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Topology identification via growing a Chow-Liu tree network

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Abstract— **We study the problem of sparse interaction topology identification using sample covariance matrix of the states of the network. We postulate that the statistics are generated by a stochastically-forced undirected consensus network with unknown topology in which some of the nodes may have access to their own states. We first propose a method for topology identification using a regularized Gaussian maximum likelihood framework where the ℓ_1 regularizer is introduced as a means for inducing sparse network topology. We also develop a method based on growing a Chow-Liu tree that is well-suited for identifying the underlying structure of large-scale systems. We apply this technique to resting-state functional MRI (FMRI) data as well as synthetic datasets to illustrate the effectiveness of the proposed approach.**

Index Terms— **Chow-Liu tree, consensus networks, coordinate descent, FMRI, Newton's method, sparse inverse covariance estimation, topology identification.**

I. Introduction

Identifying network topology and learning graphical models from partially available statistical signatures are topics of immense interest in areas ranging from machine learning to statistics to neuroscience [1]–[8]. Studying the human brain as a complex network has received significant attention recently [9]–[11]. The brain functional connectivity can be measured by computing the correlation between time-series functional magnetic resonance imaging (FMRI) data. The functional connectivity structure between different regions can be revealed by utilizing different thresholding techniques [12], [13]. In general, this is a challenging problem because it is often the case that only noisy partial network statistics are known. The goal is to develop an efficient algorithm for recovering the underlying topology of a network utilizing the limited sample data.

Recovering the underlying network topology using sample covariance matrix of the node values under structural constraints has been studied in [14]–[16]. Moreover, a rich body of literature has been devoted to the problems of designing network topology to improve performance [17]–[21]. Several algorithms can be employed to identify the underlying network structure from limited statistical data. In [22], the authors show inability of standard graphical-LASSO to identify network topology. It was demonstrated that this popular algorithm fails to recover the underlying topology even when the abundance of data is available.

In this paper, we develop a convex optimization algorithm for identifying sparse interaction topology using the sample covariance matrix of the states of the network. First, we utilize an ℓ_1-regularized Gaussian maximum likelihood estimator that has been commonly used for recovering sparse inverse covariance matrices [23]–[25]. We show that the performance of graphical-LASSO can improve significantly by imposing additional structure on the problem and using reweighting schemes [26]. In particular, our framework overcomes challenges that standard graphical-LASSO faced and performs well for the case study in [22]. Moreover, inspired by [22], we combine the Chow-Liu algorithm [27] with the techniques for growing networks developed in [28] to identify the underlying structure of an undirected consensus network. Constructing the Chow-Liu tree from statistical data does not require any matrix inversion; thereby, it is well-suited for large-scale problems. Furthermore, we have developed efficient algorithms [28] for growing connected resistive consensus networks. Herein, we demonstrate that combining these two algorithms yields an efficient method for recovering the network topology in large-scale systems.

Our presentation is organized as follows. In Section II, we discuss the properties of consensus networks and formulate the problem of topology identification using sparse inverse covariance matrix estimation. We also briefly comment on the customized second-order algorithm based on the proximal Newton method [14] to solve the ℓ_1-regularized Gaussian maximum likelihood estimation problem. In Section III, we develop an algorithm for growing a Chow-Liu tree graph in order to identify the network that yields close approximation of a given sample covariance matrix. In Section IV, we use computational experiments to illustrate features of our method. In particular, we employ our algorithm to identify the underlying functional network of the human brain using FMRI data. Finally, in Section V, we conclude with a brief summary.

II. Topology identification via structured graphical-LASSO

The problem of topology identification using a sample covariance matrix for stochastically forced undirected consensus networks has been studied in [14]. In consensus networks, each node updates its own state using localized information exchange with the neighbors. Two nodes are neighbors if an edge connects them together. Herein, we consider a network that leader nodes are equipped with absolute information about their own states. In [14], we

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showed that the underlying topology of an undirected consensus network can be identified using Gaussian maximum likelihood estimator. In this paper, we formulate the topology identification problem for undirected consensus networks with leader nodes and provide two algorithms to solve this problem.

Consider an undirected network with n nodes governed by

$$\dot{\psi}_i \;=\; \sum_{j \in \mathcal{N}_i} x_{ij}\,(\psi_j \,-\, \psi_i) \,-\, z_i\,\psi_i \,+\, w_i,$$

where each node i updates its own state using relative information exchange with its neighbors in the set $\mathcal{N}_i$. Moreover, certain nodes, the so-called leaders, have access to their own states. Here, z_i is the weight that the ith node sets for the absolute measurement, x_{ij} is the edge weight, and w_i is an exogenous stochastic disturbance. The ith node is a leader if $z_i \neq 0$ and it is a follower if $z_i = 0$. By concatenating all the states in a vector $\psi \in \mathbb{R}^n$, the consensus dynamics can be written as

$$\dot{\psi} \;=\; -\,(L_x \,+\, D_z)\,\psi \,+\, w \qquad (1)$$

Here, $L_x \in \mathbb{R}^{n \times n}$ is the graph Laplacian of the consensus network and $D_z \in \mathbb{R}^{n \times n}$ is a diagonal matrix with the ith diagonal entry z_i. The incidence matrix E of the underlying graph represents the edges in the network. The lth column of this matrix is given by

$$\xi_l \;=\; \mathrm{e}_i \,-\, \mathrm{e}_j,$$

that demonstrates the lth edge between the nodes i and j. Here, $\mathrm{e}_i \in \mathbb{R}^n$ is the ith basis vector. By using the incidence matrix, the Laplacian matrix L_x can be written as

$$L_x \;:=\; \sum_{l\,=\,1}^{m} x_l\,\xi_l\,\xi_l^T \;=\; E\,\mathrm{diag}\,(x)\,E^T$$

where $\mathrm{diag}\,(x)$ is a diagonal matrix with the edge weights $x \in \mathbb{R}^m$ in its diagonal.

Given that the covariance of the disturbance is a multiple of the identity matrix I, the steady-state covariance of ψ,

$$\Sigma \;:=\; \lim_{t\,\to\,\infty} \mathbf{E}\,(\psi\,\psi^T),$$

can be computed as the solution to the associated algebraic Lyapunov equation

$$(L_x \,+\, D_z)\,\Sigma \,+\, \Sigma\,(L_x \,+\, D_z) \;=\; 2\,I.$$

Thus, the steady state covariance can be explicitly computed as

$$\Sigma \;=\; (L_x \,+\, D_z)^{-1}. \qquad (2)$$

The inverse of the steady-state covariance matrix of the states of the system can be determined by the structure of the underlying graph that connects the n nodes. Thus, by using a sampled second-order statistics and estimating the inverse covariance matrix, the underlying topology of an undirected consensus network with leaders can be identified. The problem of sparse covariance estimation has received significant attention recently [29]–[32]. Relative to these works, our optimization problem has additional structure coming from the dynamics of undirected consensus networks. Moreover, compared to our previous work [14], we consider consensus networks with leaders and introduce a new algorithm that is convenient for solving large-scale problems.

We first generalize the proposed algorithm based on the structured graphical-LASSO in [14] to solve the problem of topology identification in undirected consensus networks with leaders. It is well-known that the estimation of the inverse covariance matrix X can be obtained as the solution to the regularized maximum log-likelihood problem [25],

$$\begin{array}{ll} \underset{X}{\text{minimize}} & -\,\log\det\,(X) \,+\, \mathrm{trace}\,(SX) \,+\, \gamma\,\|F \,\circ\, X\|_1 \\ \text{subject to} & X \,\succ\, 0, \end{array} \qquad (3)$$

where S is the sample covariance matrix, γ is a positive regularization parameter, F is the weight matrix, and $\|F \,\circ\, X\|_1 := \sum F_{ij}\,|X_{ij}|$ is the weighted ℓ_1 norm of the matrix X. By substituting the expression (2) for the inverse covariance matrix in (3) and using the incidence matrix E, the topology of a network that generates close approximation of a given sample covariance matrix can be identified by solving the following problem,

$$\begin{array}{ll} \underset{x,\,z}{\text{minimize}} & J(x,z) \,+\, \gamma_1 \displaystyle\sum_{l\,=\,1}^{m} f_l\,|x_l| \,+\, \gamma_2 \sum_{k\,=\,1}^{N} g_k\,|z_k| \\ \text{subject to} & E\,\mathrm{diag}\,(x)\,E^T \,+\, \mathrm{diag}(z) \,\succ\, 0, \end{array} \qquad \text{(NI)}$$

where

$$\begin{array}{rcl} J(x,\,z) &=& -\,\log\det\left(E\,\mathrm{diag}\,(x)\,E^T + \mathrm{diag}(z)\right) \,+ \\ && \mathrm{trace}\left(S\,(E\,\mathrm{diag}\,(x)\,E^T \,+\, \mathrm{diag}(z)\right). \end{array}$$

Moreover, $f \in \mathbb{R}^m$ and $g \in \mathbb{R}^N$ are the vectors of nonnegative weights and $(\gamma_1,\,\gamma_2)$ are the positive regularization parameters. An effective heuristic for weight selection is given by the iterative reweighted algorithm where the weights f and g are inversely proportional to the magnitudes of x and z in the previous iteration [26]. Problem (NI) is a convex but non-smooth optimization problem where the optimization variables are the vector of the edge weights $x \in \mathbb{R}^m$ and the vector of leaders weights $z \in \mathbb{R}^N$. Relative to our prior work [14], our optimization problem has additional structure induced by presence of the leader nodes.

The algorithm based on the sequential quadratic approximation of the smooth part of the objective function in [14] can be utilized for solving (NI) with minor changes. The difference is that the optimization variable size has increased form m to $m + N$. This method benefits from exploiting second-order information of the smooth part of the objective funtion and from computing the Newton direction using cyclic coordinate descent [33] over the set of active variables. For a detailed version of the algorithm; see Section III.C in [14]. We solve the problem (NI) for different values of $(\gamma_1,\,\gamma_2)$ using a path-following iterative reweighted algorithm. The topology identification then is followed by a polishing step [14] to debias the identified edge weights. We next propose an algorithm to solve the topology identification problem of large-scale networks.

III. GROWING A CHOW-LIU TREE NETWORK

In this section, we discuss an alternative algorithm for identifying the underlying network topology which is well-suited for large-scale systems. In order to find the underlying network structure using statistical data, the Chow-Liu tree algorithm [27] can be utilized. This method does not require any matrix inversion; thereby, suitable for large-scale usage. However, as discussed in [22], it causes false positives and negatives when using it for identifying the topology of disconnected networks or networks with cycles, respectively. Herein, we propose a framework in order to combine the Chow-Liu tree and the reweighted graphical-LASSO algorithms for identifying the structure of connected networks with cycles.

We consider the same consensus network in (1) and we assume that the sample covariance matrix S is given. In order to use the Chow-Liu algorithm, the mutual information matrix M should be constructed from the sample covariance matrix. Assuming Gaussian distribution for the noise w, the mutual information is given by

$$M_{ij} \;=\; \frac{1}{2}\,\log\left(\frac{S_{ii}\,S_{jj}}{S_{ii}\,S_{jj} \,-\, S_{ij}^2}\right),$$

where S_{ij} is the ijth element of the matrix S. We only use the $n\,(n\,-\,1)/2$ off-diagonal elements of this symmetric matrix to construct the Chow-Liu tree. A spanning tree of a graph with n nodes has $(n-1)$ edges. To build the Chow-Liu tree, we sort the elements of the mutual information matrix and choose the biggest $(n-1)$ of them that do not create cycles [27].

After finding the underlying tree network that generates close approximation of the sample covariance matrix, our goal is to add a certain number of edges to the tree graph in order to enhance the closed-loop performance [28]. The performance is measured by the proximity of the second-order statistical data generated by the network to the given sample covariance matrix.

Consider an undirected consensus tree network,

$$\dot{\psi} \;=\; -\,L_t\,\psi \;+\; u \;+\; w, \tag{4}$$

where w and u are the exogenous disturbance and the control input, respectively and L_t is the graph Laplacian of the tree network that is obtained using the Chow-Liu algorithm. The goal is to improve the performance of this system by growing the tree network. We approach this problem as a feedback design problem with

$$u \;=\; -\,(L_x \,+\, D_z)\,\psi, \tag{5}$$

where D_z is a diagonal matrix with the ith diagonal entry z_i and the symmetric feedback-gain matrix L_x is required to have the Laplacian structure. Since a nonzero ijth element of L_x corresponds to an edge between the nodes i and j, the communication structure in the controller graph is determined by the sparsity pattern of the matrix L_x. Moreover, the ith node is a leader if z_i is nonzero. By substituting the control input u from (5) in (4)

$$\dot{\psi} \;=\; -\,(L_t \,+\, L_x \,+\, D_z)\,\psi \;+\; w. \tag{6}$$

For a computed L_t from the Chow-Liu algorithm, our objective is to design the topology L_x and to identify the leader nodes in the network in order to achieve the desired tradeoff between the controller sparsity and the network performance. The performance is quantified by the proximity of the steady-state covariance matrix of the closed-loop system to the sample covariance matrix.

Next, we are going to establish a relation between the closed-loop graph Laplacian and the inverse covariance matrix of the network. The steady-state covariance of ψ is given by

$$\Sigma \;=\; (L_t \,+\, L_x \,+\, D_z)^{-1}, \tag{7}$$

where $L_x = E\mathrm{diag}(x)E^T$. Thus, the problem of identifying the sparse topology of a network, i.e., finding L_x and D_z, that generates close approximation of a given sample covariance matrix is equivalent to sparse inverse covariance estimation problem. This can be achieved by solving a similar regularized maximum log-likelihood problem to (3) with one main difference. The inverse covariance matrix X is the summation of the Laplacian matrices of the tree plant network L_t and the controller network $L_x + D_z$. Thus, the problem of growing a tree network in order to match the available statistical data can be formulated as

$$\begin{array}{ll} \underset{x,\,z}{\text{minimize}} & J(x,z) \;+\; \gamma_1 \displaystyle\sum_{l\,=\,1}^{m} f_l\,|x_l| \;+\; \gamma_2 \displaystyle\sum_{k\,=\,1}^{N} g_k\,|z_k| \\ \text{subject to} & L_t \,+\, E\,\mathrm{diag}\,(x)\,E^T +\; \mathrm{diag}(z) \;\succ\; 0, \end{array} \tag{8}$$

where

$$\begin{array}{rl} J(x,\,z) \;=\; & -\,\log\det\big(L_t \,+\, E\,\mathrm{diag}\,(x)\,E^T\!+\,\mathrm{diag}(z)\big) + \\ & \mathrm{trace}\,\big(S\,(E\,\mathrm{diag}\,(x)\,E^T\!+\,\mathrm{diag}(z)\big)\,. \end{array}$$

In the case of resistive networks (i.e., all the edge weights are nonnegative), since the plant network is given by a tree graph, the closed-loop network is connected; thereby, the optimization problem simplifies to

$$\begin{array}{ll} \underset{x,\,z}{\text{minimize}} & J(x,z) \;+\; \gamma_1 \displaystyle\sum_{l\,=\,1}^{m} f_l\,x_l \;+\; \gamma_2 \displaystyle\sum_{k\,=\,1}^{N} g_k\,z_k \\ \text{subject to} & x \;\geq\; 0, \quad z \;\geq\; 0. \end{array} \tag{9}$$

In this scenario, the topology identification problem turn into the problem of growing a tree network and the positive definiteness constraint simplifies to nonnegativity constraints of the vectors x and z. Thus, several optimization algorithms can be employed to solve this problem efficiently for large-scale networks.

IV. Computational experiments

We next illustrate the performance of our methods by employing them to identify the topology of an RC network with 10 nodes and a tree structure shown in Fig. 1. The voltages of the nodes form the states of the system. In this network, node 5 is grounded with $z_5 = 4$ and all other edge weights are one which implies that node 5 is a leader. This example is borrowed from [22].

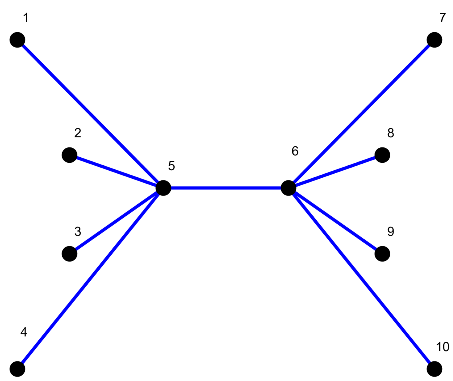

Fig. 1: The RC tree network with $n = 10$ nodes.

A. Structured graphical-LASSO algorithm

Assume that infinite samples of the nodes' voltages are available; thereby, the sample covariance matrix S is equal to the exact solution of the Lyapunov equation. Moreover, we set $\gamma_1 = \gamma_2 = \gamma$. In this case, the structured graphical-LASSO algorithm in Section II can completely recover the underlying network topology for different values of γ. This example has been previously studied in [22]. They show that when the sample covariance matrix is precise, the graphical-LASSO algorithm results in 5 false positives and negatives. However, by adding a structural constraint to the problem and using a reweighting scheme, we showed that the same algorithm can recover the network topology with zero error.

Next, we utilize our method to solve the problem by using a sample covariance matrix which is not very close to the actual covariance matrix and is constructed from only 80 samples. The algorithm is again able to recover the network topology and to identify the leader for different values of γ.

It is worth to note that the performance of this method deteriorates if we replace the reweighted ℓ_1 norm scheme with the ℓ_1 norm. In particular, by eliminating the reweighted ℓ_1 norm, we observed the effect of grounding one of the nodes with high capacitance. Although the network topology will be identified for some values of γ, by increasing γ (to very large value), the algorithm chooses the optimal edges in the same way as [22]. In particular, it ignores the connections between nodes 1 to 5 because of their low variances. In the next example, we illustrate the effectiveness of growing a Chow-Liu tree by using it on a synthetic dataset.

B. Topology identification via growing a Chow-Liu tree

In this section, the second method is utilized to identify the underlying structure of a network with cycles. The original plant network is shown in Fig. 2a. We first assume that the sample covariance matrix S is equal to the exact solution of the Lyapunov equation. We form the mutual information matrix and construct the Chow-Liu tree accordingly which is shown in Fig. 2b. We next grow this tree network in order to enhance the performance of the closed-loop system. In particular, we solve the problem (8) to find the leader nodes and the Laplacian matrix of the controller graph L_x. In this case, our algorithm can completely recover the underlying network topology for different values of γ. Next, we employ this algorithm to identify the topology of a larger network with real data to evaluate its performance.

C. FMRI dataset

The FMRI technique detects the activity of a region in the brain by measuring the blood flow to that region. Since the blood flow increases in an active part of the brain, the functioning regions can be identified by monitoring the blood flow. The functional connectivity structure between different regions can be revealed by utilizing different thresholding techniques [12], [13]. The results indicate that different regions of the brain that are not anatomically connected act closely together and are functionally linked. Moreover, the previous studies have shown that the human brain has small-world network properties [13].

In this section, we employ the second algorithm based on growing a Chow-Liu tree to identify the underlying functional network of the human brain. The sample covariance matrix is computed using the resting-state FMRI data of 20 healthy patients [13]. In the resting-state FMRI, the patients are asked to close their eyes and try not to think. The studies have shown that even in the rest state, the brain is highly active and different regions of the brain are communicating with each other [34]. We collect 134 samples from 140 cortical brain regions (nodes) in the right hemisphere. The sample correlation matrix for each patient is a 140×140 matrix and can be computed using the time series data. The sample covariance matrices are not invertible since the number of samples is smaller than the number of the nodes in the network. Thus, we use our proposed algorithm to estimate the inverse covariance matrix and to identify the underlying network structure of the human brain.

First, we form the mutual information matrix and construct the Chow-Liu tree Fig 3a. Next, we grow the obtained tree network to identify the remained edges and improve the performance of the closed-loop system. We set $\gamma_1 = \gamma_2 = \gamma$. The identified networks for a randomly chosen patient are shown in Fig 3. In particular, as the sparsity promoting parameter γ increases, the identified network gets sparser.

This example has been previously studied in [35]. Their results show that the nodes that are located in the lower left corner of the graphs are highly connected to their neighboring nodes. They compare this pattern of connectivity with the

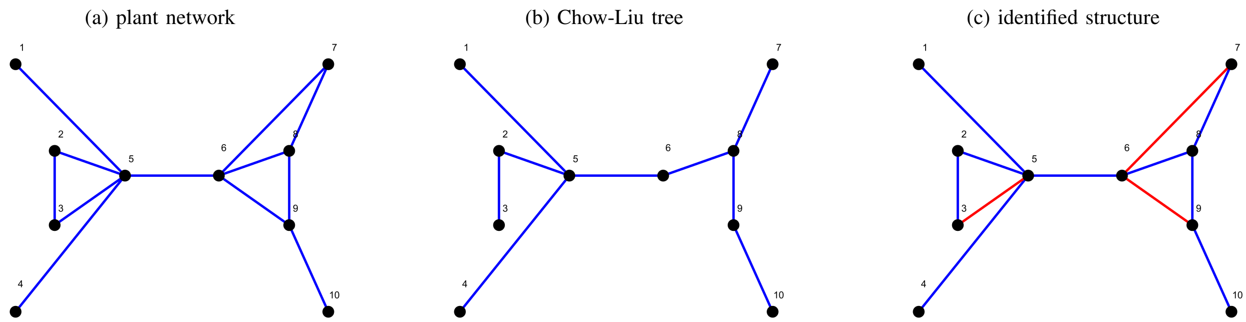

Fig. 2: (a) Plant network; (b) constructed Chow-Liu tree network; and (c) the identified network from growing the Chow-Liu tree.

false positives created by their algorithm in a synthetic RC circuit and conclude that the high number of edges in that area is false positives created by the same phenomenon in the circuit example. However, by adding a structural constraint to the problem and using a reweighting scheme, we showed that the underlying network can be recovered without high connectivity in the lower left corner. Moreover, the general shape of the identified network is consistent with the results reported in [13]. Furthermore, the small-world properties such as high clustering and high efficiency coefficients can be seen in the identified networks.

To conclude, it seems that using both an additional structural constraint and the reweighted ℓ_1 norm scheme can improve the performance of the graphical-LASSO algorithm significantly. Unlike the Chow-Liu algorithm that can be employed to construct tree networks only, our algorithm is more general and overcomes the challenges associated with the conventional algorithms proposed in [35].

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V. Concluding remarks

We have studied the problem of sparse topology identification of an undirected consensus network with leaders using second-order statistical data. The goal is to identify a sparse interaction topology using sample covariance matrix of the network state. We have introduced two algorithms based on regularized Gaussian maximum likelihood and growing a Chow-Liu tree. In the first algorithm, we propose a structured graphical-LASSO algorithm that uses the weighted ℓ_1 regularizer as a proxy for inducing sparse network topology. The other method is based on growing a Chow-Liu tree that is well-suited for identifying the underlying structure of large-scale networks. Several examples have been provided to demonstrate the performance of our framework.

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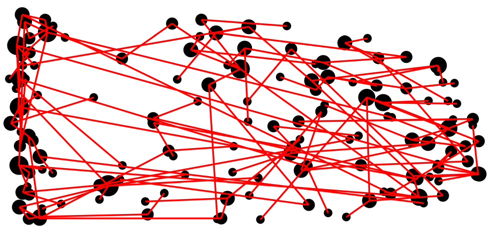
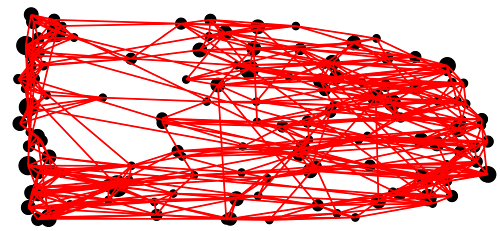
(a) Chow-Liu tree graph with 139 edges



(b) $\gamma = 0.1$



(c) $\gamma = 1$

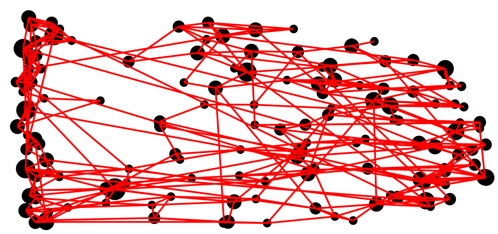


Fig. 3: The identified networks for different values of γ.

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