PRODUCT GRAPH LEARNING FROM MULTI-ATTRIBUTE GRAPH SIGNALS WITH INTER-LAYER COUPLING

Chenyue Zhang, Yiran He, Hoi-To Wai

Department of SEEM, The Chinese University of Hong Kong, Shatin, Hong Kong SAR of China

ABSTRACT

This paper considers learning a product graph from multi-attribute graph signals. Our work is motivated by the widespread presence of multilayer networks that feature interactions within and across graph layers. Focusing on a product graph setting with homogeneous layers, we propose a bivariate polynomial graph filter model. We then consider the topology inference problems thru adapting existing spectral methods. We propose two solutions for the required spectral estimation step: a simplified solution via unfolding the multi-attribute data into matrices, and an exact solution via nearest Kronecker product decomposition (NKD). Interestingly, we show that strong inter-layer coupling can degrade the performance of the unfolding solution while the NKD solution is robust to inter-layer coupling effects. Numerical experiments show efficacy of our methods.

Index Terms—graph signal processing, product graph learning, multi-attribute graph signals, network inference

1. INTRODUCTION

In recent years, there has been a growing trend in data science to develop tools for learning and making inference from signals or data observed on networks. The latter is also known as graph signals which form the subject of investigation in the emerging field of graph signal processing (GSP). Through modeling real-world networks as graphs and encoding the network data as filtered graph signals, an emerging trend is to develop tools for learning the latent graph topology from these network data; see [1, 2] and the references therein. These tools have widespread applications in the studies of social, financial, and biology networks [3].

Previous works on topology learning with GSP models have focused on mono-layer networks that consist of a single network ‘layer’, and the tools developed are applicable to single-way data. However, this may not yield a faithful model for many complex systems since networks and graphs do not live in isolation. Instead, many networked systems are better described by multi-layer networks featuring coupling interactions within and across network layers. Examples include: opinion dynamics on correlated topics [4], multi-dimensional diffusion [5], protein-protein interactions [6], animal networks [7], and relations in image pixels [8], etc. Observations made on these complex systems are usually generated from two or more coupled networks, and they give rise to multi-attribute observations on nodes, i.e., multi-way graph signals. Naturally, the graph structure embedded in these network data shall be treated using a multilayer graph model as they can not be captured by simple individual networks or flattened networks without structure.

This paper is motivated by the above to develop an inter-layer coupling aware GSP framework for learning an accurate graph structure from multi-way data. As a special case, we focus on modeling a product graph [9] with homogeneous graph layers. We also develop the corresponding inference algorithms. In light of this, we contribute to both modeling and algorithm aspects in GSP with:

• We adopt a general product graph filter for modeling multi-attribute (a.k.a. multi-way) graph signals. The model uses a bivariate polynomial graph filter to describe interactions over the physical and coupling graphs. We show that it encompasses a number of common dynamics on multilayer networks.

• We develop inference algorithms for topology reconstruction and blind centrality detection in learning the product graph model. Our development relies on an observation that the eigenvectors of graph signals’ covariance can be written as Kronecker product of respective eigenvectors of coupling and physical graphs. Leveraging this observation, we suggest spectral methods by proposing two solutions based on the layer/node-wise unfolding and nearest Kronecker product decomposition (NKD). We compare the two solutions by analyzing the effects of inter-layer coupling and show that NKD yields an exact solution under milder assumptions.

Lastly, we present numerical experiments on synthetic and real data to corroborate with our analysis. The experiments highlight the effects of inter-layer coupling strengths on topology inference.

Related Works. The closest works to ours are [10, 11] which studied product graph learning from multi-way graph signals focusing on a smoothness condition defined with the Cartesian product graph. Such conditions restricted the application of these techniques to a special form of coupling mechanism in the multi-way data. Our general product graph filter model relaxes these restrictions. Besides graph learning, [12, 13] proposed a time-vertex GSP framework.
modeling the temporal evolution of graph signals. These models can be regarded as a special case of our model where the coupling graph is fixed as a path graph. Moreover, [14–16] studied models for the generic multi-way GSP with possibly heterogeneous graph layers. While the graph model is considerably more generic, these works focused on simple graph filters, which do not account for a number of inter-layer coupling mechanisms. Lastly, we note that [17] studied an alternative multigraph GSP model without multi-way data. To our best knowledge, the current paper introduces the first product graph model with general inter-layer coupling accompanied by a suite of topology inference algorithms.

2. MULTI-ATTRIBUTE GRAPH SIGNALS

This section introduces a generative model for multi-attribute graph signals inspired by network dynamic processes on multiplex graphs with homogeneous graph layers. In particular, our development involves a product graph model [9] and a general multi-dimensional graph signal/filter model based on the former.

Product Graph Model. The center of our study is a product graph $G = (G^1, G^2)$ formed by two undirected graphs, denoted respectively as $G^1 = (V^1, E^1, A^1)$, $G^2 = (V^2, E^2, A^2)$ with $|V^1| = M$, $|V^2| = N$. Note that $A^1, A^2$ are weighted adjacency matrices associated with the respective graphs of the edge sets $E^1 \subseteq V^1 \times V^1$, $E^2 \subseteq V^2 \times V^2$. We adopt the interpretation of $G$ as a multi-layer graph such that each node in $V^2$ corresponds to a physical entity, e.g., individual on a social network, etc., and each node in $V^1$ corresponds to a layer/attribute of these physical entities. In this way, $G^2$ will be referred as the physical graph, while $G^1$ is the coupling graph between layers/attributes; see Fig. 1 (left).

Compared to conventional single graph layer models, an important feature of $G$ is that it explicitly models inter-layer coupling where all $N$ nodes co-exist in the $M$ interacting layers. It is then instrumental to define the interaction graph $G^{i,j}$ with the node set $V^{i,j} = V^i \times V^j$. Notice that $|V^{i,j}| = NM$ and the edge set of $G^{i,j}$ can then be encoded into the adjacency matrix:

$$A^{i,j} = \gamma_1 I \otimes A^j + \gamma_2 A^i \otimes I + \gamma_3 A^i \otimes A^j,$$

where $\gamma = (\gamma_1, \gamma_2, \gamma_3) \geq 0$ satisfying $\sum_{i=1}^{3} \gamma_i = 1$ are the coupling parameters of the generalized product graph, and $\otimes$ denotes Kronecker product. Different combinations of $\gamma$ can lead to different interaction patterns among the nodes in $V$ [18]. For example, with $\gamma = (\frac{1}{3}, \frac{1}{3}, 0)$, $A^i$ describes the Cartesian product graph and the matrix is also known as the supra-adjacency matrix; with $\gamma = (0, 0, 1)$, $A^i$ describes the Kronecker product graph; with $\gamma = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$, $A^i$ describes the strong product graph; see Fig. 1 (right).

Multi-attribute Graph Signals. We concentrate on modeling multi-attribute graph signals living on $G^j$ where the graph filter is induced by the graph factors $A^i, A^j$ and takes an excitation signal as its input. For example, the filter can be a function of $A^1$. We consider a general formulation of multi-layer graph filter [19]:

$$H(A^i, A^j) = \sum_{t=0}^{T} \sum_{s=0}^{T} h_{ij}(\lambda^1)^s \otimes (\lambda^2)^t,$$

where $h_{ij} \in \mathbb{R}$ are the filter coefficients and $T_i, T_c \in \mathbb{Z} + \{\infty\}$ are the orders of the bivariate filter polynomial. The multi-attribute (a.k.a. multi-way) graph signals are then modeled as:

$$y^{(s)} = H(A^i, A^j)x^{(s)} + w^{(s)},$$

where $s \in \mathbb{N}$ denotes the sample index, $x^{(s)}, w^{(s)} \in \mathbb{R}^{MN}$ are the excitation signals and observation noise, respectively. Note that $y = (y_1, \ldots, y_M) \in \mathbb{R}^{NM}$ whose $m$th block, $y_m$, corresponds to observations on the nodes $\{(m, i) : i \in V^j\}$ and the graph signals have been organized in a layer-by-layer fashion.

It is obvious that for all coupling parameters $\gamma$, any polynomial of $A^2$ can be written as (2). Notably, it is common [5] to use the supra-adjacency matrix, $A^2$ with $\gamma = (\frac{1}{3}, \frac{1}{3}, 0)$, to describe interactions in a multi-layer graph, and subsequently consider the polynomial of $A^1$ as the graph filter. However, this is not sufficient to describe certain interactions on $G$, e.g., a polynomial of $A^1 \otimes A^2$ cannot be expressed as a polynomial of $A^2$ with $\gamma = (\frac{1}{3}, \frac{1}{3}, 0)$.

We conclude this section by showcasing two example dynamic processes to illustrate the generality of our graph filter model:

Example 1. Consider the Friedkin-Johnsen multi-dimensional opinion dynamics [4, 20]. At time $t \geq 0$ and the $th$ discussion, the multi-dimensional opinions for agents in $V^2$ evolve as:

$$x(t + 1) = (A^C \otimes A^3)x(t) + x^{(s)}$$

such that the $th$ block of $x(t)$ represents the opinions of $N$ agents on the $th$ topic. The weighted adjacency matrices $A^C, A^3$ represent the logical dependencies between the $M$ topics, and the mutual trusts between the $N$ agents, respectively. They are properly scaled such that the vector $(I_{NM} - A^C \otimes A^3) > 0$ represents the self trusts of each agent on the topic. Moreover, $x^{(s)}$ is the initial belief of the agents. Under the above premises, we have:

$$y^{(s)} = \lim_{t \to \infty} x(t) = (I_{NM} - A^C \otimes A^3)^{-1}x^{(s)},$$

where we note that $(I_{NM} - A^C \otimes A^3)^{-1}$ is a special case of (2) since the latter is a function of $A^2$ with $\gamma = (0, 0, 1)$.

Example 2. The diffusion process in [5] describes dynamics such as social contact, epidemic, etc., on a multi-layer graph. In particular, with the excitation $x^{(s)}$, the states of nodes at time $t$ evolve as:

$$\frac{dx(t)}{dt} = -Ax(t) + (A^C \otimes I_N + I_M \otimes A^3)x(t) + x^{(s)}.$$

With properly scaled $A^C, A^3$, the above has a unique equilibrium:

$$y^{(s)} = (I_{NM} - A^C \otimes I_N - I_M \otimes A^3)^{-1}x^{(s)},$$

where we note that $(I_{NM} - A^C \otimes I_N - I_M \otimes A^3)^{-1}$ is a special case of (2) since the latter is a function of $A^2$ with $\gamma = (\frac{1}{3}, \frac{1}{3}, 0)$.

Graph filter models in the form of (2) may also be found in other data scenarios such as the graph causal processes [21]. These models may be based on other types of interaction graphs $G^2$ such as strong product, but they can nevertheless be covered by (2).

3. PRODUCT GRAPH LEARNING

We aim to infer the product graph model through observing the multi-attribute graph signals in (3). We concentrate on learning the coupling and physical graphs $A^i, A^j$. Our idea is to apply spectral methods with reliable performance regardless of the graph filter (2).

To fix ideas, we denote the eigenvalue decompositions (EVDs) for the adjacency matrices by:

$$A^C = V^C\Lambda^C(V^C)^\top, A^3 = V^3\Lambda^3(V^3)^\top,$$

where $V^C, V^3$ are orthogonal and $\Lambda^C, \Lambda^3$ are diagonal matrices. Without loss of generality, the eigenvalues are sorted in decreasing order. For example, the $th$ column vector of $V^C$, denoted $v_i^C$, corresponds to the $th$ largest eigenvalue $\lambda_i^C$ in $\Lambda^C$. We assume that:

**H1.** For any $i = 1, \ldots, N$, $j = 1, \ldots, M$, the magnitudes of frequency response $|h(\lambda_i^C, \lambda_j^3)|$ have distinct values, where we defined $h(\lambda_i^C, \lambda_j^3) := \sum_{t=0}^{T} \sum_{s=0}^{T} h_{ij}(\lambda_i^C)^s (\lambda_j^3)^t$ according to (2).

1. Note that the issue boils down to the non-existence of a polynomial $\tilde{h}(\cdot)$ such that $h(ab) = \tilde{h}(a + b)$ for all $h(\cdot), a, b$.  

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The above assumption holds for cases when the graph filter is a function of $A^k$ where $A^2, A^3$ have distinct eigenvalues. Consequently, the EVD of the graph filter (2) is derived as (cf. [14]):

$$H(A^2, A^3) = (V^2 \otimes V^3)H(A^2, A^3)(V^2 \otimes V^3)^\top,$$

such that $H(A^2, A^3)$ is a diagonal matrix. Under standard white noise conditions for $x^{(s)}, w^{(s)}$, i.e., both are zero-mean and satisfy $E[x^{(s)}(x^{(s)})^\top] = I$, $E[w^{(s)}(w^{(s)})^\top] = \sigma^2 I$, the graph signal covariance $C_y = E[y^{(s)}(y^{(s)})^\top]$ can be derived as:

$$C_y = (V^2 \otimes V^3)H(A^2, A^3)^2(V^2 \otimes V^3)^\top + \sigma^2 I.$$

Eq. (10) makes an important observation about the covariance matrix $C_y$. When $\sigma = 0$, the eigenvectors of $C_y$ are given by the columns of $V^2 \otimes V^3$. We will demonstrate in §3.1 that $V^2, V^3$ can be retrieved by decomposing the eigenvectors of $C_y$.

For suppose for now that the matrices $V_i^2, V_i^3$ with possibly permuted columns of $V^2, V^3$ are given, we can recover the graph topology and/or detect central nodes in $G_i, G_j$ through adapting the spectral methods developed in several existing works. In particular:

**P1. Topology Reconstruction.** It is shown in [22] that graph topologies can be reconstructed from the spectral template of graph shift operator (GSO). For example, the following problem recovers $A^2$:

$$\min_{A^2, A^3} \|\text{vec}(A^2)\|_1 + \frac{\rho}{2} \|A^2 - \widetilde{V}^2 \text{Diag}(A^3)(\widetilde{V}^3)^\top\|_F^2$$

s.t. $[\text{diag}(A^3)] \leq 1, A^2 \geq 1,$

where $\rho > 0, \epsilon > 0$ are regularization parameters, and $\text{vec}()$ is the vectorization operator. Similar formulation can be applied for $A^3$.

**P2. Centrality Estimation.** It is observed [23–25] that eigenvector centrality can be inferred from graph signals under mild conditions. Their idea can be adapted for product graphs by noting $v_i^2 \otimes v_j^3$ is the only positive eigenvector in $C_y$. Under the premise that the latter can be decomposed (cf. §3.1), we propose:

$$\tilde{v}^2 = \tilde{v}_i^2 \otimes \tilde{v}_j^3$$

and $i^* = \arg\min_{i} \|P_i(\tilde{v}_i^2)\| = \min \{\|x - (x)^+\|, \|x + (x)^-\|\}, x = \max(0, x),$ and $P_i(x) = 0$ if $x$ is all-positive or all-negative. Notice $\tilde{v}_i$ denotes the $i$th eigenvector of $C_y$.

3.1. Recovering $V^2, V^3$ from $C_y$

Our remaining task is to recover the eigenvectors in $V^2, V^3$ individually from observed data $y^{(s)}$. For simplicity, we consider the same conditions leading to (10) with $\sigma = 0$ and propose two solutions.

**Exact Solution by NKD.** Observe that the diagonal entries in $|H(A^2, A^3)|^2$ of (10) may not be sorted in descending order. Applying EVD on $C_y$ thus produces the eigenvector matrix:

$$\tilde{V} = (V^2 \otimes V^3)\Pi = \cdots \vec{v}_{i=1}^{(s)}(i) \otimes \vec{v}_{j=1}^{(s)}(i) \cdots,$$

where $\Pi$ is a permutation matrix that orders the columns of $V^2 \otimes V^3$ according to the magnitude of frequency response. For any $i = 1, \ldots, N M_j$, $\pi_i^2(i), \pi_i^3(i)$ are indices of eigenvectors for $V_i^2, V_i^3$ of the $i$th highest frequency response in $|H(A^2, A^3)|^2$, i.e., $\tilde{v}_i$.

The structure illustrated in (13) indicates that every column vectors of $\tilde{V}$ can be written as a Kronecker product. To this end, we observe the classical result adapted from [26, Theorem 2.1]:

**Proposition 1.** Consider $M \in \mathbb{R}^M \times \mathbb{R}^P$, $A \in \mathbb{R}^M \times \mathbb{R}^P$, $B \in \mathbb{R}^P \times \mathbb{R}^Q$. If $M = A \otimes B$, then $R(M) = \text{vec}(A)\text{vec}(B)^\top$, where

$$R(M) = \begin{bmatrix} M_1 \\ \vdots \\ M_P \end{bmatrix}, \quad M_i = \begin{bmatrix} \text{vec}(M_{i,1})^\top \\ \vdots \\ \text{vec}(M_{i,P})^\top \end{bmatrix}, \quad i = 1, \ldots, P.$$
with the spectrum as \(-1, 1, 2\) for \(G^c\), then \(C^\text{node}\) has repeated eigenvalues if \(\{0, -1.27\}\) are in the spectrum of \(G^c\).

On the other hand, a sufficient condition for \(C^\text{node}\) to admit distinct eigenvalues hinges on the separable filter property [13]. Concretely, we need \(h(x^c, x^c) = h(x^e) h(x^e)\) for all \(x^c, x^c\). For example, when \(h(x^c, x^c) = e^\frac{3}{2}(x^c + x^c)^2\), the interaction graph is free of the direct Kronecker product. In this case, the eigenvectors of \(C^\text{layer}\), \(C^\text{node}\) serve as good surrogates for \(V^c, V^e\), respectively.

4. NUMERICAL EXPERIMENTS

Synthetic Data. We consider graph filters that are based on \(A^i\) in (1) with the parameters \(\gamma = (\gamma_1, 2\gamma_1, 1 - 3\gamma_1)\). As \(\gamma_1 \downarrow 0\), the interaction graph has strong inter-layer coupling of Kronecker product form. We fix \(G^c\) to be the tree graph in Fig. 1 with \(M = 3\) where \(A^c\) is the unweighted adjacency matrix; while \(A^e\) will be the unweighted adjacency matrix for \(G^c\) to be determined below.

Example 1: Topology Reconstruction. This example examines the performance of product graph topology reconstruction (P1). We generate \(G^c\) as an Erdos-Renyi graph with connection probability of \(p = 0.4\). We benchmark the proposed ‘NKD’ based Algorithm 1 against ‘Unfold’ which estimates \(V^c, V^e\) from the layer-wise/node-wise unfolded graph signals; ‘PGL’ refers to the product graph learning method based on smoothness of layer-wise/node-wise unfolded graph signals in [10]; ‘Flatten’ refers to applying [22] directly to \(C^c\). For the SpectrExp problem (11) in Algorithm 1, ‘Unfold’, and ‘Flatten’, we take \(p = 40\), \(\epsilon = 10^{-6}\) and solve (11) by cvx

We consider synthetic data generated from (3) with the graph filter given by \(H(A^e, A^c) = e^{cA^e}\), where \(A^i\) is parameterized by \(\gamma_1 \in [0, \frac{1}{3}]\) as described. We also set \(\tau = 1/\max x_i, d_i, d_i = \sum_{j=1}^{N} A^c_{i,j}\). Excitation and noise signals satisfy \(x^{(s)} \sim N(0, I)\), \(w^{(s)} \sim N(0, 0.01I)\). Fig. 2 compares the performance of topology reconstruction in terms of the \(F_1\) score against the sample size \(S\) and graph size \(N\). We assume known \(\gamma_1\) and evaluate the \(F_1\) scores by comparing the ground truth to \(A^i\) reconstructed by (1) using the estimated \(A^c, A^c\). We observe that ‘NKD’ recovers the graph topology for a wide range of sample sizes and graph sizes, regardless of the coupling parameter \(\gamma_1\). Meanwhile, ‘Unfold’ and ‘PGL’ are sensitive to \(\gamma_1\) – they perform better than Algorithm 1 when \(\gamma_1 = \frac{1}{3}\), but their performances degrade noticeably when \(\gamma_1 = 0.01\). In all cases, ‘Flatten’ fails to estimate the graph topology.

Example 2: Central Nodes Detection. The next example examines the performance of central node detection (P2). We focus on detecting the central nodes of \(G^c\) using (12), where \(G^c\) is generated as a core-periphery graph [28]. The node set \(V^c = \{1, \ldots, N\}\) is partitioned into \(V^c\) = \{1, \ldots, 10\}, \(V^c_{\text{in}} = V^c \setminus V^c_{\text{out}}\). For every pair

Fig. 2. Topology Reconstruction. \(F_1\) score against (Left) sample size \(S\) with \(N = 10\); (Right) graph size \(N\) with \(S = 1000\).

Fig. 3. Central Nodes Detection. Error rate against (Left) sample size \(S\) with \(N = 80\); (Right) graph size \(N\) with \(S = 5MN\).

Fig. 4. US Senate Rollcalls Data. (Left) Estimated Senate topology \(G^c\) color coded by the two communities found by spectral clustering on \(A^e\). (Right) Estimated coupling graph of the topics of rollcalls. (i, j) \(\in V^c \times V^c\), edges are assigned randomly with probability \(1\) if \(i, j \in V^c_{\text{in}}\); with probability \(0.2\) if \(i \in V^c_{\text{in}}, j \in V^c_{\text{out}}\); with probability \(0.05\) if \(i, j \in V^c_{\text{out}}\). Our goal is to detect the 10 nodes in \(V^c_{\text{in}}\) based on the observed multi-attribute graph signals. We focus on comparing the proposed ‘NKD’ based Algorithm 1 with ‘Unfold’ which estimates \(V^c, V^e\) from the node-wise unfolded graph signals.

We consider synthetic data modeled after (3) with two graph filters: (a) \(H^{\text{inv}}(A^e, A^c) = (I - \tau A^i)^{-1}\), (b) \(H^{\text{exp}}(A^e, A^c) = e^{\tau_2 A^c}\) with \(\tau_1 = 1/\max x_i, \tau_2 = 10\). We set \(x^{(s)} \sim N(0, I)\), \(w^{(s)} \sim N(0, 0.01I)\). Fig. 3 compares the error rate in identifying the central nodes \(V^c_{\text{in}}\) as top-10 central nodes (12). As seen, ‘NKD’ delivers lower error rate with smaller number of samples for the strong coupling scenario \(\gamma_1 = 0.01\). The result corroborates with Proposition 2 as the covariance with node/layer-wise unfolded signals have close (or repeated) eigenvalues, significantly increasing the sample complexity in eigenvector estimation.

Real Data: US Senate Rollcalls. We apply Algorithm 1 to reconstruct the topology (P1) from the 113th-116th US Senate rollcalls [available: https://voteview.com/data]. We first apply NMF [29] to perform topic modeling on rollcalls’ descriptions to get \(\gamma_1 \in [0, \frac{1}{3}]\) as described. We also set \(\tau = 1/\max x_i, d_i, d_i = \sum_{j=1}^{N} A^c_{i,j}\). Excitation and noise signals satisfy \(x^{(s)} \sim N(0, I)\), \(w^{(s)} \sim N(0, 0.01I)\). Fig. 2 compares the performance of topology reconstruction in terms of the \(F_1\) score against the sample size \(S\) and graph size \(N\). We assume known \(\gamma_1\) and evaluate the \(F_1\) scores by comparing the ground truth to \(A^i\) reconstructed by (1) using the estimated \(A^c, A^c\). We observe that ‘NKD’ recovers the graph topology for a wide range of sample sizes and graph sizes, regardless of the coupling parameter \(\gamma_1\). Meanwhile, ‘Unfold’ and ‘PGL’ are sensitive to \(\gamma_1\) – they perform better than Algorithm 1 when \(\gamma_1 = \frac{1}{3}\), but their performances degrade noticeably when \(\gamma_1 = 0.01\). In all cases, ‘Flatten’ fails to estimate the graph topology.

Conclusions. This paper considered the problem of learning from multi-attribute graph signals by proposing a general product graph filter model and developing its inference algorithms. Future works include analyzing the sampling complexity of Algorithm 1 and studying the effects of layer-wise/node-wise unfolding of graph signals on sampling complexity or identifiability.
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