Learning Multiplex Graph with Inter-layer Coupling

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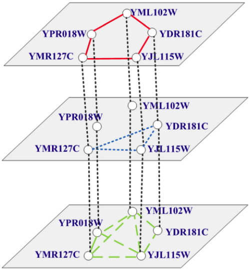
Motivation

[Source: NETWORK MANAGEMENT]

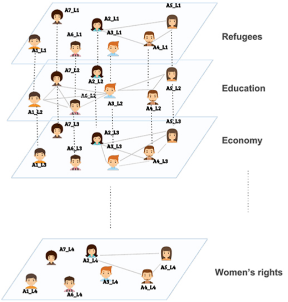
[Source: Sapien Labs]

- Graphs are natural ways to represent *social*, *biology*, *transportation*, *power* networks, and others.
- **Graph Signal Processing (GSP)** — extends *signal processing* to graph data and enables 'interpretable' inference of data.

Motivation



Multilayer protein networks [Source: [Zhao et al., 2016]]



Multilayer social network [Source: [Hanteer and Rossi, 2019]]

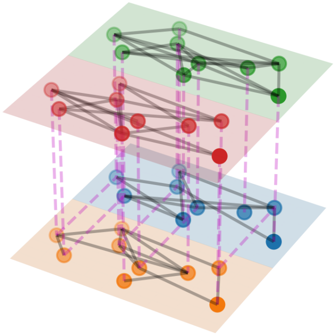
- Prior works consider **closed systems** with single layer of networks, but *networks do not live in isolation [Kivelä et al., 2014]*.
- A general model is **multiplex graph** – a node is present on ≥ 2 **layers of graphs**, each with different topology – e.g., opinion dynamics on ≥ 2 topics, weather measurement stations, brain signals, etc.
- Note: We focus on *multi-attribute graph signals*.

Goals and Contributions

To extend GSP methods to multiplex graphs: signal analysis, topology learning, etc. — we focus on **graph topology learning**.

Contributions:

- **Multiplex Graph Filter** for *multi-attribute* graph signals with nonlinear intra-/inter-layer couplings.
- Interpret TV/smoothness criterion as a **matched filter** criterion – extend to handle inter-layer couplings.
- **Alternating Optimization Procedure** for efficient multiplex graph learning.

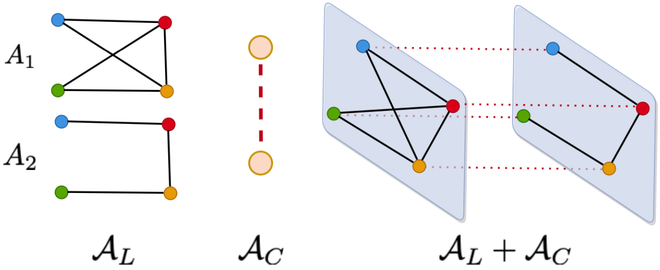


Related Works

- **Models for multi-way graph signals** (on multiplex graphs)
  - [Zhang et al., 2023b] – **tensor GSP model**, but it lacks inter-layer coupling dynamics.
  - [Natali et al., 2020, Grassi et al., 2017] considered **product graph signal models** which is a special case of multiplex graphs.
- **Multiplex graph topology learning**
  - [Kalaitzis et al., 2013] [Kadambari and Chepuri, 2021], [Einizade and Sardouie, 2023] learn **product graphs** using graph signals via smoothness, spectral template, etc.
  - Our prior work [Zhang et al., 2023a] consider a fine-grained model for product graph learning.
- **Graph Machine Learning**
  - [Cen et al., 2019, Zhang et al., 2019] seek embeddings for graph representation on heterogeneous graph with HetGNN.
  - [Butler et al., 2023] proposed a model for convolutional learning on multigraph.
- and many others ...

Multiplex Graph Model

- $G = \langle V, \mathcal{E}, \mathcal{G}^C \rangle$ with nodes V, layer edges $\mathcal{E}$, coupling graph $\mathcal{G}^C$.
- There are $|V| = N$ nodes and L layers.
- **Layer Graphs:** For $\ell = 1, ..., L$, $\mathcal{G}_\ell$ with supernodes V_ℓ, edges E_ℓ, representing intra-layer links with adjacency $\boldsymbol{A}_\ell$.
- **Coupling Graph:** $\mathcal{G}^C$ for inter-layer links with adjacency $\boldsymbol{C}$.
- **Adjacency Matrix:** Layer-wise $\boldsymbol{\mathcal{A}}_L = \text{blkdiag}(\boldsymbol{A}_1, \ldots, \boldsymbol{A}_L)$ and coupling $\boldsymbol{\mathcal{A}}_C = C \otimes I_N$. e.g: supra-adjacency: $\boldsymbol{A} = \boldsymbol{\mathcal{A}}_L + \boldsymbol{\mathcal{A}}_C$.



Multi-attribute Graph Filter and Signals.

- We model **multi-attribute** graph signal as

$$\boldsymbol{y}^{(m)} = \mathcal{H}(\boldsymbol{\mathcal{A}}_L, \boldsymbol{\mathcal{A}}_C)\boldsymbol{x}^{(m)} + \boldsymbol{w}^{(m)} \in \mathbb{R}^{NL}, \tag{1}$$

- $\mathcal{H}(\boldsymbol{\mathcal{A}}_L, \boldsymbol{\mathcal{A}}_C)$ shall model the multiplex with distinct intra-layer and coupling dynamics $\rightarrow$ a **general** multi-attribute graph filter model[1]:

$$\mathcal{H}(\boldsymbol{\mathcal{A}}_L, \boldsymbol{\mathcal{A}}_C) = \sum_{t=0}^{T-1} \sum_{j=0}^{2^t-1} h_{t,j} \prod_{i=1}^{t} \boldsymbol{\mathcal{A}}_L^{b_{t,j}^{(i)}} \boldsymbol{\mathcal{A}}_C^{1-b_{t,j}^{(i)}}, \quad b_{t,j}^{(i)} \in \{0,1\} \tag{GF}$$

- **Remark**: the tensor GSP model [Zhang et al., 2023b] essentially takes the **polynomial filter** of supra-adjacency matrix

$$\mathcal{H}(\boldsymbol{\mathcal{A}}_L, \boldsymbol{\mathcal{A}}_C) = \sum_{t=0}^{T-1} h_t(\boldsymbol{\mathcal{A}}_L + \boldsymbol{\mathcal{A}}_C)^t. \tag{GF-t}$$

[1] Note: this is a multinomial with exponential number of coefficients. Similar observations are made in [Butler et al., 2023].

Expressibility of (GF): Multiplex Graph Dynamics

It is necessary to use the model (GF) with

$$\mathcal{H}(\boldsymbol{\mathcal{A}}_L, \boldsymbol{\mathcal{A}}_C) = \sum_{t=0}^{T-1} \sum_{j=0}^{2^t-1} h_{t,j} \prod_{i=1}^{t} \boldsymbol{\mathcal{A}}_L^{b_{t,j}^{(i)}} \boldsymbol{\mathcal{A}}_C^{1-b_{t,j}^{(i)}}, \quad b_{t,j}^{(i)} \in \{0,1\}$$

Supra-diffusion Process:

- E.g., dynamics of epidemics [Kivelä et al., 2014]:

$$\frac{d\boldsymbol{y}_\ell(t)}{dt} = -\boldsymbol{y}_\ell(t) + \underbrace{\boldsymbol{A}_\ell \boldsymbol{y}_\ell(t)}_{\text{intra-layer}} + \underbrace{\textstyle\sum_{\ell'=1}^{L} C_{\ell,\ell'} \boldsymbol{y}_{\ell'}(t)}_{\text{inter-layer}} + \boldsymbol{x}_\ell^{(m)}.$$

- Steady-state of the diffusion process:

$$\boldsymbol{y}^{(m)} = \lim_{t\to\infty} \boldsymbol{y}(t) = (\boldsymbol{I}_{NL} - (\boldsymbol{\mathcal{A}}_L + \boldsymbol{\mathcal{A}}_C))^{-1} \boldsymbol{x}^{(m)},$$

- **Fine with** (GF) and (GF-t).

Expressibility of (GF): Multiplex Graph Dynamics

It is necessary to use the model (GF) with

$$\mathcal{H}(\boldsymbol{\mathcal{A}}_L, \boldsymbol{\mathcal{A}}_C) = \sum_{t=0}^{T-1} \sum_{j=0}^{2^t-1} h_{t,j} \prod_{i=1}^{t} \boldsymbol{\mathcal{A}}_L^{b_{t,j}^{(i)}} \boldsymbol{\mathcal{A}}_C^{1-b_{t,j}^{(i)}}, \quad b_{t,j}^{(i)} \in \{0,1\}$$

Opinion Dynamics:

- Evolution with mutual trust $\boldsymbol{C}$ and logical matrix $\boldsymbol{A}_\ell$:

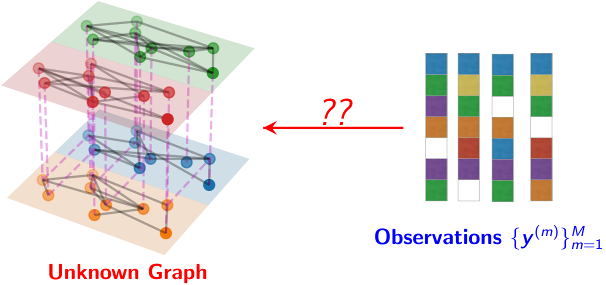
$$\boldsymbol{y}_\ell(t+1) = \underbrace{\boldsymbol{A}_\ell \sum_{\ell'=1}^{L} C_{\ell,\ell'} \boldsymbol{y}_{\ell'}(t)}_{\textbf{coupled}\text{ inter- and intra-layer}} + \boldsymbol{x}_\ell^{(m)},$$

- Steady-state opinions:

$$\boldsymbol{y}^{(m)} = \lim_{t\to\infty} \boldsymbol{y}(t) = (\boldsymbol{I}_{NL} - \boldsymbol{\mathcal{A}}_L \boldsymbol{\mathcal{A}}_C)^{-1} \boldsymbol{x}^{(m)}.$$

- **Fine with** by (GF) **but not** (GF-t).

Multiplex Graph Learning



Task: Given graph signals $\{\boldsymbol{y}^{(m)}\}_{m=1}^{M}$, estimate multiplex graph $\boldsymbol{\mathcal{A}}_L$, $\boldsymbol{\mathcal{A}}_C$.

- **General idea**: Following [Dong et al., 2016], exploit smoothness of multi-attribute graph signals → how to leverage (GF)?

TV Objective and Matched Graph Filter

(Let's take a slight detour ...)

- Let $\boldsymbol{S} \in \mathbb{R}^{N \times N}$ be the pairwise distance matrix of graph signals and we aim at learning the (simple) graph adjacency $\boldsymbol{A}$.
- Consider the **Dirichlet energy criterion** in [Berger et al., 2020][2]:

$$\mathrm{TV}(\hat{\boldsymbol{A}}) := \sum_{i,j=1}^{N} \hat{A}_{ij} \frac{1}{M} \|\boldsymbol{y}_i - \boldsymbol{y}_j\|^2 = \sum_{i,j=1}^{N} \hat{A}_{ij} S_{ij} = \langle \hat{\boldsymbol{A}} | \boldsymbol{S} \rangle. \qquad (2)$$

With $\boldsymbol{y}^{(m)} \approx \mathcal{H}(\boldsymbol{A})\boldsymbol{x}^{(m)}$ and under mild condition

$$\min_{\hat{\boldsymbol{A}}} \mathrm{TV}(\hat{\boldsymbol{A}}) \overset{approx.}{\Longleftrightarrow} \max_{\hat{\boldsymbol{A}}} \langle \hat{\boldsymbol{A}} \,|\, \mathcal{H}^2(\boldsymbol{A}) \rangle.$$

- If $\mathcal{H}^2(\boldsymbol{A})$ is a low-pass graph filter [Ramakrishna et al., 2020], then its **first order approximation**[3] is given by $\mathcal{H}^2(\boldsymbol{A}) \approx \boldsymbol{A}$.
- Criterion (2) can be interpreted as a **matched filter** criterion.

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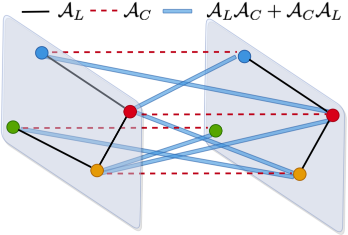
[2] Graph learning methods based on quadratic TV such as [Dong et al., 2016] can be interpreted similarly.

[3] In general $\mathcal{H}(\boldsymbol{A})$ is not known a-priori, 1st order approx is the best we can do.

Tractable Approximation to (GF)

- (GF) is **intractable** in general $\because$ exponential no. of parameters.
- Inspired by the examples, consider the **approximation**[4]:

$$\mathcal{H}(\boldsymbol{\mathcal{A}}_L, \boldsymbol{\mathcal{A}}_C) \approx \overline{\mathcal{H}}_1(\boldsymbol{\mathcal{A}}_L) + \overline{\mathcal{H}}_2(\boldsymbol{\mathcal{A}}_C) + \overline{\mathcal{H}}_3(\boldsymbol{\mathcal{A}}_L \boldsymbol{\mathcal{A}}_C + \boldsymbol{\mathcal{A}}_C \boldsymbol{\mathcal{A}}_L) \quad \text{(a-GF)}$$



- $\overline{\mathcal{H}}_1, \overline{\mathcal{H}}_2, \overline{\mathcal{H}}_3$ are polynomials.
- $\overline{\mathcal{H}}_1(\boldsymbol{\mathcal{A}}_L)$, $\overline{\mathcal{H}}_2(\boldsymbol{\mathcal{A}}_C)$ model intra- and inter-layer graph dynamics,
- $\overline{\mathcal{H}}_3$ captures two-hops neighbors and cross-layer interactions.

[4] Also assume that $\mathcal{H}(\boldsymbol{\mathcal{A}}_L, \boldsymbol{\mathcal{A}}_C)\mathcal{H}(\boldsymbol{\mathcal{A}}_L, \boldsymbol{\mathcal{A}}_C)^\top$ obeys a similar form.

Matched Graph Filter for Multiplex Graph Learning

- $\boldsymbol{S} \in \mathbb{R}^{NL \times NL}$ = pairwise distance matrix of **multi-attribute** signals.
- Consider a **generalized Dirichlet energy criterion**

$$\mathrm{TV}(\boldsymbol{\mathcal{A}}_L, \boldsymbol{\mathcal{A}}_C) := \sum_{i,j=1}^{NL} \left[\hat{h}(\boldsymbol{\mathcal{A}}_L, \boldsymbol{\mathcal{A}}_C)\right]_{ij} S_{ij} = \langle \hat{h}(\boldsymbol{\mathcal{A}}_L, \boldsymbol{\mathcal{A}}_C) \,|\, \boldsymbol{S} \rangle. \quad (3)$$

- With (a-GF), we have

$$\boldsymbol{S} \approx \overline{\mathcal{H}}_1(\boldsymbol{\mathcal{A}}_L) + \overline{\mathcal{H}}_2(\boldsymbol{\mathcal{A}}_C) + \overline{\mathcal{H}}_3(\boldsymbol{\mathcal{A}}_L \boldsymbol{\mathcal{A}}_C + \boldsymbol{\mathcal{A}}_C \boldsymbol{\mathcal{A}}_L).$$

- **Assumption H1**: $\overline{\mathcal{H}}_1(\cdot), \overline{\mathcal{H}}_2(\cdot), \overline{\mathcal{H}}_3(\cdot)$ are **low-pass graph filters**.
- Under H1, the matched multiplex graph filter design:

$$\hat{h}(\boldsymbol{\mathcal{A}}_L, \boldsymbol{\mathcal{A}}_C) = \boldsymbol{\mathcal{A}}_L + \boldsymbol{\mathcal{A}}_C + \lambda(\boldsymbol{\mathcal{A}}_C \boldsymbol{\mathcal{A}}_L + \boldsymbol{\mathcal{A}}_L \boldsymbol{\mathcal{A}}_C).$$

$\rightarrow$ A **high-order smoothness** metric!

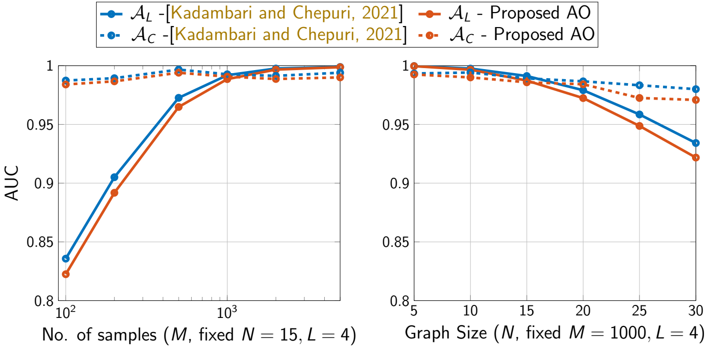
Multiplex Graph Learning - Algorithm

Under H1, we formulate the **bi-convex** problem:

$$\min_{\hat{\mathcal{A}}_L, \hat{\mathcal{A}}_C \in \mathcal{A}} \left\langle \widehat{\mathcal{A}}_L + \widehat{\mathcal{A}}_C + \lambda \left(\widehat{\mathcal{A}}_L \widehat{\mathcal{A}}_C + \widehat{\mathcal{A}}_C \widehat{\mathcal{A}}_L \right) \mid \boldsymbol{S} \right\rangle + \alpha \left(\|\widehat{\mathcal{A}}_L\|_F^2 + \|\widehat{\mathcal{A}}_C\|_F^2 \right) \tag{4}$$

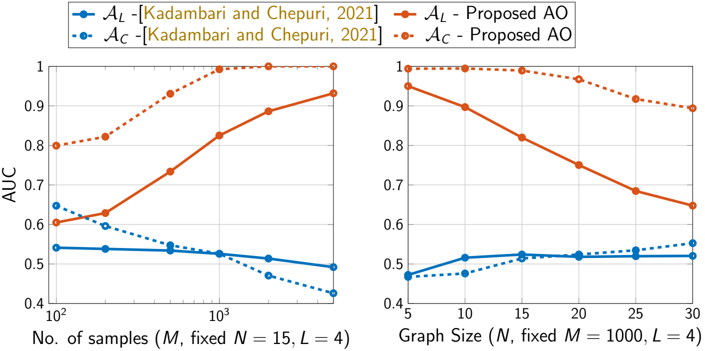
- **Algorithm**: alternating optimization (AO) can be applied:
  - Fix $\widehat{\mathcal{A}}_C$ and solve for $\widehat{\mathcal{A}}_L \rightarrow$ fix $\widehat{\mathcal{A}}_L$ and solve for $\widehat{\mathcal{A}}_C \rightarrow \cdots$
- The AO subproblems are separable and tractable – each involves **convex** problems size of $N \times N$ or $L \times L$.
- AO finds a stationary point of (4) as iteration number goes to ∞ [Grippo and Sciandrone, 2000].
- **Remark**: when $\lambda = 0$, the problem reduces into that of [Kadambari and Chepuri, 2021].

Topology Reconstruction under strong coupling



- Weak coupling: $\mathcal{H}_{\text{wk}}(\boldsymbol{\mathcal{A}}_L, \boldsymbol{\mathcal{A}}_C) = (\boldsymbol{I} - \tau_{\text{wk}}(\boldsymbol{\mathcal{A}}_L + \boldsymbol{\mathcal{A}}_C))^{-1}$.
- Observation: AUC performance generally improves as M increases/deteriorates as N increases.
- Proposed AO ($\lambda = 0.1$) attains **similar** performance to the benchmark.

Topology Reconstruction under strong coupling



- Strong coupling: $\mathcal{H}_{\text{str}}(\boldsymbol{\mathcal{A}}_L, \boldsymbol{\mathcal{A}}_C) = (\boldsymbol{I} - \tau_{\text{str}} \boldsymbol{\mathcal{A}}_L \boldsymbol{\mathcal{A}}_C)^{-1}$.
- Benchmark fails in estimating graph topologies under strong coupling.
- Proposed AO ($\lambda = 5$) recovers topology effectively regardless of layer coupling **robustly**.

Summary

Takeaway: Distinct **inter-layer and intra-layer interactions** dynamics require careful modeling for multiplex graph learning.

We have introduced a method for learning multiplex network structures from multi-attribute graph signals:

- General multiplex graph filter to model complex signal interactions.
- Matched filter perspective to graph learning by smoothness $\rightarrow$ a **high-order smoothness metric** aimed at inter-layer coupling.
- An efficient AO procedure for learning graph topologies.

- **Future work**: modeling of multiplex graph signals, adopting other GSP tools, ...

Thank you!

Contact me at htwai@cuhk.edu.hk if you are interested.

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