Efficient Variational Bayesian Structure Learning of Dynamic Graphical Models

Hang Yu, Member, IEEE, Songwei Wu, and Justin Dauwels, Senior Member, IEEE

Abstract—Estimating a sequence of dynamic graphical models, in which adjacent graphs share similar structures, are of paramount importance in various social, financial, biological, and engineering systems, since the evolution of such networks can be utilized for example to spot trends, detect anomalies, predict vulnerability, and evaluate the impact of interventions. Existing methods for learning dynamic graphical models require the tuning parameters that control the graph sparsity and the temporal smoothness to be selected via brute-force grid search. Furthermore, these methods are computationally burdensome with time complexity $O(NP^3)$ for $P$ variables and $N$ time points. As a remedy, we propose a low-complexity tuning-free Bayesian approach, named BADGE. Specifically, we impose temporally dependent spike and slab priors on the graphs such that they are sparse and varying smoothly across time. An efficient variational inference algorithm based on natural gradients is then derived to learn the graphs from the data in an automatic manner. Owning to the pseudo-likelihood and the mean-field approximation, the time complexity of BADGE is only $O(NP^2)$. To cope with the local maxima problem of variational inference, we resort to simulated annealing and propose a method based on bootstrapping of the observations to generate the annealing noise. We provide numerical evidence that BADGE outperforms existing methods on synthetic data in terms of structure estimation, while being more efficient especially when the dimension $P$ becomes high. We further apply the approach to the stock return data of 78 banks from 2005 to 2013 and find that the number of edges in the financial network as a function of time contains three peaks, in coincidence with the 2008 global financial crisis and the two subsequent European debt crisis. On the other hand, by identifying the frequency-domain resemblance to the time-varying graphical models, we show that BADGE can be extended to learning frequency-varying inverse spectral density matrices, and further yields graphical models for multivariate stationary time series. As an illustration, we analyze scalp EEG signals of patients at early stages of Alzheimer’s disease (AD) and show that the brain networks extracted by BADGE can better distinguish between the patients and the healthy controls.

Index Terms—Dynamic graphical models, structure learning, variational inference, simulated annealing, bootstrapping, inverse spectral density matrices

1 INTRODUCTION

The recent decades have witnessed a rapid development of graphical models, since they provide a refined language to describe complicated systems and further facilitate the derivation of efficient inference algorithms [2]. While an extensive literature revolves around learning static graphical models that are time invariant (see [3]-[11] and references therein), the change of interdependencies with a covariate (e.g. time or space) is often the rule rather than the exception for real-world data, such as friendships between individuals in a social community, communications between genes in a cell, equity trading between companies, and computer network traffic. Furthermore, such dynamic graphical models can be leveraged to spot trends, detect anomalies, classify events, evaluate the impact of interventions, and predict future behaviors of the systems. For instance, estimating time-varying functional brain networks during epileptic seizures can show how the dysrhythmia of the brain propagates, and analyzing the network evolution can help to detect epilepsy and assess the treatment of epilepsy [12]. We therefore focus on learning dynamic graphical models in this study.

In the case where all variables follow a joint Gaussian distribution, the graphical model structure is directly defined by the precision matrix (i.e., the inverse covariance matrix). Specifically, a zero element corresponds to the absence of an edge in the graphical model or the conditional independence between two variables. Therefore, our objective is to learn a time-varying precision matrix. Existing works on learning the time-varying precise matrix can be categorized into three groups. The first one [13]-[16] considers the temporal dependence by smoothing the empirical covariance matrix across time using kernels. Given the temporally dependent covariance matrix, the sparse precision matrix is then estimated individually at each time point. The estimation problem can be solved by maximizing the likelihood with an $\ell_1$-norm penalty on the precision matrix. However, unexpected variability may arise between two adjacent networks since each network is estimated independently [17]. To mitigate this issue, the second group of dynamic network models [17]-[24] further captures the temporal dependence by enforcing $\ell_1$, $\ell_2$, or Frobenius norm constraints on the difference between two consecutive precision matrices. As an alternative, instead of imposing separate constraints for the sparsity and the smoothness across time of the precision
matrices, the third group \cite{25} employs the local group lasso penalty to promote sparsity and smoothness together.

Unfortunately, the dynamic graphical models inferred by all three categories of methods are sensitive to the tuning parameters, including the kernel bandwidth and the penalty parameters that control the sparsity and smoothness. Classical brute-force grid search approaches for selecting these parameters are cross validation (CV), Akaike information criterion (AIC) and Bayesian information criterion (BIC) \cite{14, 15, 17, 18, 22}-\cite{25}. However, heavy computational burdens come along with these methods; the learning algorithm needs to be run once for every combination of all possible values of the tuning parameters in a predefined candidate set before the one associated with the largest score is chosen. Moreover, it has been demonstrated in \cite{26} that these parameter selection approaches yield unsatisfactory results for graphical model selection, especially when the number of variables is large. Apart from the large number of runs for parameter selection, the computational cost in each run is also large. The time complexity of the current three groups of methods is $O(NP^3)$, where $P$ denotes the dimension (i.e., number of variables) and $N$ denotes the sample size. In practice, these methods are fraught with difficulties of daunting computational cost when tackling problems with more than 100 variables.

To address these problems, we propose a novel approach named BADGE (BAyesian inference of Dynamic Graphical modEls) to learn the time-varying graphical models that is free of tuning while having a low time complexity of $O(NP^2)$. In particular, we focus on Gaussian graphical models, and consequently, our objective is to infer the time-varying precision matrix. To this end, we impose a temporally dependent spike and slab prior \cite{27, 28} on the off-diagonal entries of the precision matrix at each time point. Specifically, each off-diagonal entry of the precision matrix can be factorized as the product of a Bernoulli and a Gaussian distributed variable; the former is coupled over time via a binary Markov chain while the latter a Gaussian-Markov chain (i.e., a thin-membrane model \cite{29}). To facilitate the derivation of the variational inference algorithm, we replace the exact likelihood of the precision matrix at each time instant by the pseudo-likelihood that consists of the conditional distributions of one variable conditioned on the remaining variables. We then develop an efficient variational inference algorithm based on natural gradients to learn the variational distribution of the time-varying precision matrix. Due to the use of the pseudo-likelihood and the mean-field approximation in the variational inference, the time complexity of BADGE is only $O(NP^2)$. To cope with the problem of local maxima during the variational inference, we resort to simulated annealing \cite{30} and propose a method based on bootstrapping to generate the annealing noise. Numerical results show that when compared with the three groups of frequentist methods, BADGE achieves better performance in terms of structure estimation with significantly less amount of computational time. We further apply BADGE to construct financial networks from the stock return data of 78 banks worldwide during the 2008 Great recession. We find that the network becomes denser during the crisis, with clear peaks during the Great financial crisis and each wave of the subsequent European debt crisis.

Interestingly, BADGE can be extended to inferring graphical models for multiple stationary time series in frequency domain in a straightforward manner. Before explaining this approach, we briefly review the relevant literature on graphical models for stationary time series below. In \cite{31}, it is shown that for jointly Gaussian time series, the conditional independencies between time series are encoded by the common zeros in the inverse spectral density matrices at all frequencies. Given this insight, hypothesis tests are then performed in \cite{31}-\cite{34} to test the conditional independence between every pair of time series. However, such methods are limited to problems with low dimensions and the true graphical model cannot be very sparse. On the other hand, Bach and Jordan \cite{35} further show that by leveraging the Whittle approximation \cite{35} the Fourier transform of the time series at a certain frequency can be regarded as samples drawn from the complex Gaussian distribution whose covariance matrix is the spectral density matrix at the same frequency. As a result, an appealing approach is to first estimate the smoothed spectral density matrix given the Fourier transform of the time series and then to infer the sparse inverse spectral density matrix by maximizing the $\ell_1$ norm penalized likelihood \cite{37}. However, this approach requires extensive tuning. A variant of this approach for autoregressive processes is proposed in \cite{38}. Apart from the frequentist methods, Bayesian methods have also been proposed in \cite{39}. Unfortunately, this method can only learn decomposable graphs from the data. It is also quite time-consuming since Monte-Carlo Markov Chain is used to learn the Bayesian model. Note that the time complexity of all aforementioned methods is at least $O(NP^3)$ for $P$-variate time series with length $N$. In this paper, in analogy to estimating the time-varying inverse covariance matrix, we learn the frequency-varying inverse spectral density matrix using BADGE based on the Fourier transform of the time series, and then define the graphical model for the multivariate time series by identifying the common zero pattern of all inverse spectral density matrices. Different from the aforementioned methods, BADGE is tuning free and scales gracefully with the dimension with time complexity $O(NP^2)$. We compare BADGE with the frequentist method GMS (graphical model selection) proposed in \cite{37} on synthetic data. Similar to the results in the time domain, BADGE can better recover the true graphs while being more efficient. We further apply BADGE to the scalp EEG signals of patients at early stages of AD, and build a classifier based on the estimated graphical models to differentiate between the patients and the controls. The classification accuracy resulting from BADGE is higher than that from GMS.

This paper is structured as follows. We present our Bayesian model for time-varying graphical models in Section 2 and derive the natural gradient variational inference algorithm in Section 3. We then extend the proposed model to frequency domain to infer graphical models for stationary time series in Section 4. In Section 5, we show the numerical results for both synthetic and real data. Finally, we close this paper with conclusions in Section 6.
2 Bayesian Formulation of Time-Varying Graphical Models

We are concerned with undirected graphical models $G = (\mathcal{V}, \mathcal{E})$ in this paper, where $\mathcal{V}$ denotes a set of vertices relating to variables and $\mathcal{E}$ denotes the edge set that encodes the conditional dependencies between the variables. Each node $j \in \mathcal{V}$ is associated with a random variable $x_j$. An edge $(j, k) \in \mathcal{E}$ is absent if and only if the corresponding two variables $x_j$ and $x_k$ are conditionally independent:

$$ p(x_j, x_k | x_{\neg j-k}) = p(x_j | x_{\neg-j}) p(x_k | x_{\neg-j}), \quad \text{where } -j-k \text{ denotes all the nodes in } \mathcal{V} \text{ except } j \text{ and } k. $$

When all variables $x = [x_1, \cdots, x_P]$ are jointly Gaussian distributed, the resulting graphical model is referred to as a Gaussian graphical model. Let $\mathcal{N}(\mu, \Sigma)$ denote a Gaussian distribution with mean $\mu$ and covariance $\Sigma$. The distribution can be equivalently parameterized as $\mathcal{N}(\text{K}^{-1}h, \text{K}^{-1})$, where $\text{K} = \Sigma^{-1}$ is the precision matrix (the inverse covariance) and $h = K\mu$ is the potential vector. The density function can be expressed as:

$$ p(x) \propto \text{det}(K)^{\frac{1}{2}} \exp \left( -\frac{1}{2} x'Kx + h'x \right), \quad (1) $$

where $x'$ denotes the transpose of $x$. Under this scenario, the conditional dependencies are characterized by the precision matrix, that is, $x_j$ and $x_k$ are conditionally independent if and only if $K_{jk} = 0$. As a result, for Gaussian graphical models, we target at inferring a sparse precision matrix from the data.

For time-varying graphical models, we assume that the observation $x^{(t)}$ at time $t$ is drawn from the graphical model with precision matrix $K^{(t)}$ for $t = 1, \cdots, T$, and $K^{(t)}$ changes smoothly with $t$. Without loss of generality, we further assume that $\mu^{(t)} = 0$ in our model, and so $h^{(t)} = 0$.

The likelihood of $K^{(t)}$ can then be expressed as:

$$ p(x^{(t)} | K^{(t)}) \propto \text{det}(K^{(t)})^{\frac{1}{2}} \exp \left( -\frac{1}{2} x^{(t)}'K^{(t)}x^{(t)} \right). \quad (2) $$

To facilitate the derivation of the variational inference algorithm, we propose to use the pseudo-likelihood instead of the exact likelihood (2) in the Bayesian formulation. More specifically, the pseudo-likelihood is derived from the conditional distributions of one variable $x_j$ conditioned on the remaining variables $x_{\neg j}$:

$$ p(x_j | x_{\neg j}, K_{jj}, K_{\neg j}) \propto \sqrt{K_{jj}} \exp \left[ -\frac{1}{2} K_{jj} (x_j' + K_{jj}^{-1} K_{\neg j-j} x_{\neg j})^2 \right], \quad (3) $$

where $K_{\neg j-j}$ denotes row $j$ in $K$ excluding $K_{jj}$, and $-K_{jj}^{-1} K_{\neg j-j} x_{\neg j}$ and $K_{jj}^{-1}$ are respectively the mean and the variance of the conditional distribution $p(x_j | x_{\neg j})$. Here, we regard (3) as a Gaussian distribution of $x_j$ whose mean and variance are parameterized by $K_{jj}$ and $K_{\neg j-j}$. In other words, it is a likelihood function of $K_{jj}$ and $K_{\neg j-j}$. This pseudo-likelihood of $K$ has been frequently explored in the literature [3]-[7], [18], [25], for Gaussian graphical model selection. It simplifies the determinant term in (2) that typically leads to heavy computational burden of $O(P^3)$, and so improves the computational efficiency. Indeed, the time complexity of the proposed method BADGE is only $O(P^2)$ w.r.t. (with regard to) $P$, owning to the pseudo-likelihood. Furthermore, the pseudo-likelihood typically results in more accurate and robust results when learning the graph structure [6], [7], [23].

Next, we impose priors on both $K_{jj}$ and $K_{\neg j-j}$ in order to construct a full Bayesian model. We first focus on the off-diagonal elements $K_{jk}$. To guarantee that the off-diagonal parts of the precision matrices $K^{(t)}$ are sparse while varying smoothly across time, we resort to the temporally dependent spike and slab prior [27], [28]. Concretely, a spike and slab prior on $K_{jk}^{(t)}$ can be defined as [40]:

$$ K_{jk}^{(t)} \sim \pi_{jk}^{(t)} N(\mu_{jk}^{(t)}, \nu_{jk}^{(t)}) + (1 - \pi_{jk}^{(t)}) \delta_0, \quad (4) $$

where $N(\mu_{jk}^{(t)}, \nu_{jk}^{(t)})$ is a Gaussian distribution with mean $\mu_{jk}^{(t)}$ and variance $\nu_{jk}^{(t)}$, $\delta_0$ is a Kronecker delta function, and $\pi_{jk}^{(t)} \in [0, 1]$ determines the probability of $K_{jk}^{(t)} = 0$ (i.e., the spike probability). By decreasing $\pi_{jk}^{(t)}$ to 0, this prior would shrink $K_{jk}^{(t)}$ to 0, thus encouraging sparsity in $K^{(t)}$. The above expression can also be equivalently written as [27]:

$$ K_{jk}^{(t)} = s_{jk}^{(t)} J_{jk}^{(t)}, \quad J_{jk}^{(t)} \sim N(\mu_{jk}^{(t)}, \nu_{jk}^{(t)}), \quad s_{jk}^{(t)} \sim \text{Ber}(\pi_{jk}^{(t)}), \quad (5) $$

where $\text{Ber}(\pi_{jk}^{(t)})$ is a Bernoulli distribution with success probability $\pi_{jk}^{(t)}$. To obtain $K^{(t)}$ that changes smoothly with $t$, we need to impose smoothness priors on both $s_{jk}^{(t)}$ and $J_{jk}^{(t)}$. For $s_{jk}^{(t)}$, we assume that it is drawn from a binary Markov chain defined by the initial state and the transition probabilities:

$$ p(s_{jk}^{(1)}:N) = p(s_{jk}^{(1)}) \prod_{t=2}^{N} p(s_{jk}^{(t)} | s_{jk}^{(t-1)}), \quad (8) $$

where

$$ p(s_{jk}^{(1)}) = \pi_1 \delta(s_{jk}^{(1)}=1) (1 - \pi_1) \delta(s_{jk}^{(1)}=0), \quad (9) $$

$$ p(s_{jk}^{(t)} | s_{jk}^{(t-1)}) = A_0 \delta(s_{jk}^{(t-1)}=0, s_{jk}^{(t)}=0) (1 - A_0) \delta(s_{jk}^{(t-1)}=0, s_{jk}^{(t)}=1) \cdot A_1 \delta(s_{jk}^{(t-1)}=1, s_{jk}^{(t)}=1) (1 - A_1) \delta(s_{jk}^{(t-1)}=1, s_{jk}^{(t)}=0), \quad (10) $$

and $\delta(\cdot)$ denotes the indicator function that yields 1 when the condition in the bracket is satisfied and 0 otherwise. We further assume $\pi_1$, $A_0$, and $A_1$ follow uniform distributions $\text{Be}(1, 1)$, where $\text{Be}(1, 1)$ denotes a Beta distribution with shape parameters one.
The resulting prior on Markov chain, in particular, a thin-membrane model [29].

\[ \alpha_{jk} \propto \exp \left( -\frac{\alpha_{jk}}{2} \sum_{t=2}^{N} (J_{jk}^{(t)} - J_{jk}^{(t-1)})^2 \right) \]

\[ \propto \exp \left( -\frac{\alpha_{jk}}{2} J_{jk}^{(1:N)} K_{TM} J_{jk}^{(1:N)} \right), \]

where \( \alpha_{jk} \) is the smoothness parameter and \( \alpha_{jk} K_{TM} \) is the precision matrix of this Gaussian graphical model. We further impose a non-informative Jeffreys’s prior on \( \alpha_{jk} \), that is, \( p(\alpha_{jk}) \propto 1/\alpha_{jk} \). The difference between \( J_{jk}^{(t-1)} \) and \( J_{jk}^{(t)} \) at every two consecutive time points \( t - 1 \) and \( t \) is controlled by the smoothness parameter \( \alpha_{jk} \), suggesting that \( \alpha_{jk} \) determines the smoothness of \( J_{jk}^{(t)} \) across \( t \).

We also notice that \( K_{TM} \) is the graph Laplacian matrix corresponding to the Markov chain: the diagonal entry \( [K_{TM}]_{jj} \) equals the number of neighbors of node \( j \), while the off-diagonal entry \( [K_{TM}]_{jk} \) equals \(-1\) if node \( j \) and \( k \) are adjacent and 0 otherwise. As a result, \( K_{TM} \) is a tri-diagonal matrix in our case. Furthermore, it follows from the properties of the Laplacian matrix that \( K_{TM}^2 = 0 \), where 1 denotes a vector of all ones. In other words, the thin-membrane model is invariant to the addition of \( c \mathbf{1} \), where \( c \) is an arbitrary constant, and it allows the deviation from any overall mean level without having to specify the overall mean level itself. Such desirable properties make the thin-membrane model a popular smoothness prior in practice.

For diagonal entries in the time-varying precision matrix, since they can only take positive values, we reparameterize \( K_{jj}^{(t)} \) as \( K_{jj}^{(t)} = \exp(\kappa_{jj}^{(t)}) \). To promote the smooth variation of \( \kappa_{jj}^{(t)} \) across \( t \), we assume that \( \kappa_{jj}^{(1:N)} \) follows a thin-membrane model with smoothness parameter \( \beta \). We also impose the Jeffreys’s prior on \( \beta \).

Altogether, the proposed Bayesian model is summarized as a graphical model in Fig. 1. The joint distribution of all variables can be factorized as:

\[
\begin{align*}
    p(x^{(1:N)}, s^{(1:N)}, J^{(1:N)}, \kappa^{(1:N)}, \pi_1, A_{00}, A_{11}, \alpha, \beta) &= p(x^{(1:N)} | s^{(1:N)}, J^{(1:N)}, \kappa^{(1:N)}) p(s^{(1:N)} | \pi_1, A_{00}, A_{11}) \cdot p(J^{(1:N)} | \alpha) p(\kappa^{(1:N)} | \beta) p(\pi_1) p(A_{00}) p(A_{11}) p(\alpha) p(\beta) \\
    &= \prod_{j=1}^{P} \prod_{t=1}^{N} p(x_{j}^{(t)} | \kappa_{j}^{(t)}, J_{j-1}^{(t)}, s_{j-1}^{(t)}) \cdot \prod_{j=1}^{P} \prod_{k=j+1}^{P} \left[ p(s_{jk}^{(1:N)} | \pi_1, A_{00}, A_{11}) p(J_{jk}^{(1:N)} | \alpha_{jk}) p(\alpha_{jk}) \right] \cdot \prod_{j=1}^{P} p(\kappa_{j}^{(1:N)} | \beta) p(\pi_1) p(A_{00}) p(A_{11}) p(\beta).
\end{align*}
\]

3 Variational Inference

In this section, we develop a variational inference algorithm to learn the above Bayesian model. We begin with an introduction to variational inference. We then derive the low-complexity variational inference algorithm for BADGE. Since the variational inference algorithm is often sensitive to local maxima, we further present how to utilize simulated annealing to help the algorithm escape from local maxima.

3.1 Variational Inference and Natural Gradients

Suppose that variables \( x, z_1, \) and \( z_2 \) form a hierarchical Bayesian model, in which \( x \) is observed whereas \( z_1 \) and \( z_2 \) are the latent variables. The joint distribution can be factorized as:

\[
p(x, z_1, z_2) = p(x | z_1) p(z_1 | z_2) p(z_2).\]

The ultimate goal of the variational inference is to approximate the exact but intractable posterior \( p(z_1, z_2 | x) \) by a tractable variational distribution \( q(z_1, z_2) \) that is closest in Kullback-Leibler (KL) divergence to \( p(z_1, z_2 | x) \). Minimizing the KL divergence is equivalent to maximizing a lower bound of the evidence log \( p(x) \), that is [41]:

\[
\mathcal{L} = \mathbb{E}_q(z_1, z_2) [\log p(x, z_1, z_2)] - \mathbb{E}_q(z_1, z_2) [\log q(z_1, z_2)],
\]

where \( \mathbb{E}_q(z_1, z_2) \) is the expectation over the distribution \( q(z_1, z_2) \) and \( \mathcal{L} \) is often referred to as evidence lower bound (ELBO) [41, 42]. The inequality stems from Jensen’s inequality and the equality holds when \( q(z_1, z_2) = p(z_1, z_2 | x) \).

Typically, we apply the mean-field approximation and factorize the variational distribution as \( q(z_1, z_2) = q(z_1) q(z_2) \). Next, we choose \( q(z_1) \) and \( q(z_2) \) that maximize the ELBO \( \mathcal{L} \). In the case where all distributions in the Bayesian model are from the exponential family and are conditionally conjugate, the classical expectation-maximization variational Bayes algorithm [41, 42] provides an efficient tool to update the variational distributions. Suppose that \( p(z_2) \) takes the following exponential form:

\[
p(z_2) \propto \exp \{ \gamma' \phi(z_2) \},
\]

where \( \gamma \) is a vector of natural parameters (a.k.a. canonical parameters) and \( \phi(z_2) = [\phi_1(z_2), \ldots, \phi_m(z_2)] \) denotes the vector of sufficient statistics. Since the prior \( p(z_2) \) is conjugate to the likelihood \( p(z_1 | z_2) \), we can express the likelihood in the same functional form as the prior w.r.t. \( z_2 \):

\[
p(z_1 | z_2) \propto \exp \{ \phi(z_2)' \psi(z_1) \},
\]

where \( \phi(z_2) \) denotes the natural parameters, and \( \psi(z_1) \) depending on \( z_1 \) only denotes the sufficient statistics. The
variational distribution \( q(z_i) \) for \( i \in \{1, 2\} \) that maximizes \( \mathcal{L} \) can be derived as [41], [42]:

\[
q(z_i) \propto \exp \left\{ \mathbb{E}_{q(z_i)} [\log p(x, z_1, z_2)] \right\}
\] (16)

Note that the expectation inside the exponential is taken over all latent variables except the one whose variational distribution is to be updated. The expectation-maximization variational Bayes algorithm then cycles through the update rules for \( q(z_1) \) and \( q(z_2) \) until convergence. This algorithm fully exploits the geometry of the posterior and implicitly adopts natural gradients, resulting in simple close-form update rules and faster convergence than standard gradients [42]-[44]. However, (16) yields a distribution with a close-form expression only under the conjugate scenario.

In the case where the pair of prior and the likelihood is not conjugate, we first specify the functional form of the variational distribution, compute the natural gradient w.r.t. the natural parameters of the distribution, and then follow the direction of the natural gradients to update these parameters. Concretely, we still specify the variational distribution to be the exponential family distributions, due to their generality and many useful algebraic properties. As such, \( q(z_2) \) can be expressed as:

\[
q(z_2; \theta) = \exp \left\{ \theta^T \phi(z_2) - A(\theta) \right\},
\] (17)

where \( \theta \) is a vector of natural parameters and \( A(\theta) = \log \int \exp[\theta^T \phi(z_2)]dz_2 \) is the log-partition function. We call the above representation minimal if all components of the vector of sufficient statistics \( \phi(z_2) = [\phi_1(z_2), \cdots, \phi_m(z_2)] \) are linearly independent for all \( z_2 \). Minimal representation suggests that every distribution \( q(z_2; \theta) \) has a unique natural parameterization \( \theta \). We further define the mean parameter vector as \( \eta = \mathbb{E}[\phi(z_2)] \). It is easy to show that:

\[
\eta = \nabla_\theta A(\theta).
\] (18)

Note that this mapping is one-to-one if and only if the representation is minimal. Next, we consider optimizing the natural parameters \( \theta \) of the variational distribution following the direction of the natural gradient. The natural gradient pre-multiples the standard gradient by the inverse of the Fisher information matrix \( \mathcal{I} \). In particular for distributions in the minimal exponential family (i.e., \( q(z_2; \theta) \)), the resulting Fisher information matrix is given by:

\[
\mathcal{I}(\theta) = -\mathbb{E}_{q(z_2)} [\nabla_\theta^T \log q(z_2; \theta)] = \nabla_\theta A(\theta) = \frac{\partial \eta}{\partial \theta}.
\] (19)

The last equality follows directly from [15]. Thus, the natural gradient of \( \mathcal{L} \) w.r.t. \( \theta \) can be simplified as:

\[
\mathcal{I}(\theta)^{-1} \nabla_\theta \mathcal{L} = \mathcal{I}(\theta)^{-1} \frac{\partial \eta}{\partial \theta} \nabla_\eta \mathcal{L} = \nabla_\eta \mathcal{L}.
\] (20)

In other words, for variational distributions in the minimal exponential family, the natural gradient of the ELBO \( \mathcal{L} \) w.r.t. to the natural parameters \( \theta \) is equivalent to the standard gradient of \( \mathcal{L} \) w.r.t. the corresponding mean parameters \( \eta \). We further notice that the second term in \( \mathcal{L} \) [15] is the entropy of \( q(z_2; \theta) \) and its gradient w.r.t. \( \eta \) is \( -\theta \). As a result, let \( \mathcal{L}_1 = \mathbb{E}_{q(z_1, z_2)} [\log p(x, z_1, z_2)] \) denote the first term in \( \mathcal{L} \) [15] and \( 0 < \rho \leq 1 \) be the step size, the update rule of \( \theta \) for the natural gradient algorithm is:

\[
\theta^{(i+1)} = (1 - \rho) \theta^{(i)} + \rho \nabla_\eta \mathcal{L}_1(\theta^{(i)}).
\] (21)

Note that the above natural gradient update rule amounts to the expectation-maximization update rule in (16) when \( p(z_2) \) and \( p(z_1 | z_2) \) are conjugate as in [14] and \( \rho = 1 \). For instance, the update rule for \( q(z_2) \) resulting from both algorithms is the same and can be written as:

\[
q(z_2) \propto \exp \left\{ [\gamma + \langle \psi(z_1) \rangle] \phi(z_2) \right\}.
\] (22)

In other words, the expectation-maximization algorithm is a special case of the natural gradient algorithm when the Bayesian model is conditionally conjugate. The natural gradient variational inference algorithm is guaranteed to achieve linear convergence with a constant step size \( \rho \) under mild conditions [43]. In practice, to further accelerate the convergence, we follow [43] to set \( \rho = 1 \) for the conjugate pairs (i.e., applying the expectation-maximization variational Bayes update rule in (16)) and to use the line search method to determine the step size \( \rho \) for the non-conjugate pairs. The convergence with this step size scheme can be easily proven as in [45], since the ELBO is guaranteed to increase in every iteration.

### 3.2 Variational Inference for BADGE

Our objective is to approximate the intractable posterior distribution \( p(s^{(1:N)}, j^{(1:N)}, \kappa^{(1:N)}, \pi_1, A_{00}, A_{11}, \alpha, \beta | x^{(1:N)}) \) by a tractable variational distribution, that is, \( q(s^{(1:N)}, j^{(1:N)}, \kappa^{(1:N)}, \pi_1, A_{00}, A_{11}, \alpha, \beta) \). Specifically, we apply the mean-field approximation and factorize the variational distribution as:

\[
q(s^{(1:N)}, j^{(1:N)}, \kappa^{(1:N)}, \pi_1, A_{00}, A_{11}, \alpha, \beta) = \prod_{j=1}^{P} \prod_{k=1}^{P} \left[ q(s_{jk}^{(1:N)}) q(j_{jk}^{(1:N)}) q(\alpha_{jk}) \right] \prod_{j=1}^{P} q(\kappa_{j}^{(1:N)}) q(\pi_1)
\]

\[
q(A_{00}) q(A_{11}) q(\beta).
\] (23)

The first term in the ELBO can be expressed as in [44].

We then proceed to derive the update rules for the variational distribution. In the proposed Bayesian model [12], all pairs of prior and likelihood are conjugate except the prior and likelihood of \( \kappa^{(1:N)} \). We first concentrate on the conjugate pairs; the corresponding variational distribution can be derived following the expectation-maximization variational Bayes update rule in (16). Specifically, for \( s_{jk}^{(1:N)} \),

\[
q(s_{jk}^{(1:N)}) \propto \exp \left[ \sum_{t=2}^{N} \varphi_0^s(s_{jk}^{(t)}) + \sum_{t=2}^{N} \varphi_0^s(s_{jk}^{(t-1)}) \right],
\] (41)

where the node potential \( \varphi_0^s \) and edge potential \( \varphi_0^e \) of the binary Markov chain are defined in [27]-[28] in Table [1]. The marginal and pairwise densities, \( q(s_{jk}^{(t)}) \) and \( q(s_{jk}^{(t)}, s_{jk}^{(t-1)}) \), can then be computed via message passing in the binary Markov chain (i.e., the forward-backward algorithm) with time complexity \( O(N) \). Given \( q(s_{jk}^{(t)}) \) and \( q(s_{jk}^{(t)}, s_{jk}^{(t-1)}) \), the variational distributions of the initial state \( \pi_1 \) and the transition probabilities \( A_{00} \) and \( A_{11} \) can be written as:

\[
q(\pi_1) = \text{Be}(a, b),
\]

\[
q(A_{00}) = \text{Be}(c_0, d_0),
\]

\[
q(A_{11}) = \text{Be}(c_1, d_1).
\] (44)
\[ \mathcal{L}_1 = \sum_{t=1}^{N} \sum_{j=1}^{P} \left[ \frac{1}{2} \left( \exp \left( \kappa_j^{(t)} \right) \right) s_{j,k}^{(t)} - \frac{1}{2} \left( \exp \left( - \kappa_j^{(t)} \right) \right) \left( K_{j,k} s_{j,k}^{(t)} - \frac{1}{2} \left( \exp \left( - \kappa_j^{(t)} \right) \right) \left( K_{j,k} s_{j,k}^{(t)} \right) \right) \right] + \sum_{j=1}^{P} \sum_{k=1}^{K} \left[ \delta(s_{j,k}^{(t)}) = 1 \right] \left( \log \pi_1 \right) + \left[ \delta(s_{j,k}^{(t)}) = 0 \right] \left( \log \left( 1 - \pi_1 \right) \right) \right] + \sum_{j=1}^{P} \sum_{k=1}^{K} \left[ \delta(s_{j,k}^{(t-1)}) = 1, s_{j,k}^{(t)} = 0 \right] \left( \log \left( 1 - \pi_0 \right) \right) + \left[ \delta(s_{j,k}^{(t-1)}) = 0, s_{j,k}^{(t)} = 1 \right] \left( \log \left( 1 - \pi_0 \right) \right) \right] + \left[ \delta(s_{j,k}^{(t-1)}) = 1, s_{j,k}^{(t)} = 1 \right] \left( \log \left( 1 - \pi_{opp} \right) \right) + \left[ \delta(s_{j,k}^{(t-1)}) = 0, s_{j,k}^{(t)} = 0 \right] \left( \log \left( 1 - \pi_{opp} \right) \right) \right] \]

\[ \Rightarrow \left( \frac{N}{2} - 1 \right) \sum_{j=1}^{P} \sum_{k=1}^{K} \left( \log \alpha_{jk} + \left( \frac{P(N-1)}{2} - 1 \right) \log \beta \right) \]

\[ \frac{\partial \mathcal{L}_1}{\partial \left( K_{j,k}^{(t)} \right)} = -2 \alpha_{jk} \left( \frac{\exp(-\kappa_j^{(t)})}{\left( \exp(-\kappa_j^{(t)}) \right)^2} \right) s_{j,k}^{(t-1)} - \frac{1}{2} \left( \exp(-\kappa_j^{(t)}) \right) \left( K_{j,k} s_{j,k}^{(t)} \right) \]

\[ \frac{\partial \mathcal{L}_1}{\partial \left( K_{j,k}^{(t)} \right)} = \delta \left( s_{j,k}^{(t)} = 1 \right) \left( \log \pi_1 \right) + \delta \left( s_{j,k}^{(t)} = 0 \right) \left( \log \left( 1 - \pi_1 \right) \right) - \left( \frac{\partial \mathcal{L}_1}{\partial \left( K_{j,k}^{(t)} \right)} \left( \frac{1}{2} \cdot \frac{\partial \mathcal{L}_1}{\partial \left( K_{j,k}^{(t)} \right)} \right) \right) \]

\[ \right] \]

\[ \Rightarrow \left( \frac{N}{2} - 1 \right) \sum_{j=1}^{P} \sum_{k=1}^{K} \left( \log \alpha_{jk} + \left( \frac{P(N-1)}{2} - 1 \right) \log \beta \right) \]

\[ \frac{\partial \mathcal{L}_1}{\partial \left( K_{j,k}^{(t)} \right)} = -2 \alpha_{jk} \left( \frac{\exp(-\kappa_j^{(t)})}{\left( \exp(-\kappa_j^{(t)}) \right)^2} \right) s_{j,k}^{(t-1)} - \frac{1}{2} \left( \exp(-\kappa_j^{(t)}) \right) \left( K_{j,k} s_{j,k}^{(t)} \right) \]

\[ \frac{\partial \mathcal{L}_1}{\partial \left( K_{j,k}^{(t)} \right)} = \delta \left( s_{j,k}^{(t)} = 1 \right) \left( \log \pi_1 \right) + \delta \left( s_{j,k}^{(t)} = 0 \right) \left( \log \left( 1 - \pi_1 \right) \right) - \left( \frac{\partial \mathcal{L}_1}{\partial \left( K_{j,k}^{(t)} \right)} \left( \frac{1}{2} \cdot \frac{\partial \mathcal{L}_1}{\partial \left( K_{j,k}^{(t)} \right)} \right) \right) \]

\[ \right] \]

\[ \Rightarrow \left( \frac{N}{2} - 1 \right) \sum_{j=1}^{P} \sum_{k=1}^{K} \left( \log \alpha_{jk} + \left( \frac{P(N-1)}{2} - 1 \right) \log \beta \right) \]

\[ \frac{\partial \mathcal{L}_1}{\partial \left( K_{j,k}^{(t)} \right)} = -2 \alpha_{jk} \left( \frac{\exp(-\kappa_j^{(t)})}{\left( \exp(-\kappa_j^{(t)}) \right)^2} \right) s_{j,k}^{(t-1)} - \frac{1}{2} \left( \exp(-\kappa_j^{(t)}) \right) \left( K_{j,k} s_{j,k}^{(t)} \right) \]

where the shape parameters \( a, b, c_0, c_1, d_1 \) of the Beta distributions can be updated as in (35)-(40).

The other hand, the variational distribution \( q(J_{jk}^{(1:N)}) \) corresponds to a Gauss-Markov chain that can be decomposed into node and edge potentials as:

\[ q(J_{jk}^{(1:N)}) \propto \exp \left[ \sum_{t=1}^{N} \varphi_{\mathcal{V}}(J_{jk}^{(t)}) + \sum_{t=2}^{N} \varphi_{\mathcal{E}}(J_{jk}^{(t)}, J_{jk}^{(t-1)}) \right] \]

where the node potentials \( \varphi_{\mathcal{V}}(J_{jk}^{(t)}) \) and edge potentials \( \varphi_{\mathcal{E}}(J_{jk}^{(t)}, J_{jk}^{(t-1)}) \) are defined in (29) and (30) in Table 1.

Again, the mean and variance for each \( J_{jk}^{(t)} \) and the pairwise covariance of \( J_{jk}^{(t)} \) and \( J_{jk}^{(t-1)} \) can be obtained via message passing (a.k.a. belief propagation) with complexity \( O(N) \).

We can then update the variational distribution of \( \alpha_{jk} \) as:

\[ q(\alpha_{jk}) = \text{Ga} \left( \frac{N-1}{2}, \sum_{t=2}^{N} \left( (J_{jk}^{(t)} - J_{jk}^{(t-1)})^2 \right) \right) \]

where \( \text{Ga}(a,b) \) denotes a Gamma distribution with shape parameter \( a \) and rate parameter \( b \). The expectation of \( \alpha_{jk} \) is \( (N-1)/(\sum_{t=2}^{N} ((J_{jk}^{(t)} - J_{jk}^{(t-1)})^2) \).

Finally, let us turn our attention to \( \kappa_j^{(1:N)} \), whose prior and likelihood are not conjugate. As mentioned in the previous subsection, we need to specify the functional form of \( q(\kappa_j^{(1:N)}) \), compute the natural gradients, and then update the natural parameters of \( q(\kappa_j^{(1:N)}) \) following (21). Here, we choose \( q(\kappa_j^{(1:N)}) \) to be Gaussian. Owing to the thin-layer membrane priors on \( \kappa_j^{(1:N)} \), \( q(\kappa_j^{(1:N)}) \) is also associated with a Gauss-Markov chain, in the same fashion as \( q(J_{jk}^{(1:N)}) \).
Therefore, we can parameterize $q(\boldsymbol{\kappa}_j^{(1:N)})$ as:

$$q(\boldsymbol{\kappa}_j^{(1:N)}) \propto \exp \left[ \sum_{t=1}^{N} \varphi^\psi_t(\kappa_j^{(t)}) + \sum_{t=2}^{N} \varphi^\xi_t(\kappa_j^{(t)} - \kappa_j^{(t-1)}) \right]$$

$$\propto \exp \left[ \sum_{t=1}^{N} \left( - \frac{\Omega_t \kappa_j^{(t)}}{2} + h_t \kappa_j^{(t)} \right) - \sum_{t=2}^{N} \Omega_{t,t-1} \kappa_j^{(t)} \kappa_j^{(t-1)} \right],$$

where $\Omega$ denotes the $N \times N$ tri-diagonal precision matrix and $h$ is the $N$-dimensional potential vector. In light of (21), $\Omega$ and $h$ can be updated as in (33)-(34). Note that the step size $\rho$ in (33)-(34) is chosen via line search. After obtaining the mean, the variance and the pairwise covariance of $\kappa_j^{(1:N)}$ via message passing in the Gauss-Markov chain, we can update $q(\beta)$ as $q(\beta) = \text{Ga}((N - 1)P/2, \sum_{t=1}^{N} \sum_{j=1}^{N} (\kappa_j^{(t)} - \kappa_j^{(t-1)})^2)/2$. Detailed derivation of the variational inference algorithm can be found in the supplementary material.

### 3.3 Time Complexity

We notice that the most expensive operations in the update rules in Table 1 are the products $\langle k_{j,j}^{(t)} \rangle x_{-j}^{(t)}$ and $\langle K_{k,j}^{(t)} \rangle x_{-j}^{(t)}$ in (25) and $\langle K_{k,j}^{(t)} \rangle x_{-j}^{(t)}$ in (51). The time complexity of these operations is $O(P)$. The last product is used for updating one diagonal element $K_{j,j}^{(t)}$, and hence, the time complexity for updating all NP diagonal elements in $K^{(1:N)}$ is $O(NP^2)$. On the other hand, the first two products are used for updating one off-diagonal element $K_{k,j}^{(t)}$. Take into account all $O(NP^2)$ off-diagonal elements in $K^{(1:N)}$, and the overall time complexity of BADGE should be $O(NP^3)$. However, instead of computing these products every time when updating an off-diagonal element $K_{k,j}^{(t)}$, we can first keep a record of $\langle K_{k,j}^{(t)} \rangle x_{-j}^{(t)}$ for $j = 1, \ldots, P$ at the beginning of BADGE. Next, for each off-diagonal element $K_{k,j}^{(t)}$, the products can be computed as $\langle K_{k,j}^{(t)} \rangle x_{-j}^{(t)} = \langle K_{k,j}^{(t)} \rangle x_{-j}^{(t)} - \langle K_{k,j}^{(t)} \rangle x_{k}^{(t)}$ and likewise for $\langle K_{k,j}^{(t)} \rangle x_{-j}^{(t)}$. After updating the variational distribution of this off-diagonal element, we can then update the record as $\langle K_{k,j}^{(t)} \rangle x_{-j}^{(t)} = \langle K_{k,j}^{(t)} \rangle x_{-j}^{(t)} + \langle K_{k,j}^{(t)} \rangle x_{k}^{(t)}$ and likewise for $\langle K_{k,j}^{(t)} \rangle x_{-j}^{(t)}$. As a consequence, we can cycle through all off-diagonal elements in $K^{(1:N)}$ without recomputing the products every time. The resulting time complexity of BADGE can be reduced to $O(NP^2)$.

### 3.4 Simulated Annealing

The ELBO is non-convex, and thus, the variational inference algorithm suffers from the issue of local maxima. To counteract this problem, we employ simulated annealing and modify the update rule of the variational inference in (21) as (30):

$$\tilde{\theta} = (1 - \rho) \theta^{(i)} + \rho \frac{1}{T^{(i)}} \nabla_\theta L_1(\theta^{(i)}) + \left(1 - \frac{1}{T^{(i)}} \right) \epsilon^{(i)},$$

where $T^{(i)}$ denotes the annealing temperature in iteration $i$, and $\epsilon^{(i)}$ denotes the annealing noise vector. This modification applies to both the natural gradient and the expectation-maximization update rule, as the expectation-maximization update rule is a special case of the natural gradient update rule in the conjugate case when $\rho = 1$. Note that $T^{(i)} \rightarrow 1$ as $i \rightarrow \infty$. The update $\tilde{\theta}$ is accepted with the probability:

$$p(\theta^{(i+1)} = \tilde{\theta}) = \min \left\{ 1, \exp \left[ \frac{L(\theta^{(i)}) - L(\tilde{\theta}^{(i)})}{1 - 1/T^{(i)}} \right] \right\},$$

otherwise $\theta^{(i+1)} = \theta^{(i)}$. When the temperature $T^{(i)}$ is high, $\tilde{\theta}$ is sufficiently volatile to avoid shallow local maxima. As $T^{(i)}$ decreases to 1, the algorithm mimics the original variational inference and converges.

Next, we discuss how to build the noise vector $\epsilon^{(i)}$. Currently, there is no generic rule for specifying the noise distribution. In this work, we only add noise when updating the natural parameters of $q(s_{jk}^{(1:N)})$, $q(J_{jk}^{(1:N)})$, and $q(\kappa_j^{(1:N)})$, since the update rules for these parameters are more complicated than the others and so the resulting estimates are more likely to converge to local maxima. Let $\nabla_{\eta} L_1(\theta^{(i)})$ denote the natural gradient of $L_1$ in (24) w.r.t. the natural parameters $\theta$ of $q(s_{jk}^{(1:N)})$, $q(J_{jk}^{(1:N)})$, and $q(\kappa_j^{(1:N)})$. It can be observed from the corresponding update rules (cf. Eqs. (25)-(34) in Table 1) that $\nabla_{\eta} L_1(\theta^{(i)})$ can be decomposed into two terms: $\nabla_{\eta} L_1(\theta^{(i)}) = \nabla_{\eta} L_1(\theta^{(i)}, x^{(1:N)}) + \nabla_{\eta} L_1(\theta^{(i)}, \xi)$, where $\nabla_{\eta} L_1(\theta^{(i)}, x^{(1:N)})$ is a function of the observations $x^{(1:N)}$, and $\nabla_{\eta} L_1(\theta^{(i)}, \xi)$ is a function of the hyperparameters $\xi = \{\pi_1, A_{00}, A_{11}, \alpha, \beta\}$. Correspondingly, we decompose the noise vector as $\epsilon^{(i)} = \epsilon^{(i)}(x^{(1:N)}) + \epsilon^{(i)}(\xi)$. For the hyperparameters $\xi$, we utilize their variational distributions to obtain the noise $\epsilon^{(i)}(\xi)$. Concretely, we draw a random sample $\xi$ of $\xi$ from the variational distribution in each iteration, and compute the noise vector as $\epsilon^{(i)}(\xi) = \nabla_{\eta} L_1(\theta^{(i)}, \xi)$.

On the other hand, for the function of the observations, let $\nabla_{\eta} L_1(\theta^{(i)}, x^{(1:N)}) = \nabla_{\eta} L_1(\theta^{(i)}, x^{(1:N)})/T^{(i)} + (1 - 1/T^{(i)}) \epsilon^{(i)}(x^{(1:N)})$ denote the noisy gradient that is corrupted by the annealing noise. As $T^{(i)} \rightarrow 1$, $\nabla_{\eta} L_1(\theta^{(i)}, x^{(1:N)})$ becomes less noisy and converges to the exact gradient $\nabla_{\eta} L_1(\theta^{(i)}, x^{(1:N)})$. Here, instead of proposing a distribution for $\epsilon^{(i)}(x^{(1:N)})$, we specify the noisy gradient $\nabla_{\eta} L_1(\theta^{(i)}, x^{(1:N)})$ directly by replacing the observations $x^{(1:N)}$ in $\nabla_{\eta} L_1(\theta^{(i)}, x^{(1:N)})$ with its bootstrapped
sample set $\hat{x}^{(1:N)}$. Such bootstrapped sets are often used for
time-invariant graphical model selection \cite{25,40,47} so as
to find a network that is robust to bootstrapping. We borrow
this idea and provide an empirical distribution for $x^{(1:N)}$ by
bootstrapping the original observations. More specifically,
for each time point $t$, we set $\hat{x}^{(t)} = x^{(t)}$ by sampling $\tau$ 
uniformly from a window around $t$ with width $w$, namely,
$\{t - w, t - w + 1, \ldots , t + w\}$. The noisy gradient can then
be computed as $\nabla_\eta \hat{L}_1(\theta^{(t)}, x^{(1:N)}) = \nabla_\eta L_1(\theta^{(t)}, \hat{x}^{(1:N)})$.
Furthermore, we set $w = (1 - 1/T^{(1)})N/2$ such that the
variance of the noisy gradient $\nabla_\eta \hat{L}_1(\theta^{(t)}, x^{(1:N)})$ decreases 
with the decreases of $T$ and $\nabla_\eta \hat{L}_1(\theta^{(t)}, x^{(1:N)})$ converges
to the exact gradient $\nabla_\eta L_1(\theta^{(t)}, x^{(1:N)})$ as $T^{(1)} \to 1$.

In practice, we increase $R^{(1)} = 1/T^{(1)}$ instead of decreasing $T^{(1)}$ as $i$ increases. More concretely, we first estimate the number of iterations for simulated annealing as $N_a$. We then begin the algorithm with $N^{(1)} = 0$ (i.e., $T^{(1)} = \infty$) and increases $R^{(1)}$ by $10/N_a$ in every 10th iteration. After $N_a$ iterations, $R^{(1)}N_a = 1$ (i.e., $T^{(1)}N_a = 1$). In the following experiments, we set $N_a = 500$ unless stated otherwise.

For the detailed implementation of the proposed simulated annealing technique, we refer the readers to the overall algorithm summarized in Algorithm 1 in the supplementary material.

In order to demonstrate the usefulness of the proposed simulated annealing approach, we depict the convergence results of BADGE with and without simulated annealing in Fig. \ref{fig: convergence}. Here, we consider a synthetic data set. The true time-varying graph corresponding to this data set is given. We then randomly select 100 true edges and 100 absent edges from the true graph and check how the corresponding $s^{(1)}_{jk}$ changes as the algorithm proceeds. The initial values for all parameters are the same in both cases. It is obvious that BADGE equipped with simulated annealing can better separate the true edges from false ones.

4 Graphical Models for Stationary Time Series

In this section, we discuss how to exploit BADGE to learn interactions among $P$ univariate stationary Gaussian processes (i.e., time series) $y^{(1:N)}_{1:P}$. A graphical model $G = (V, E)$ for $y^{(t)}$ is constructed by letting an edge $(j, k) \notin E$ denote that the two entire time series $y^{(1:N)}_{j}$ and $y^{(1:N)}_{k}$ are conditionally independent given the remaining collection of time series $y^{(1:N)}_{-jk}$ \cite{48}, that is,

$$
cov(y^{(t)}_{j}, y^{(t+\tau)}_{k}) = 0, \quad \forall \tau. \quad (49)
$$

In other words, the lagged conditional covariance equals 0 for all time lags $\tau$. On the other hand, the conditional dependence can also be defined in frequency domain of the time series. Concretely, we first define the spectral density matrix as the Fourier transform of the lagged covariance matrix $\text{cov}(y^{(t)}_{j}, y^{(t+\tau)}_{k})$:

$$
S^{(\omega)} = \sum_{\tau} \text{cov}(y^{(t)}_{j}, y^{(t+\tau)}_{k}) \exp(-i\omega\tau), \quad (50)
$$

for $\omega \in [0, 2\pi]$. Let $K^{(\omega)} = [S^{(\omega)})^{-1}$, the conditional dependence between $y^{(1:N)}_{j}$ and $y^{(1:N)}_{k}$ holds if and only if $K^{(\omega)}_{jk} = 0, \quad \forall \omega$. \quad (51)

This suggests that one common zero entry in the inverse spectral density matrices across a certain frequency band is equivalent to the conditional independence between the corresponding two time series in this frequency band. Therefore, for a multivariate time series, we aim to infer the inverse spectral density matrices $K^{(\omega)}$.

Here, we follow the state-of-the-art Whittle approximation framework \cite{35}: Suppose that $f^{(\omega)}_{1:P}$ is the discrete Fourier transform of $y^{(1:P)}_{1:P}$ at frequency $\omega$:

$$
f^{(\omega)}_{j} = \sum_{t} y^{(t)}_{j} \exp(-i\omega t), \quad (52)
$$

then $f^{(\omega)}$ are independent complex Gaussian random variables with mean zero and precision matrix given by the inverse spectral density matrix $K^{(\omega)}$ at the same frequency:

$$
f^{(\omega)}_{1:P} \sim \mathcal{N}(0, K^{(\omega)}_{-1}). \quad (53)
$$

As a result, we can learn $K^{(\omega)}$ that changes smoothly with $\omega$ from $f^{(\omega)}$ using BADGE. In this scenario, the covariance is the frequency $\omega$. It should be stressed that the complex Gaussian distribution in \cite{35} can be written as:

$$
p(f^{(\omega)} | K^{(\omega)}_{-1}) \propto \det(K^{(\omega)}_{-1}) \exp\left( -f^{(\omega)*} K^{(\omega)} f^{(\omega)} \right), \quad (54)
$$

where $f^{(\omega)*}$ denotes the complex conjugate transpose of $f^{(\omega)}$. The above density function does not have the operation of square root as in the density function of the Gaussian distribution for real numbers \cite{2}. The corresponding pseudo-likelihood of $K^{(\omega)}$ can then be expressed as:

$$
p(f^{(\omega)} | K^{(\omega)}_{jj}, K^{(\omega)}_{j\cdot j}) \propto K^{(\omega)}_{jj} \exp\left( -K^{(\omega)}_{jj} f^{(\omega)} f^{(\omega)*} \right) - \sum_{j\neq j} K^{(\omega)}_{jj} f^{(\omega)} f^{(\omega)*} - f^{(\omega)} K^{(\omega)} f^{(\omega)} - K^{(\omega)}_{jj} f^{(\omega)} f^{(\omega)*} K^{(\omega)}_{jj} f^{(\omega)} K^{(\omega)}_{jj} f^{(\omega)*}, \quad (55)
$$

where $f^{(\omega)}$ is the complex conjugate of $f^{(\omega)}$. In addition, the prior distribution on $K^{(\omega)}$ is also a complex Gaussian distribution. We therefore modify the ELBO $\mathcal{L}$ and the corresponding update rules accordingly. The detailed update rules is summarized in Table 1 in the supplementary material.

5 Experimental Results

In this section, we compare the proposed BADGE algorithm with the state-of-the-art methods in the literature. Specifically, for the problem of learning time-varying graphical models, we consider three benchmark methods:

1) KERNEL \cite{13,14,16}: Kernel-smoothed covariance matrices $S^{(t)}$ are first estimated, and then a graphical model is inferred at each time point by solving the graphical lasso problem:

$$
K^{(t)} = \arg\min_{K^{(t)}} \text{tr}(S^{(t)} K^{(t)}) - \log \det (K^{(t)}) + \lambda_1 ||K^{(t)}||_1, \quad (K^{(t)} \geq 0)
$$

This suggests that one common zero entry in the inverse spectral density matrices across a certain frequency band is equivalent to the conditional independence between the corresponding two time series in this frequency band. Therefore, for a multivariate time series, we aim to infer the inverse spectral density matrices $K^{(t)}$.
where $\lambda_1$ controls the sparsity of $K^{(t)}$.

2) SINGLE [17, 19, 20]: It further controls the smoothness of $K^{(t)}$ over $t$ by imposing penalty on the difference between the precision matrices at every two consecutive time points:

$$K^{(t)} = \arg\min_{K^{(t)} \geq 0} \sum_{t=1}^{N} \left[ \text{tr}(S^{(t)}K^{(t)}) - \log \det K^{(t)} + \lambda_1 |K^{(t)}|_1 \right] + \lambda_2 \|K^{(t)} - K^{(t-1)}\|_1. \quad (56)$$

3) LOGGLE [25]: It exploits the local group lasso penalty to promote the sparsity of $K^{(t)}$ and the smoothness across time simultaneously:

$$K^{(t)} = \arg\min_{K^{(t)} \geq 0} \sum_{t} \text{tr}(S^{(t)}K^{(t)}) - \log \det K^{(t)} + \lambda_1 \sum_{j \neq k} \left[ \sum_{\tau \in D(t,d)} K_{jk}^{(\tau)} \right]^{\frac{1}{2}}, \quad (57)$$

where $D(t,d) = \{ \tau : |\tau - t| \leq d \}$ denotes neighborhood around $t$ with width $d$. The exact likelihood in the above expression is replaced by the pseudo-likelihood in the implementation to achieve better performance [25].

The time complexity of the above three methods is $O(NP^3)$. On the other hand, for the problem of learning graphical models for stationary time series in frequency domain, we compare BADGE with the GMS approach proposed in [37], which can be regarded as the counterpart of KERNEL in the frequency domain.

5.1 Time-Varying Graphical Models (Time Domain)

5.1.1 Synthetic Data

Given the dimension $P$, the number of time points $N$, and the average number of edges $N_e$, we simulate synthetic Gaussian distributed data from time-varying graphical models as follows. We first generate the off-diagonal elements in the precision matrices $K^{(1:N)}$ using the following function:

$$K_{jk}^{(t)} = A_{jk} \sin \left( \frac{\pi t}{2N} \right) + B_{jk} \cos \left( \frac{\pi t}{2N} \right) + C_{jk} \sin \left( \frac{\pi (t + D_{jk})}{2N} \right), \quad (58)$$

where for all $j$ and $k$, $A_{jk}$, $B_{jk}$, and $C_{jk}$ are drawn uniformly from $[-1, -0.5] \cup [0.5, 1]$, and $D_{jk}$ follows a uniform distribution in $[-0.25, 0.25]$. We then set a threshold and zero out the off-elements whose magnitude is smaller than the threshold such that the average number of edges in $K^{(1:N)}$ is $N_e$. Next, we compute the diagonal entries as $K_{jj}^{(t)} = \sum_{k \neq j} |K_{jk}^{(t)}| + 0.1$ to guarantee the positive definiteness of $K^{(1:N)}$. Finally, we draw a sample $x^{(t)}$ at each time point $t$ from $N(0, K^{(t)})$.

We compare all methods in terms of precision, recall, $F_1$-score, and the computational time. Precision is defined as the proportion of correctly estimated edges to all the edges in the estimated graph; recall is defined as the proportion of correctly estimated edges to all the edges in the true graph; $F_1$-score is defined as 2-precision-recall/(precision+recall), which is a weighted average of the precision and recall. For the benchmark methods, since the ground truth is given, we first select the tuning parameters that maximize the $F_1$-score and refer to the results as oracle results (a.k.a. optimal results). We also show the results when the tuning parameters are selected via cross validation (CV), which is commonly used in existing works [14, 17, 23-25]. More specifically, for all three frequentist methods, we choose the kernel bandwidth $h$ from 5 candidates $\{\exp(-4)N, \exp(-3)N, \ldots, N\}$ and $\lambda_1$ from 5 candidates $\{\exp(-4), \exp(-3), \ldots, 1\}$. We further select $\lambda_2$ from $\{\exp(-4), \exp(-2), \ldots, \exp(4)\}$ for SINGLE and $d$ from $\{\exp(-4)N, \exp(-3)N, \ldots, N\}$ for LOGGLE. We show the results for graphs with different dimensions $P$, different sample sizes $N$, and different graph densities (characterized by the average number of edges $N_e$) respectively in Table 2, Table 3, and Table 4. The results are averaged over 5 trials and the standard deviation is presented in the brackets.

We observe that BADGE typically obtains the highest $F_1$-score with the least amount of computational time, regardless of the dimension, the sample size, and the graph density. In other words, BADGE can well recover the time-varying graph structure in an automated fashion. On the other hand, the oracle results of LOGGLE and SINGLE are comparable to that of BADGE. However, in practice, we have no information on the true graphs and therefore cannot choose the tuning parameters that maximize the $F_1$-score (i.e., minimize the difference between the true and estimated graphs). As mentioned before, one practical approach to choosing the tuning parameters is CV. Unfortunately, as can be observed from Table 4, the CV results are typically worse than the oracle results, indicating that CV cannot always find the optimal tuning parameters. Additionally, we can see that LOGGLE and SINGLE outperform KERNEL in terms of $F_1$-score after capturing the temporal dependence across $K^{(t)}$. Nevertheless, they become prohibitively slow when $P \geq 100$, severely hindering their applications to large-scale problems in practice. By contrast, BADGE improves the estimation accuracy while being more efficient. Indeed, as shown in Fig. 3, the computational time of BADGE approximately increases quadratically with
TABLE 2: Graph recovery results from different methods for synthetic data with different dimensions \((P = 20, 100, 500, N = 1000, N_r = P)\). The standard deviations are shown in the brackets.

| Methods          | \(P = 20\)                          | \(P = 100\)                         | \(P = 500\)                          |
|------------------|-------------------------------------|-------------------------------------|-------------------------------------|
| Precision        | Recall                              | \(F_1\)-score                       | Time(s)                            |
| BADGE            | 0.89 (5.06e-2)                      | 0.86 (2.31e-2)                      | 0.82 (4.06e-2)                     |
| KERNEL (oracle)  | 0.83 (1.76e-2)                      | 0.88 (1.94e-2)                      | 0.87 (1.96e-2)                     |
| KERNEL (CV)     | 0.53 (1.76e-2)                      | 0.86 (2.58e-2)                      | 0.53 (1.76e-2)                     |
| SINGLE (oracle) | 0.86 (2.58e-2)                      | 0.9 (2.06e-2)                       | 0.86 (2.58e-2)                     |
| SINGLE (CV)     | 0.63 (1.76e-2)                      | 0.86 (2.58e-2)                      | 0.63 (1.76e-2)                     |

TABLE 3: Graph recovery results from different methods for synthetic data with different size \((P = 20, 500, 1000, 2000, N_r = P)\). The standard deviations are shown in the brackets.

| Methods          | \(N = 500\)                          | \(N = 1000\)                         | \(N = 2000\)                         |
|------------------|-------------------------------------|-------------------------------------|-------------------------------------|
| Precision        | Recall                              | \(F_1\)-score                       | Time(s)                            |
| BADGE            | 0.85 (7.32e-2)                      | 0.87 (1.32e-2)                      | 0.89 (1.32e-2)                     |
| KERNEL (oracle)  | 0.62 (4.52e-2)                      | 0.83 (1.32e-2)                      | 0.83 (1.32e-2)                     |
| KERNEL (CV)     | 0.53 (1.76e-2)                      | 0.86 (2.58e-2)                      | 0.53 (1.76e-2)                     |
| SINGLE (oracle) | 0.86 (2.58e-2)                      | 0.9 (2.06e-2)                       | 0.86 (2.58e-2)                     |
| SINGLE (CV)     | 0.7 (1.32e-2)                       | 0.86 (2.58e-2)                      | 0.7 (1.32e-2)                      |

TABLE 4: Graph recovery results from different methods for synthetic data with different density \((P = 20, N = 500, 1000, 2000, N_r = P)\). The standard deviations are shown in the brackets.

| Methods          | \(N_r = 30\)                          | \(N_r = 60\)                         | \(N_r = 100\)                        |
|------------------|-------------------------------------|-------------------------------------|-------------------------------------|
| Precision        | Recall                              | \(F_1\)-score                       | Time(s)                            |
| BADGE            | 0.89 (9.88e-2)                      | 0.9 (4.18e-2)                       | 0.9 (4.18e-2)                      |
| KERNEL (oracle)  | 0.85 (7.32e-2)                      | 0.87 (1.32e-2)                      | 0.89 (1.32e-2)                     |
| KERNEL (CV)     | 0.53 (1.76e-2)                      | 0.86 (2.58e-2)                      | 0.53 (1.76e-2)                     |
| SINGLE (oracle) | 0.86 (2.58e-2)                      | 0.9 (2.06e-2)                       | 0.86 (2.58e-2)                     |
| SINGLE (CV)     | 0.7 (1.32e-2)                       | 0.86 (2.58e-2)                      | 0.7 (1.32e-2)                      |
analyzed the volatilities of 96 banks in the world’s top 150 and further constructed time-varying networks by inferring sparse vector autoregressive approximation models in sliding windows of the volatility data. The three peaks were also observed in their experiment; the range of the three peaks in [52] is shown in Fig. 4a. Here we learn networks from the stock return data by means of BADGE, instead of extracting them from volatilities, yet we obtain similar results. As opposed to BADGE, the three peaks are not very obvious for KERNEL, SINGLE, and LOGGLE. The results of these methods may become better by selecting the tuning parameters from a larger set of candidates, at the expense of increased computational time. Unfortunately, the computational time for KERNEL, SINGLE, and LOGGLE is already 1.48e5, 4.90e7, and 8.06e6 seconds respectively, and testing more candidates of the tuning parameters will make these methods distressingly slow. On the other hand, BADGE only takes 3.08e4 seconds to converge. In summary, BADGE can better capture the changes in the financial networks in less amount of computational time.

Next, let us delve into the results given by BADGE. We plot the estimated financial networks at the beginning of each year from 2005 to 2013 in Fig. 5. In this figure, the banks are clustered according to their regions automatically, as banks in the same region are expected to have more interactions. We further choose the cluster of US, Europe (including UK), and Asia-Pacific and depict the average number of connections for banks in each cluster as a function of time in Fig. 4b. Both Fig. 4b and Fig. 5 tell us that number of connections for US and European banks is larger than that of banks in Asia-Pacific. In light of the theory of system risk, the financial institutions with more
TABLE 5: Graph recovery results from BADGE and GMS for synthetic time series with different dimensions ($P = 20, 100$, $N = 1000$, $N_c = P$). The standard deviations are shown in the brackets.

| Methods   | $P = 20$ |           |           |           | $P = 100$ |           |           |           |
|-----------|----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| BADGE     | 0.90 (3.14e-2) | 0.88 (4.23e-2) | 2.18e2 (2.10e1) | 0.88 (4.90e-2) | 0.71 (3.92e-2) | 0.78 (4.22e2) | 4.75e3 (2.85e2) |
| GMS (oracle) | 0.93 (1.05e-2) | 0.77 (2.76e-2) | 3.36e3 (5.13e-1) | 0.71 (1.94e-2) | 0.79 (2.02e2) | 0.75 (7.21e3) | 4.16e5 (6.20e3) |
| GMS (CV)  | 0.63 (1.02e-1) | 0.78 (1.29e-1) | 4.22e2 (7.98e2) | 0.71 (7.66e-2) | 0.68 (2.53e-2) | 0.68 (3.96e-2) | 5.06e5 (9.36e3) |

TABLE 6: Graph recovery results from BADGE and GMS for synthetic time series with different lengths ($P = 20$, $N = 500, 1000, 2000$, $N_c = P$). The standard deviations are shown in the brackets.

| Methods   | $N = 500$ |           |           |           | $N = 1000$ |           |           |           | $N = 2000$ |           |           |           |
|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| BADGE     | 0.90 (6.51e-2) | 0.91 (9.38e-2) | 1.10e2 (8.28) | 0.90 (1.31e-2) | 0.88 (4.23e-2) | 2.16e2 (2.10e1) | 0.90 (6.40e-2) | 0.91 (3.92e-2) | 0.92 (4.44e2) (5.56e3) |
| GMS (oracle) | 0.90 (1.15e-1) | 0.70 (1.09e-1) | 1.70e3 (1.06) | 0.83 (1.01e-1) | 0.72 (2.76e-2) | 3.36e3 (5.13e1) | 0.80 (7.24e2) | 0.73 (1.12e-1) | 0.76 (6.04e2) | 7.26e3 (5.12e2) |
| GMS (CV)  | 0.90 (1.37e-1) | 0.76 (1.14e-1) | 5.54e3 (1.55e2) | 0.63 (1.02e-1) | 0.78 (1.29e-1) | 4.22e2 (7.93e2) | 0.75 (7.56e2) | 0.73 (1.01e-1) | 0.74 (7.36e2) | 9.01e3 (9.76e2) |

connections are central institutions (i.e., sit in the center of the financial system). Such institutions are more sensitive to financial crises, and conversely, their failure can lead to the breakdown of the entire system with a larger probability [49]. With this theory in mind, we can now analyze how the networks changed during the financial crisis. Before the Lehman bankruptcy, the average number of connections for US banks first increased in 2006, due to the Government’s unexpected decision to tighten monetary policy in May and June that year [52]. There was no other major shock in 2006 though, and therefore, the average number of connections for US banks decreased later in 2006 [52]. In early 2007, the collapse of several mortgage originators led to the sharp increase of connections in US [50]. Due to the large number of connections between banks in US and Europe, the European banks also lost a tremendous amount on toxic assets and from bad loans. Consequently, the connections for European banks also increased. In late 2007 and 2008, the 2007 subprime mortgage crisis in US finally led to the global financial crisis [50], since US sat in the center of the network. We can see that the entire financial network in 2008 (see Fig. [53] and Fig. 5) is much denser than the one before and after the crisis (see Fig. 5a and Fig. 5b). In the post-Lehman period, the US market calmed after the government injected a massive amount of capital into major US banks [50]. Thus, the number of connections for US banks decreased correspondingly. On the other hand, the European debt crisis occurred in Greece in late 2009 and further spread to Ireland and Portugal [53]. The delay of the rescue package for Greece caused the second peak of connections for European banks in May 2010. Later in 2011, the debt crisis further affected Spain and Italy [53], leading to the third peak for Europe from June to August in 2011 in Fig. 4b. Note that the number of connections for US banks was low when the debt crisis first happened in 2009. However, due to risk contagion in the financial network, the number of connections for US banks also reached another peak in 2011. On the other hand, since there is fewer number of connections between Asia-Pacific countries and US and Europe (see Fig. 5), the financial crisis did not impact Asia-Pacific countries as severely as US and Europe.

5.2 Graphical Models for Time Series (Frequency Domain)

5.2.1 Synthetic Data
To test the proposed method for inferring graphical models in the frequency domain, we consider simulated time series with length $N$ generated from a first order vector autoregressive process for $P$ variables. Specifically, we simulate data from the model

$$y^{(t)} = Ay^{(t-1)} + \epsilon^{(t)},$$

where $y^{(t)} \in \mathbb{R}^P$, $A \in \mathbb{R}^{P \times P}$, and $\epsilon^{(t)} \sim \mathcal{N}(0, I)$. The inverse spectral density of the process is then given by

$$K^{(\omega)} = I + A' A + \exp(-i\omega) A + \exp(i\omega) A'.$$

We consider time series with different dimensions, sample sizes, and graph density, and compare the results given by BADGE with those of GMS [37]. The graph density is characterized by the number of non-zero elements in $A$, which is denoted as $N_c$ in the sequel. For GMS, the kernel bandwidth $h$ is selected from $\{\exp(-4)N, \exp(-2)N, \ldots, \exp(4)N\}$ and $\lambda_1$ is chosen from $\{\exp(-4), \exp(-3), \ldots, 1\}$. Again, we select the tuning parameters by maximizing the $F_1$-score between the estimated and true graphs (i.e., the oracle results) as well as using CV. Before applying these methods, we first normalize the data $y^{(1:N)}$ to have unit variance. We then apply the normalized Fourier transform to obtain the Fourier coefficients $f^{(1:N)}_{1:P}$ such that the variance of $f^{(1:N)}_{1:P}$ does not increase with $N$. The results averaged over 5 trials are summarized in Table 7.

The results are similar to those in the time domain. Hence, we only provide a brief summary of the results here. BADGE yields the best performance in the terms of the $F_1$-score with the least amount of computational time in all cases. The oracle results are the second best. CV cannot always select the optimal tuning parameters, and so the CV results are worse than the oracle results. We can also observe that the increase of dimension $P$ or the graph density $N_c$ deteriorates the performance, whereas the increase of the sample size $N$ improves the performance, as expected. The computational time of BADGE and GMS is approximately a linear function of $N^2P^2$ and $N^3P^3$, respectively.

5.2.2 Scalp EEG of AD Patients
In this section, we consider the problem of inferring functional brain networks from scalp EEG recordings. Specifically, we analyze two data sets. The first one contains 22
TABLE 7: Graph recovery results from BADGE and GMS for synthetic time series with different graph density \((P = 20, N = 1000, N_c = 10, 20, 40)\). The standard deviations are shown in the brackets.

| Methods       | \(N_c = 10\)  | \(N_c = 20\)  | \(N_c = 40\)  |
|---------------|---------------|---------------|---------------|
|               | Precision     | Recall        | \(F_1\)-score | Time(s) | Precision     | Recall        | \(F_1\)-score | Time(s) | Precision     | Recall        | \(F_1\)-score | Time(s) |
| BADGE         |               |               |               |         |               |               |               |         |               |               |               |         |
|               | 0.93 (1.16e-1) | 0.97 (8.86e-2) | 2.26e2 (1.18e1) |         | 0.90 (3.14e-2) | 0.88 (4.23e-2) | 2.11e2 (1.10e1) |         | 0.93 (4.20e-2) | 0.72 (2.89e-2) | 2.04e2 (7.90e1) |     |
| GMS (oracle)  | 0.90 (6.63e-2) | 0.81 (2.64e-2) | 0.85 (7.77e-2) |         | 0.83 (9.41e-2) | 0.72 (8.72e-2) | 0.76 (7.37e-2) |         | 0.74 (7.61e-2) | 0.68 (2.10e-2) | 0.71 (4.12e-2) | 3.66e3 (3.32e1) |
| GMS (CV)      | 0.79 (1.62e-1) | 0.80 (3.60e-2) | 0.79 (8.55e-2) |         | 0.63 (1.22e-1) | 0.78 (1.26e-1) | 0.69 (8.18e-2) |         | 0.74 (7.61e-2) | 0.68 (2.10e-2) | 0.71 (4.12e-2) | 3.06e3 (7.26e2) |

Fig. 6: Boxplots of the number of edges given by BADGE and GMS for the first data set with MCI patients.

Fig. 7: Boxplots of the number of edges given by BADGE and GMS for the second data set with Mild AD patients.

patients with mild cognitive impairment (MCI, a.k.a. predementia) and 38 healthy control subjects [54]. The patients complained of the memory problem, and later on, they all developed mild AD (i.e., the first stage of AD). The ages of the two groups are 71.9 ± 10.2 and 71.7 ± 8.3, respectively. We provide some more details in the recording setup. Ag/AgCl electrodes (disks of diameter 8mm) were placed on 21 sites according to the 10-20 international system, with the reference electrode on the right ear-lobe. EEG was recorded with Biotop 6R12 (NEC San-ei, Tokyo, Japan) at a sampling rate of 200Hz.

The second data set consists of 17 patients with mild AD and 24 control subjects [55]. The ages of the two groups are 77.6 ± 10.0 and 69.4 ± 11.5, respectively. The patient group underwent full battery of cognitive tests (Mini Mental State Examination, Rey Auditory Verbal Learning Test, Benton Visual Retention Test, and memory recall tests). The EEG time series were recorded using 21 electrodes positioned according to Maudsley system, similar to the 10-20 international system, at a sampling frequency of 128 Hz. Although AD cannot be cured at present, existing symptoms-delaying medications are proven to be more effective at early stages of AD, such as MCI and mild AD [54]. On the other hand, scalp EEG recording systems are inexpensive and potentially mobile, thus making it a useful tool to screen a large population for the risk of AD. As a result, it is crucial to identify the patients from scalp EEG signals at early stages of AD.

We first perform the normalized Fourier transform on all channels of EEG signals to obtain \(f(\omega)\). We only consider \(f(\omega)\) in the frequency band \(4 – 30\)Hz in order to filter out the noise in the signal. \(K(\omega)\) is then inferred from \(f(\omega)\) by applying the proposed BADGE algorithm. We further split \(K(\omega)\) into three frequency ranges: \(4 – 8\)Hz, \(8 – 12\)Hz, and \(12 – 30\)Hz, as suggested by previous works on the same data sets [54], [55]. For each frequency band, we infer the corresponding graphical models by finding the common zero patterns of all \(K(\omega)\) for \(\omega\) in this band. We compare BADGE with GMS (CV) in this experiment to check which method can yield graphs that can better distinguish between the patients and the control subjects. The candidate set of the kernel bandwidth \(h\) and the penalty parameter \(\lambda_1\) for GMS (CV) is respectively \(\{\exp(-3)N, \exp(-2.5)N, \cdots, \exp(-1)N\}\) and \(\{\exp(-5), \exp(-4.5), \cdots, \exp(-0.5)\}\).

First, we count the number of edges in the graphical models, which can be regarded as a measure of synchrony between different EEG channels. We observe that graphical models in 4 – 8Hz can best distinguish between patients and controls for both data sets and both methods. We depict in Fig. 7 the boxplots of the number of edges in the graphical models. Clearly, the graphical models for patients are more sparse than that for healthy people, and this phenomenon becomes more pronounced for Mild AD patients. Such findings are consistent with the loss of synchrony within the EEG signals for AD patients as reported in the literature [54], [55]. We further conduct the Mann-Whitney test on the number of edges in the two sets of graphical models, respectively for the patients and the controls. The resulting p-value given by BADGE for the two data sets is respectively \(7.55 \times 10^{-3}\) and \(1.49 \times 10^{-3}\), which are statistically significant. As a comparison, the p-value resulting from GMS is \(3.99 \times 10^{-1}\) for the MCI data and \(9.26 \times 10^{-2}\) for the Mild AD data. Next, we further train a random forest classifier based on the estimated brain networks to differentiate between the patients and the controls. The input to the classifier is the estimated brain networks to differentiate between the patients and the controls. The classifier. The accuracy yielded by BADGE for the two data sets is respectively 65.85% and 70%. On the other hand, the computational time averaged over all subjects is \(3.50 \times 10^2\) seconds for BADGE and \(1.40 \times 10^4\) seconds for GMS. Apparently, BADGE can more accurately describe the perturbations in the EEG synchrony for MCI and mild AD patients, while being more efficient.
We propose a novel Bayesian model BASED to solve the problem of estimating dynamic graphical models. In contrast to the existing methods that a have high time complexity of $O(NP^3)$ and require extensive parameter tuning, the time complexity of BASED is only $O(NP^2)$ and it is free of tuning. Specifically, we develop a novel gradient based variational inference algorithm to learn the Bayesian model. To deal with the problem of local maxima, we resort to simulated annealing and propose to use bootstrap to generate the annealing noise. In comparison with the existing methods, BASED can better recover the true graphs with the least amount of computational time. We then apply BASED to analyze the stock return data of 78 banks worldwide, and observe that the resulting financial network becomes denser during the 2008 global financial crisis and the subsequent European debt crisis. On the other hand, we find the resemblance between inferring time-varying inverse covariance matrices and frequency-varying inverse spectral density matrices, and extend BASED to learn graphical models among a multitude of stationary time series in frequency domain. Numerical results from EEG data of MCI and mild AD patients show that the proposed model may help to diagnose AD from scalp EEG at an early stage.

As BASED can only tackle Gaussian distributed data at present, we intend to extend it to non-Gaussian data by means of Gaussian copulas in future work. Additionally, it is interesting to extend BASED to deal with piecewise constant graphical models. In this case, the data can be partitioned into a certain number of time segments. The graph within each segment remains unchanged, but the graphs for every two consecutive segments can be completely different. Such piece-wise constant graphical models also find wide applications in practice.

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