

Robust Signal-Structure Reconstruction

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Abstract—This paper focuses on the reconstruction of the signal structure of a system in the presence of noise and nonlinearities. Previous results on polynomial time reconstruction in this area were restricted to systems where target specificity was part of the inherent structure, [5]. This work extends these results to all reconstructible systems and proposes a faster reconstruction algorithm along with an improved model selection procedure. Finally, a simulation study then details the performance of this new algorithm on reconstructible systems.

I. INTRODUCTION

The process of network reconstruction is the attempt to determine the structure and dynamics of a networked system. The simplest representation of a linear time-invariant system is its transfer function, G . The process for determining a system's transfer function from input-output data is known as system identification, (see Figure 1). Unfortunately, a system's transfer function contains very little information about the internal structure of a network.

A linear time-invariant system's state space realization offers a more detailed representation of a system's structure. Although rich in information, the process of reconstruction from input-output dynamics to the state space realization, (A, B, C, D) , known as the realization process (see Figure 1), is ill-posed since there are many possible state space realizations for a single transfer function matrix.

Another representation of the structure of a network is a system's dynamical structure function, (Q, P) , which was originally introduced in [4]. Dynamical structure functions (DSF) contain more information about a system's structure than the transfer function, while requiring only weak a priori information, compared to the state space realization, to reconstruct from input-output dynamics.

The DSF describes the network structure of a system in the sense that the matrix Q can be interpreted as the weighted adjacency matrix of a directed graph 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 DSF is referred to as the signal structure of the system.

The DSF of a system denotes the structure and dynamics of a linear time-invariant system at a resolution consistent

with the number of measured states. This means if less states are measured, the structure of the DSF would relate closely to the structure of a system's transfer function, while more measured states implies that the structure of the DSF is closer to the structure given by the state space representation of the system.

As with a system's state space, the process of determining a system's DSF from input-output data is ill-posed without any a priori information about the network. However, given a DSF of a system (Q, P) , the transfer function for that system is uniquely defined as $G = (I - Q)^{-1}P$, [4].

Definition 1. A system's DSF is considered reconstructible if there exists a priori information about the network that creates a bijection between a system's transfer function and its DSF.

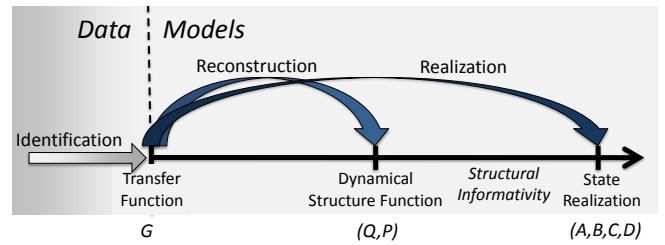


Fig. 1: System Representations Organized by Structural Informativity

In [6], a robust reconstruction method was presented that allowed for the reconstruction of the signal structure of a network when noise and nonlinearities were present in the system. This approach calculates the optimal dynamical structure function for all possible Boolean structures, i.e. all possible ways of connecting the network, and then uses a model selection technique to determine the best possible Boolean structure. Unfortunately, iterating over all possible Boolean structures involves a computational complexity of $O(2^p)$, which greatly restricts its usage to that of small networks, e.g. networks with less than three or four measured states.

Several algorithms were proposed in [5] that improved the computational complexity of the robust reconstruction method from exponential to polynomial. However, the algorithms proposed are for systems which are target specific, meaning for each measured state there exists a corresponding input that perturbs that measured state, possibly through a hidden (unmeasured) state, and that input does not perturb

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any other measured states except through the corresponding measured state. In [1], necessary and sufficient conditions for network reconstruction were proposed that show that target specificity is sufficient, but not necessary for reconstruction. This implies that there exist reconstructible networks for which the target specificity assumption fails. This paper extends the polynomial time algorithm to these cases, which can be common, for example, in proteomics and other applications.

In Section II, we extend the robust reconstruction problem to include all reconstructible networks, not only those that meet the target specificity assumption. In Section III, we extend the polynomial time algorithm for dynamical structure functions to all reconstructible networks and propose a new reconstruction algorithm that reduces the computational complexity of the reconstruction process. Section IV provides an improved model selection procedure. Section V contains the results of simulation studies. Finally, in Section VI we present our conclusions.

II. ROBUST RECONSTRUCTION FOR DYNAMICAL STRUCTURE FUNCTIONS

Previous robust reconstruction results in [6] use a method that requires target specificity. The results in this paper remove the requirement of target specificity to allow for the robust reconstruction of all possible reconstructible networks, [3].

To model the input-output data with noise and nonlinearities, we begin by considering an additive uncertainty on the control structure P , as seen in Figure 2. In this framework, the “true” system is given by $(I - Q)^{-1}(P + \Delta)$, where Δ represents unmodeled dynamics, including noise and nonlinearities. Given this uncertainty, we define the distance from data to a particular Boolean structure to be $\|\Delta\|$, in an appropriate norm.

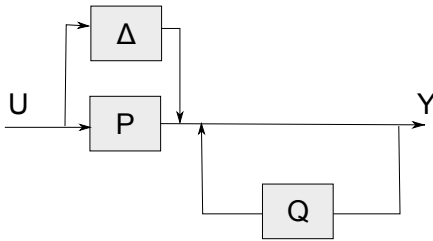


Fig. 2: Additive uncertainty on P

Figure 2 illustrates the relationship:

$$Y = (I - Q)^{-1}(P + \Delta)U.$$

This can be rewritten as:

$$\Delta U = Y - [Q \ P] \begin{bmatrix} Y \\ U \end{bmatrix}.$$

We can then exploit the fact that U is a diagonal matrix, based on the way experiments are performed in which only one input is affected at a time, which gives us:

$$\|\Delta U\| = \|c\Delta I\| = \|c\Delta\| = |c|\|\Delta\|,$$

where $c \neq 0$ is the amount each input is perturbed. Thus, we note that minimizing $\|\Delta U\|$ is equivalent to minimizing $\|\Delta\|$.

We highlight that this method of determining the correct structure of a network makes the following assumptions:

- 1) experiments are performed sequentially, with each input taking a turn,
- 2) the size of the perturbation on each input is of equal magnitude.

The purpose of minimizing $\|\Delta\|$ is to determine the Boolean structure with the smallest distance from given input-output data from experiments performed on the system. Therefore, we want to solve the following problem:

$$\delta = \min_{Q, P} \|Y - [Q \ P] \begin{bmatrix} Y \\ U \end{bmatrix}\|$$

Stacking the unknowns from Q and P into a vector x , this can be written as $w - Lx$, where w is the matrix Y stacked into a vector row by row and

$$L = \begin{bmatrix} y_2 \dots y_n & 0 & \dots & 0 & u_1 \dots u_n & 0 & \dots & 0 \\ 0 & \dots & 0 & \ddots & 0 & 0 & \dots & 0 \\ 0 & \dots & 0 & 0 & y_1 \dots y_{n-1} & 0 & \dots & 0 \end{bmatrix} \quad (1)$$

where y_i and u_i are the i^{th} columns of Y^T and U^T , respectively. Note that we remove a column of y on each row of L because the definition of Q from [4] states that the diagonal values of Q are known to be zero. This means that there are $p^2 - p$ possible Boolean structures of Q and pm possible Boolean structures of P , yielding $pm + p^2 - p$ possible Boolean structures for x .

If we index the possible combinations of Boolean structures with $v = 1, \dots, pm + p^2 - p$, then consider the v^{th} Boolean dynamical structure function and denote (Q_v, P_v) as a dynamical structure function with this Boolean structure. We can then reorganize the problem so that it becomes:

$$\delta_v^2 = \inf_{x \in \chi_v} \|w - Lx\|_2^2 \quad (2)$$

where χ_v is the set of all x that satisfy the constraints of the v^{th} Boolean structure.

It is well known that this problem is ill-posed, since L is not full column rank. As proposed in [1], certain elements of x must be known a priori in order for the system to be reconstructible, this information is contained in a $(pm + p^2 - p) \times k$ transformation matrix T so that $x = Tz$, where z is the reduced number of unknowns such that LT has full column rank, meaning $k \leq p^2$. The information contained in T could come from knowing how inputs affect the system or how states within the system interact (or fail to interact) with each other. For example, if we knew that the system was target specific, then we know that P is square and diagonal, which is information that can be incorporated into T . The complete necessary and sufficient conditions for reconstructibility are provided in [1].

Therefore, the robust reconstruction problem can finally be stated as:

$$\delta_c^2 = \inf_{z \in \zeta_c} \|w - Mz\|_2^2 \quad (3)$$

where $M = LT$ and $\zeta_c \subset \chi_v$ is the set of all z that satisfy the constraints of the c^{th} Boolean structure, where $c = 1, \dots, k$.

III. POLYNOMIAL TIME RECONSTRUCTION ALGORITHM

Assuming our system meets the requirements to be reconstructible, we now develop a polynomial time algorithm for robust reconstruction. A greedy polynomial-time algorithm for the reconstruction of networks with target specificity was given in [5].

The extension of the algorithm to all reconstructible networks, including those that may fail target specificity, requires the redefinition of several terms in the algorithm. First, we redefine the term S , which originally represented the Boolean structure of Q in [5], to be the Boolean structure of the vector z , which could contain elements of both P and Q . Furthermore, we note that we utilize δ as defined in Equation 3 rather than δ as defined in [5]. The superscripts on S and δ in Algorithm M_2 and M_3 refer to the number of links (i.e. non-zero elements) for that Boolean structure, unless otherwise stated.

Algorithm M_2

Set S^k to the fully-connected structure.

for $j = k \rightarrow 1$ **do**

Remove one link of S^j at a time to obtain a set of j structures with $j - 1$ links and calculate δ^{j-1} for each of these structures.

Set S^{j-1} as the minimum- δ^{j-1} structure.

end for

Set S^0 as the decoupled structure.

Apply a model selection procedure to the set $\mathbb{S} = \{S^j\}$.

We now propose a new algorithm, similar to the one above, which takes advantage of two important facts:

- 1) Algorithm M_2 is a greedy algorithm that keeps a record of only one structure for each possible structure with j links, where j ranges from 0 to k and
- 2) As noted in [6], the structures with more links have lower δ scores since they have more degrees of freedom.

The algorithm will also make use of the following definition:

Definition 2. The term *full* refers to the Boolean structure of the fully-connected network, i.e. a $k \times 1$ vector of ones. The term *full- x* , where x is a positive integer less than k , refers to a Boolean structure with x links missing, i.e. x entries of full- x are zeros, the rest are ones.

Example 1. If the full Boolean structure of a system is given by $[1 \ 1 \ 1]^T$, then the possible full-1 Boolean structures are: $[0 \ 1 \ 1]^T$, $[1 \ 0 \ 1]^T$, and $[1 \ 1 \ 0]^T$.

First, we use an iterative procedure to determine which links are the least likely to occur in the correct network. The full-1 Boolean structure with the j^{th} value set to zero is denoted S_j^1 and its associated δ from Equation 3 we denote δ_j^1 . Then, another iterative procedure determines a candidate

set \mathbb{S} , with one structure (S^k) for each level of sparsity (k links). Finally, a model selection procedure is applied to this reduced set to select a single solution.

Algorithm M_3

Set S^k to the fully-connected structure.

for $j = k \rightarrow 1$ **do**

Set the j^{th} position of S_j^1 to 0 and calculate δ_j^1 .

Store S_j^1 , δ_j^1 , and j in F .

end for

Sort F by δ_j^1 in descending order.

Set S to the fully-connected structure.

for $d = k \rightarrow 1$ **do**

Remove from S the link corresponding to the 0 location of the d^{th} structure from F .

Set S^d to S .

Calculate δ^d for S^d .

end for

Set S^0 as the decoupled structure.

Apply a model selection procedure to the set $\mathbb{S} = \{S^d\}$

Algorithm M_3 reduces the overall number of structures that need to be considered from $O(p^4)$ for Algorithm M_2 to $O(p^2)$, [5].

This means that Method M_3 only needs to consider the structures circled in red in Figure 3, rather than all allowable structures considered by Method M_2 in order to determine the correct structure.

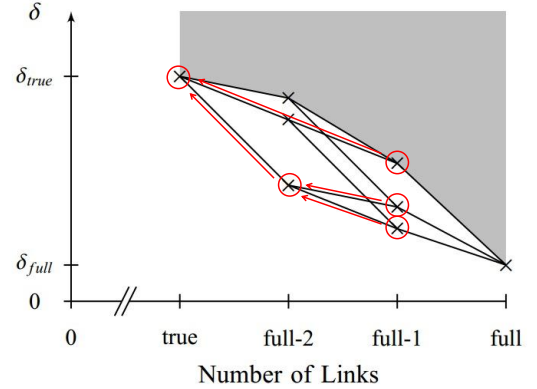


Fig. 3: An example problem showing δ values plotted against number of links for the allowable set of Method M_2 . The structures considered by Method M_3 are circled in red.

To determine when a solution can be found by Algorithm M_3 , we begin with the following Lemma:

Lemma 1. A given reconstruction is solvable by Method M_3 , i.e. the true structure will appear in the candidate set, if no full-1 link structure with a zero that does not appear in the true structure has a lower δ score than all full-1 link structures with zeros that appear in the true structure.

Proof. If all the full-1 link structures that have zeros in the true system have lower δ scores than every other full-1 link structure, then their combination will be selected by

Method M_3 ensuring that the true solution will appear in the candidate set. \square

Theorem 1. *If no noise is present in the system, Method M_3 will ensure that the true structure is part of the candidate set, assuming there is sufficient data for reconstruction.*

Proof. As noted in [6], due to the additional degrees of freedoms provided by extra connections, all Boolean structures S^j with zeros obtained from any ordered combination (where order refers to the iterative manner in which links were eliminated to obtain S^j) which coincide with locations of zeros in the true structure will have a cost $\delta = 0$. Furthermore, all Boolean structures that have at least one zero that does not correspond to missing links in the true structures will have $\delta > 0$.

Therefore, when no noise is present in the system all Boolean structures with one link missing that correspond to a missing link in the true structure will have δ values lower than all Boolean structures with one link missing that does not appear in the true structure. By Lemma 1, this guarantees that the true structure is part of the candidate set. \square

Corollary 1. *There exists $\epsilon > 0$ and $r > 0$, where ϵ represents the noise in the system, such that if $\epsilon < r$, Method M_3 will ensure that the true structure is part of the candidate set, assuming there is sufficient data for reconstruction.*

Proof. This follows from Theorem 1 by continuity. \square

IV. MODEL SELECTION PROCEDURE

The original robust reconstruction method in [6] noted that finding an optimal δ yields a series of candidate solutions that have more degrees of freedom than the true network due to overfitting, so a model selection procedure is required to penalize extra connections in the candidate solutions. The Akaike Information Criterion (AIC) was proposed as a model selection procedure and is defined as:

$$AIC = 2k - 2\ln(L)$$

where k is the number of parameters in the model and L is the maximized value of the likelihood function for the model, [2].

Akaike's Information Criterion with correction for finite sample sizes is defined as:

$$AICc = AIC + \frac{2k(k+1)}{n-k+1}$$

where n is the sample size.

A customized AIC was used in [6] for the minimization of the likelihood function and was defined as follows:

$$AIC_{original} = 2k + n\ln\left(\frac{2\pi L}{n} + 1\right) \quad (4)$$

However, $AIC_{original}$ did not scale well to large networks and the use of the natural logarithm heavily favored the full link structure when noise was present in the system. To overcome these issues we use a customized form of the

Akaike Information Criterion, which we will call the Chetty-Warnick Information Criterion:

$$CWIC_k = \frac{\delta_k}{N+C} + L_k$$

where δ_k is defined in Equation (2), N is the number of unknowns in Q , C is the number of unknowns in P , and L_k is the number of nonzero entries in the k^{th} Boolean structure. Dividing δ by $N+C$ scales δ by the size of the known network, since the difference in δ for the candidate solutions becomes smaller as the size of the measured network increases. Furthermore, we use only the minimized value of δ rather than the $\ln(\delta)$ because, as mentioned above, the natural logarithm heavily favors the completed connected network, making it difficult to correctly identify the true network.

$CWIC$ with correction for finite sample sizes is then given by:

$$CWIC_{c_k} = VIC_k + \frac{2L_k(L_k+1)}{N+C-L_k+1}$$

A comparison of the reconstruction process as noise variance increases using Method M_3 with $AIC_{original}$ and the $CWIC$ is given in Figure 4. The network being reconstructed is a linearized version of the single feedback loop defined in [6].

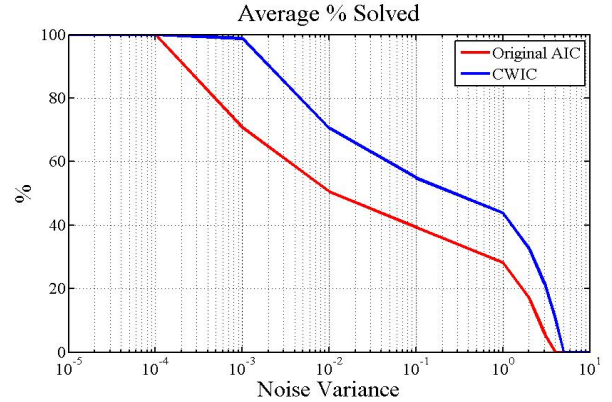


Fig. 4: Comparison of reconstruction problems successfully solved using Algorithm M_3 using the original AIC and $CWIC$ as the model selection procedure.

As Figure 4 shows, $CWIC$ performs better than the original AIC as noise variance increases.

V. SIMULATIONS

Our empirical study will focus on:

- 1) Compare the accuracy of the Method M_3 before the redefinition of variables from [5] to Method M_3 as defined in Section III of this paper,
- 2) Comparing the accuracy of Method M_2 to Method M_3 , where the model selection procedure is the $CWIC$,
- 3) Determining whether the accuracy of reconstruction is degraded by increasing the size of a network, and
- 4) Improving the accuracy of reconstruction through improved data collection techniques.

The data in these simulations are continuously sampled, with no missing data points.

A. Analyzing Non-Target Specific Reconstruction

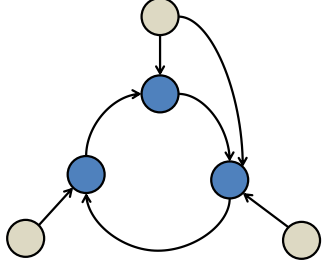


Fig. 5: Non-Target Specific Ring Network. Cream nodes represent inputs and blue nodes represent outputs.

The first simulation demonstrates why a redefinition of the reconstruction algorithm was even necessary by using a single feedback loop with a single extra edge to make it non-target specific, as seen in Figure 5. It is trivial to show that this network is reconstructible.

Figure 6 shows the results of reconstruction using Method M_3 both with and without the assumption that the non-target specific network is target specific.

As the figure shows, assuming that the system is target specific when it isn't leads to catastrophic failure in the network reconstruction procedure.

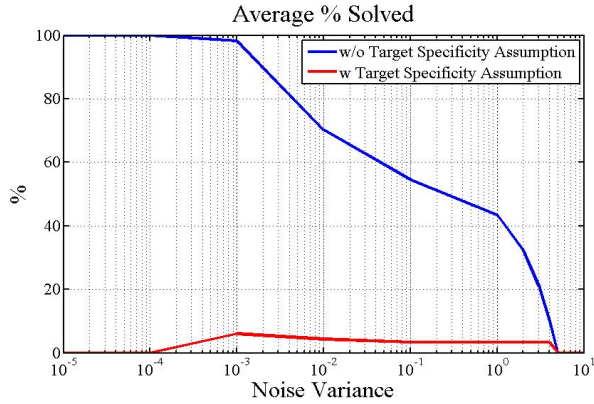


Fig. 6: Reconstruction of non-target specific network with and without the assumption that it is target specific.

B. Comparison of Polynomial Time Algorithms

Our next result comes from the comparison of Method M_2 and Method M_3 . In Figure 7, we note that the two methods seem almost indistinguishable.

We expect Method M_3 to begin failing when a *full* - 1 structure which has a zero that appears in the true structure has a larger δ value than a *full* - 1 structure which has a zero that does not appear in the true structure. In this case the true structure is not part of the candidate set provided by Method M_3 .

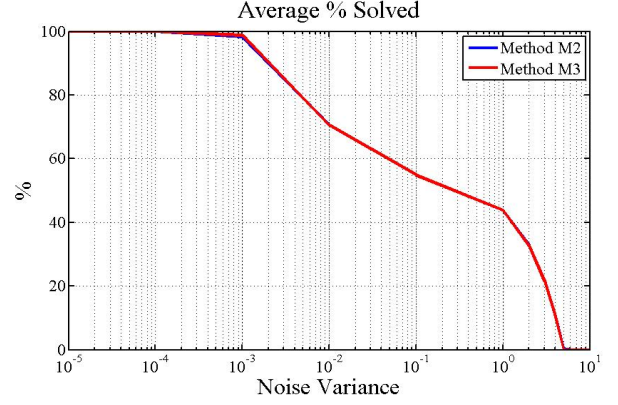


Fig. 7: Comparison of reconstruction methods M_2 and M_3 .

The true structure could potentially be found in the candidate set generated by Method M_2 if the δ value of the structure with non-true zero, mentioned above, combined with zeros that are true values is higher than the combined values of the true zero, mentioned above, with higher δ combined with the other true zero structures.

The fact that the two methods seem almost indistinguishable means that this situation probably doesn't occur for this particular example, although that may not be true in general.

C. Increasing Network Size

Now, in order to see how the accuracy of reconstruction degrades as the size of the network increases, we introduce the ring of rings network and assume target specificity in Figure 8 (inputs not shown). The rings of rings is interesting since it has a full transfer function, but, as the figure shows, it is clearly very structured.

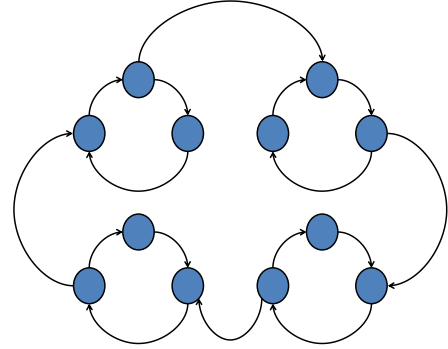


Fig. 8: Ring of Rings Network

All things being equal, we now compare the accuracy of reconstructing various subsets of the ring of rings in Figure 9. The first set is just a single loop of 3 nodes, the second is two loops of 3 nodes each with one connection between them, the third is three loops of 3 nodes each with a connection between the first and second loop and the second and third loops, and finally the fourth is the complete ring of rings network.

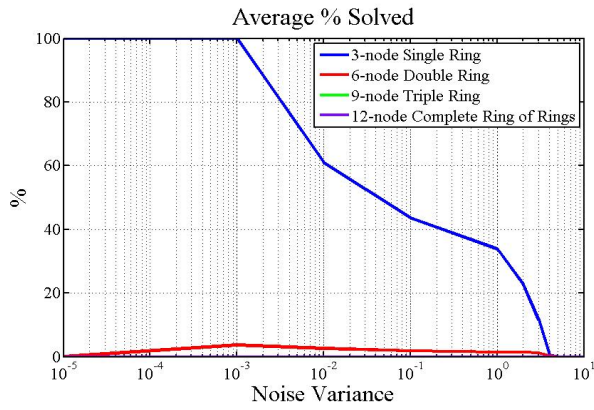


Fig. 9: Comparison of reconstruction problems for increasing network size.

As the figure shows, the network reconstruction process degrades as the size of the network grows. The point of a polynomial time algorithm is to allow for the reconstruction of large networks, so if the reconstruction process degrades with network size, the new algorithm isn't very useful. We now provide several ways in which to improve data collection so that network reconstruction of large networks is viable.

D. Improving Results

The best way to improve results is to improve data collection.

1) *Repeated Experiments*: Firstly, we note that repeating experiments on the network can drastically increase the accuracy of reconstruction by averaging out noise in the system. If the cost of experiments is high, reconstruction is still possible, but with much smaller ϵ . This is made evident in comparing reconstruction for increasing noise variance with no repeated experiments to reconstruction with noise averaging, again using a linearized single feedback loop, in Figure 10.

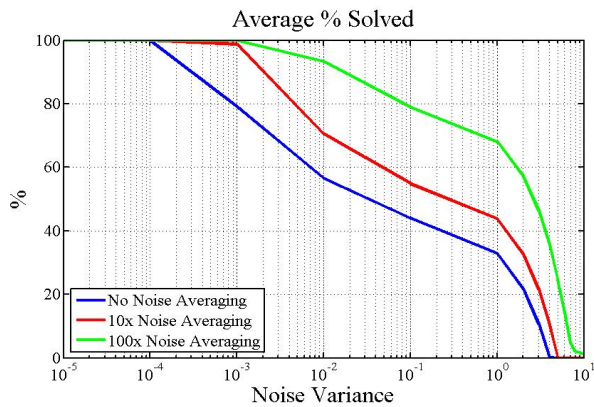


Fig. 10: Comparison of robust network reconstruction of a single feedback loop with and without noise averaging.

The figure shows that increasing the noise averaging allows for more accurate reconstruction.

2) *Increasing Data Amount*: Another way to improve the accuracy of the reconstruction process is to increase the number of data points collected during each experiment. Our conjecture is that as the size of the network grows, the number of data points that must be collected in order to accurately reconstruct must grow exponentially, though validating this conjecture is beyond the scope of this work. Figure 11 shows the increase in accuracy as the number of points collected during each experiment increases for the case of the ring of rings network.

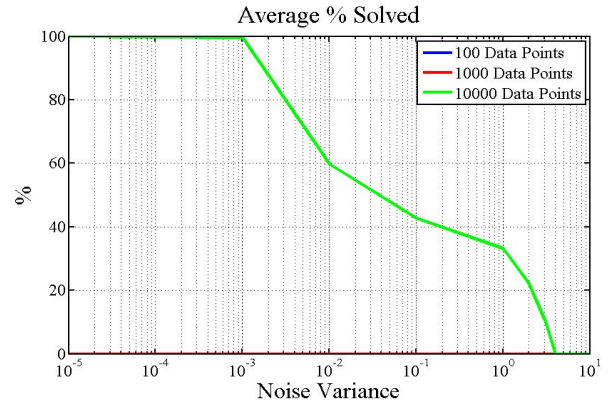


Fig. 11: Improved reconstruction with increased data collection.

VI. CONCLUSION

In this paper we extended the robust reconstruction problem beyond those networks that met the strict assumption of target specificity to include all reconstructible networks. Furthermore, we improved upon previously proposed reconstruction algorithms by further reducing the computational complexity of the reconstruction method. Then, we customized our existing model selection procedure to scale with the size of the network in order to ensure accurate reconstructions for large networks.

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