Nonlinear Models for Topology Inference and Learning over Graphs

Yanning Shen

Background. The study of networks and network phenomena has recently emerged as a major catalyst for collectively understanding the behavior of complex systems . Such systems are ubiquitous, and commonly arise in both natural and man-made settings. For example, online interactions over the web are commonly facilitated through social networks such as Facebook and Twitter, while sophisticated brain functions are the result of vast interactions within complex neuronal networks. Other networks naturally emerge in settings as diverse as financial markets, genomics and proteomics, power grids, and transportation systems, to name just a few.

Inference of directed network topologies is a well-studied problem with applications in diverse settings. For example, discovery of causal links between regions of interest in the brain is tantamount to identification of an implicit connectivity network. Studies pertaining to regulatory and inhibitory interactions among genes depend upon identification of unknown links within gene regulatory networks. Since network structures are often unobservable, in order to facilitate network analytics, one generally resorts to approaches capitalizing on measurable nodal processes to infer the unknown topology. Most contemporary graph topology inference approaches overwhelmingly rely on linear models due to their inherent simplicity and tractability, and presume that the nodal processes are directly observable.

Dimensionality reduction methods have been extensively studied by the signal processing and machine learning communities. Various algorithms have been proposed for dimensionality reduction, e.g., Principal component analysis, multi-dimensional scaling and local linear embedding. These approaches capture and preserve linear relationships between data. However, for data residing on highly nonlinear manifolds using only linear relations may not be enough. Generalizing PCA, Kernel PCA can capture nonlinear relationships between data, for a preselected kernel function. While all the aforementioned approaches have been successful in reducing the dimensionality of various types of data, they do not consider additional information during the dimensionality reduction process. This prior information may be task specific, e.g., provided by some “expert” or the physics of the problem, or it could be inferred from alternate views of the data, and can provide additional insights for the desired properties of the low-dimensional representations. In fMRI signals for instance, in addition to time series collected at different brain regions, one may also have access to the connectivity patterns among these regions. This additional information can be encoded in a graph, and incorporated into the dimensionality reduction process through graph-aware regularization.

Research Objectives. The objective of my researcch is to effect significant technical advances for nonlinear learning inference for big data from large-scale networks. On top of the theoretical foundation, my research centered around the following thrusts:

(T1) Nonlinear dimensionality reduction for big categorical data;
(T2) Nonlinear modeling and inference of dynamic networks; and,
(T3) Classification and clustering for big data over dynamic networks.

Research Highlights. Thrusts (T1)-(T3) are tightly intertwined with regard to the challenges and opportunities. A class of novel learning and inference methods with performance guarantees will be developed.

(T1) Nonlinear dimensionality reduction for big categorical data. Extracting latent low-dimensional structure from high-dimensional data is of paramount importance in timely inference tasks encountered with big data. The sheer volume of data and the fact that observations are acquired sequentially over time, motivate updating previously obtained analytics rather than recomputing new ones from scratch each time a new datum becomes available. In this context, we advocated a new framework to efficiently track the latent low-dimensional structures from incomplete and corrupt datasets typically encountered in practice. The proposed framework encompasses several fundamental learning tasks including imputation, clustering, and classification. Numerical tests for real MovieLens dataset and MINST dataset confirm the power of proposed methods [1]–[3].

(T2) Nonlinear modeling and inference of dynamic networks. Structural equation model (SEM) is a widely used method for directed network topology inference. However, SEMs are faced with three major limitations: i) SEMs assume linear dependencies among nodes; ii) SEMs require full knowledge of exogenous inputs in order to guarantee network identification, which may not be readily available in some practical settings; iii) SEMs assume that the network structure does not vary over time. Faced with these challenges, we advocate two novel topology inference approaches that could account for the nonlinear dependencies among nodes, and can identify and track the dynamic directed network topology even without such information.

T2.1) Kernel-based models for network topology inference. We generalize the SEMs and structural vector autoregressive models (SVARMs) to model (possible) nonlinear interactions among nodes, which provides a powerful tool for modeling and identifying real-world networks. The advocated approach leverages kernels as a powerful encompassing framework for nonlinear modeling, and an efficient estimator with affordable tradeoffs is put forth. Pursuit of the novel kernel-based approach yields a convex regularized estimator that promotes edge sparsity, a property exhibited by most real-world networks. Experiments on a real gene expression dataset, as well as brain data sets unveil interesting new edges that were not revealed by linear SEMs, which could shed more light on regulatory behavior of human genes, an brain dynamics at seizure onset [4]–[8].

T2.1) Tensor-based network topology inference and tracking. Conventional SEMs assume full knowledge of exogenous inputs, which may not be readily available in some practical settings. Hence, we advocate a novel SEM-based topology inference approach that entails factorization of a three-way tensor, constructed from the observed nodal data, using the well known parallel factor (PARAFAC) decomposition. Capitalizing on the uniqueness properties inherent to high-order tensor factorizations, it is shown that topology identification is possible under reasonably mild conditions. In addition, to facilitate real-time operation and inference of time-varying networks, an adaptive tensor decomposition scheme which tracks the topology-revealing tensor factors is developed. Extensive tests on simulated and real stock quote data demonstrate the merits of the novel tensor-based approach [9]–[11].

(T3) Classification and clustering for big data over dynamic networks. With the insights gained from the T1 and T2, we will further broaden the scope of our theoretical and algorithmic framework by considering online classification and clustering tasks over time-varying networks. In this context, we aims to combine the processing of streaming datasets with the analysis of dynamic networks. Our preliminary results has revealed the benefit of taking into consideration the underlying network topologies, for dimensionality reduction and clustering of data observed on graphs. Future research will focus on making use of network dynamics to enhance the performance of machine learning tasks on network processes [12].

Professional Goals. Fascinated by the theory that is inspired by and can propel real-life applications, I am determined to pursue an academic career, so that I can devote myself to both research and teaching on machine learning-, optimization-, and network science-related topics.

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