

# Joint Simplicial Complex Learning via Binary Linear Programming

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## **Introduction**

What are higher-order networks and why do we need them?

## **Problem Formulation**

What is the general formulation we follow?

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How exactly do we recover the simplicial complex?

## **Why This Works**

What justifies the method?

## **Results and Insights**

What do we learn from experiments?

# Hypergraphs: Moving beyond Graphs

- Graphs are a set of nodes and edges:

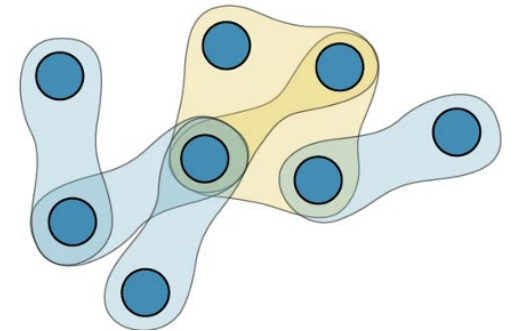
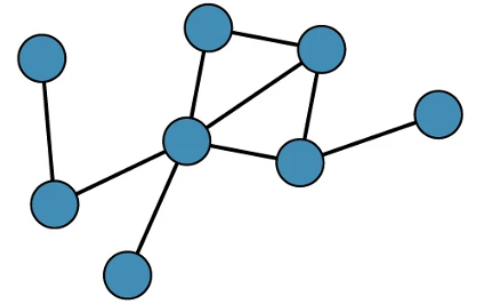
$$\mathcal{G} = (\mathcal{V}, \mathcal{E}), \text{ where } \mathcal{V} = \{v_1, v_2, \dots, v_N\} \text{ and } \mathcal{E} = \{e_1, e_2, \dots, e_K\}$$

Each edge  $e_k$  connects a pair of nodes.

- Hypergraphs are a set of nodes and hyperedges:

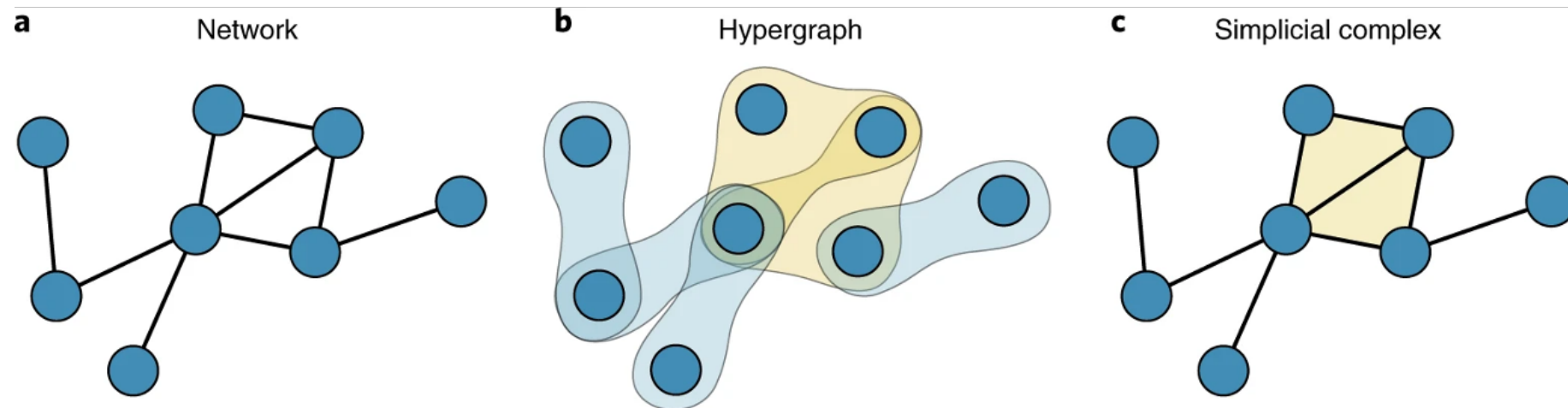
$$\mathcal{H} = (\mathcal{V}, \mathcal{F}), \text{ where } \mathcal{V} = \{v_1, v_2, \dots, v_N\} \text{ and } \mathcal{F} = \{f_1, f_2, \dots, f_K\}$$

Each hyperedge  $f_k$  connects an arbitrary number of nodes.



# Simplicial Complexes

- Simplicial Complexes are [hypergraphs with structure](#).
- For every hyperedge connecting a set of nodes, [all subsets of that set must also exist](#) in the complex.

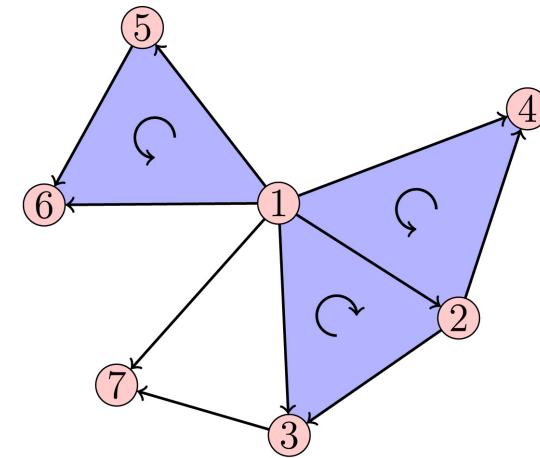
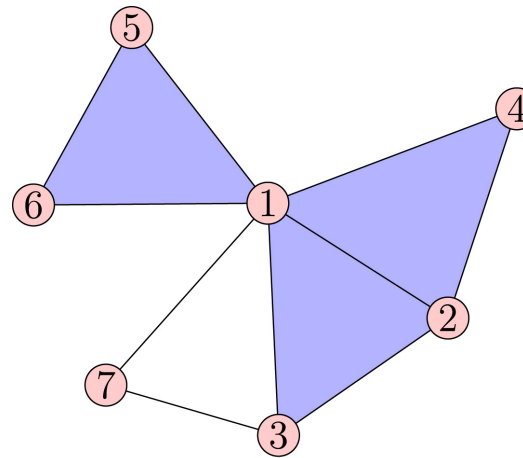


- Each hyperedge:  $k$ -simplex. 0-simplices: nodes, 1-simplices: edges, ...

Goal: identify the **topology** of the simplicial complex from **data**.

# Simplicial Complexes: Defining Topology

- Given a topology, how do we mathematically represent it?
- Incidence matrices:  $\mathbf{B}_k \in \mathbb{R}^{N_{k-1} \times N_k}$
- Map from  $k - 1$ -simplices to  $k$ -simplices



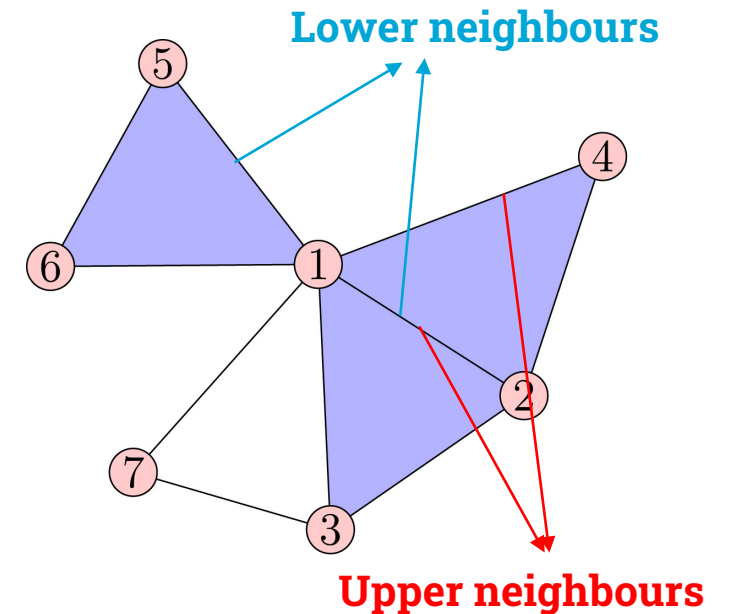
$$\mathbf{B}_1 = \begin{matrix} & \overbrace{\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 0 \end{bmatrix}}^{\text{edges}} \\ \left. \vphantom{\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 0 \end{bmatrix}} \right\} \text{nodes} \end{matrix}$$

$$\mathbf{B}_2 = \begin{matrix} & \overbrace{\begin{bmatrix} 1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}}^{\text{triangles}} \\ \left. \vphantom{\begin{bmatrix} 1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}} \right\} \text{edges} \\ 6 \end{matrix}$$

# Simplicial Complexes: Defining Topology

- A simplicial complex of order  $K$  can be defined via the Hodge Laplacians:

$$\mathbf{L}_k = \underbrace{\mathbf{B}_k^\top \mathbf{B}_k}_{\mathbf{L}_k^{\text{low}}} + \underbrace{\mathbf{B}_{k+1} \mathbf{B}_{k+1}^\top}_{\mathbf{L}_k^{\text{up}}}, \quad k = 1, \dots, K-1.$$



- Simplicial complex structural constraint:

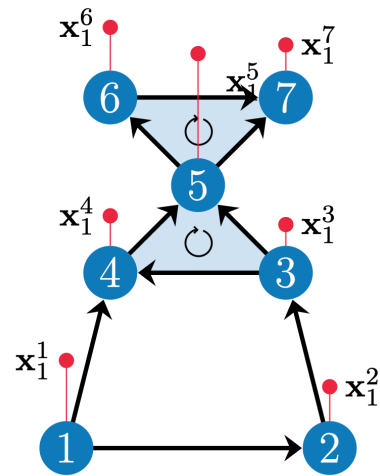
$$\mathbf{B}_k \mathbf{B}_{k+1} = \mathbf{0} \quad \forall k = 1, \dots, K-1.$$

# Simplicial Complexes: Data

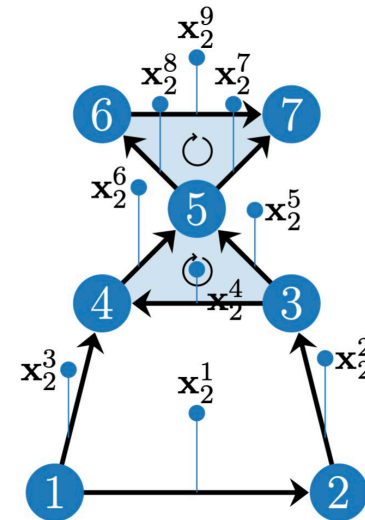
- A  $k$ -simplicial signal:  $\mathbf{X}_k \in \mathbb{R}^{N_k \times F_k}$ ,

where  $N_k$  is the number of  $k$ -simplices,

$F_k$  is the number of features per simplex.



Node signals



Edge signals

# Problem Formulation

Identify topology

Links b/w topology and signals

$$\min_{\mathbf{B}_1, \mathbf{B}_2} f_1(\mathbf{B}_1, \mathbf{X}_0) + f_2(\mathbf{B}_2, \bar{\mathbf{X}}_1)$$

s.t.  $\mathbf{B}_1 \in \mathcal{B}_1, \mathbf{B}_2 \in \mathcal{B}_2,$   $\mathbf{B}_1 \mathbf{B}_2 = \mathbf{0}.$

Subject to feasible incidence matrices

Subject to the inclusion constraint

# Problem Formulation

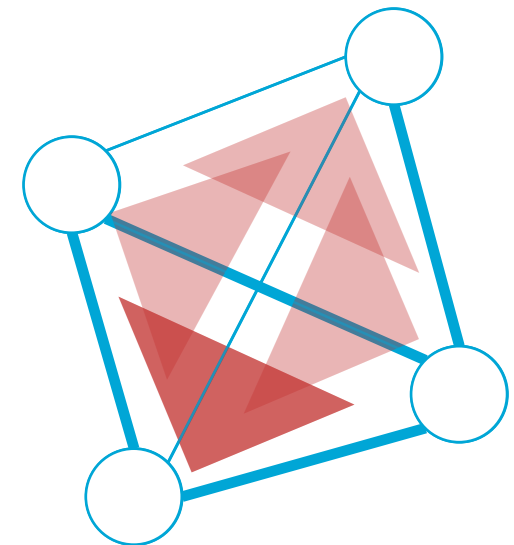
$$\begin{aligned} \min_{\mathbf{B}_1, \mathbf{B}_2} \quad & f_1(\mathbf{B}_1, \mathbf{X}_0) + f_2(\mathbf{B}_2, \bar{\mathbf{X}}_1) \\ \text{s.t.} \quad & \mathbf{B}_1 \in \mathcal{B}_1, \quad \mathbf{B}_2 \in \mathcal{B}_2, \quad \mathbf{B}_1 \mathbf{B}_2 = \mathbf{0}. \end{aligned}$$

Maintaining feasibility

# Maintaining Feasibility

- Avoid directly learning incidence matrices.
- Select simplices from full complexes [1].
- Full incidence matrices:  $\bar{\mathbf{B}}_1 \in \mathbb{R}^{N_0 \times \bar{N}_1}$  and  $\bar{\mathbf{B}}_2 \in \mathbb{R}^{\bar{N}_1 \times \bar{N}_2}$
- Select existing simplices using  $\mathbf{s}_1 \in \{0,1\}^{\bar{N}_1}$ ,  $\mathbf{s}_2 \in \{0,1\}^{\bar{N}_2}$
- Work only in the space of  $\mathbf{s}_1$ ,  $\mathbf{s}_2$
- Enforce minimum number of simplices by imposing minimum cardinality

Edge selection with  $\mathbf{s}_1$   
Triangle selection with  $\mathbf{s}_2$



# Problem Formulation

Links b/w topology and signals

Assume signals  
available on all  
possible edges

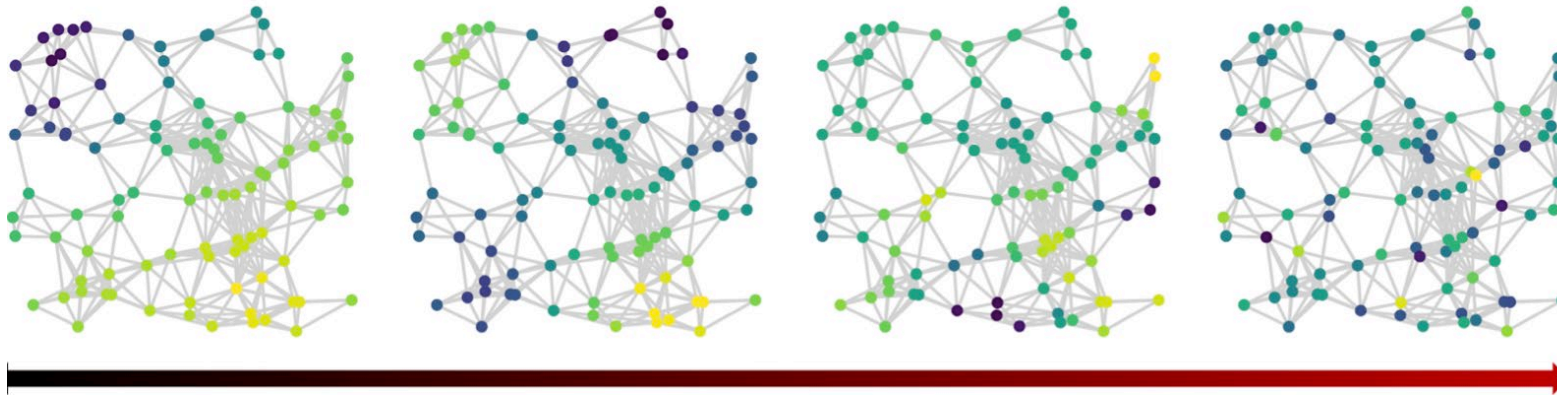
$$\begin{aligned} \min_{\mathbf{B}_1, \mathbf{B}_2} & \quad f_1(\mathbf{B}_1, \mathbf{X}_0) + f_2(\mathbf{B}_2, \bar{\mathbf{X}}_1) \\ \text{s.t.} & \quad \mathbf{B}_1 \in \mathcal{B}_1, \quad \mathbf{B}_2 \in \mathcal{B}_2, \quad \mathbf{B}_1 \mathbf{B}_2 = \mathbf{0}. \end{aligned}$$

# Smoothness: Linking topology to signals

- Linking node signals to edges:

Node signal smoothness on edges:  $\text{tr}(\mathbf{X}_0^\top \bar{\mathbf{L}}_0 \mathbf{X}_0)$ ,  $\bar{\mathbf{L}}_0 = \bar{\mathbf{B}}_1 \text{diag}(\mathbf{s}_1) \bar{\mathbf{B}}_1^\top$

Captures total variation of node signals across edges



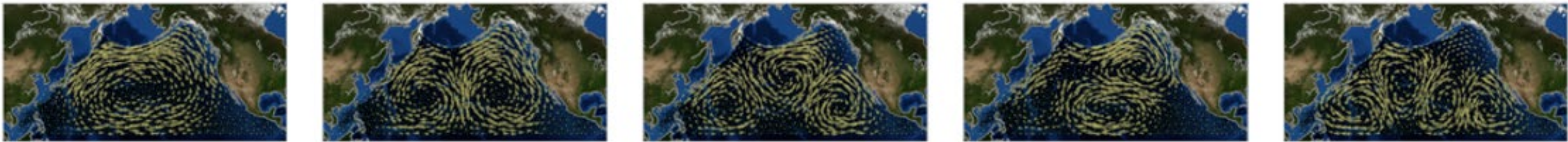
Increasing node signal variation across edges

# Smoothness: Linking topology to signals

- Linking edge signals to triangles:

Edge signal curl on triangles:  $\text{tr}(\bar{\mathbf{X}}_1^\top \bar{\mathbf{L}}_1^{\text{up}} \bar{\mathbf{X}}_1)$ ,  $\bar{\mathbf{L}}_1^{\text{up}} = \bar{\mathbf{B}}_2 \text{diag}(\mathbf{s}_2) \bar{\mathbf{B}}_2^\top$

Measures the rotational component of edge signals around triangles



Increasing edge signal curl on triangles

# Smoothness: Linking topology to signals

- Linking edge signals to triangles:

No existing measure which captures edge signal variation within a triangle

**Proposed measure:** sum of pair differences of edge signals within a triangle

$$\sum_{i=1}^{\bar{N}_2} [\mathbf{s}_2]_i \sum_{\substack{f,g \in \mathcal{F}(\sigma_2^{(i)}) \\ f < g}} \|[\bar{\mathbf{X}}_1]_{f,:} - [\bar{\mathbf{X}}_1]_{g,:}\|_2^2$$

Generalizes graph signal smoothness to higher orders.

All smoothness measures are linear in the selection variables.

# Problem Formulation

$$\begin{aligned} \min_{\mathbf{B}_1, \mathbf{B}_2} \quad & f_1(\mathbf{B}_1, \mathbf{X}_0) + f_2(\mathbf{B}_2, \bar{\mathbf{X}}_1) \\ \text{s.t.} \quad & \mathbf{B}_1 \in \mathcal{B}_1, \quad \mathbf{B}_2 \in \mathcal{B}_2, \quad \boxed{\mathbf{B}_1 \mathbf{B}_2 = \mathbf{0}.} \end{aligned}$$

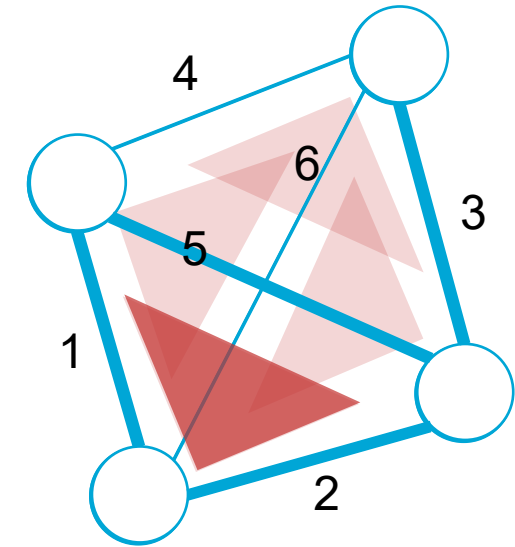
**Enforcing inclusion**

# Enforcing Inclusion

- Two main approaches currently to enforce inclusion

Hierarchical [1]: solve for edges, and then triangles.  
No need to mathematically couple simplices.

Bilinear constraint [2]:  $(\mathbf{1} - \mathbf{s}_1)^\top \bar{\mathbf{B}}_2^+ \mathbf{s}_2 = 0$   
Requires alternating approaches.



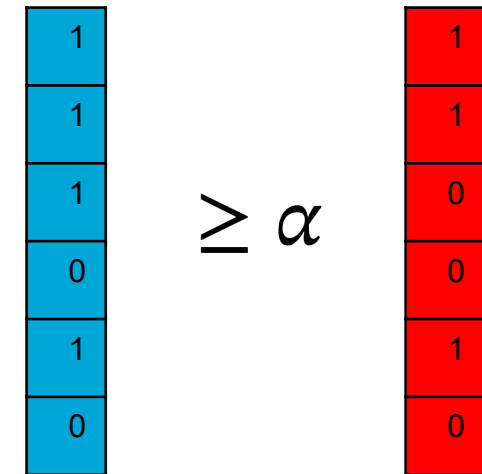
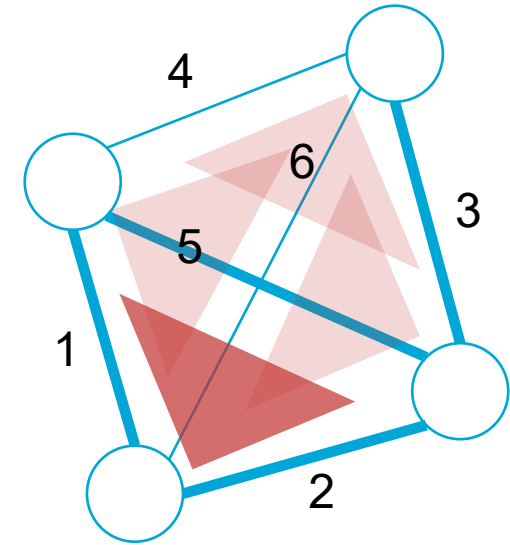
0	0	0	1	0	1
1	1	0	0	1	0

# Enforcing Inclusion

- We introduce a linear constraint to enforce inclusion

$$\mathbf{s}_1 \geq \alpha \bar{\mathbf{B}}_2^+ \mathbf{s}_2$$

- Allows for a joint approach without requiring alternating!



# Problem Formulation

$$\begin{aligned} \min_{\mathbf{B}_1, \mathbf{B}_2} \quad & f_1(\mathbf{B}_1, \mathbf{X}_0) + f_2(\mathbf{B}_2, \bar{\mathbf{X}}_1) \\ \text{s.t.} \quad & \mathbf{B}_1 \in \mathcal{B}_1, \quad \mathbf{B}_2 \in \mathcal{B}_2, \quad \mathbf{B}_1 \mathbf{B}_2 = \mathbf{0}. \end{aligned} \quad \Rightarrow$$

$$\begin{aligned} \min_{\mathbf{s}_1, \mathbf{s}_2} \quad & \mathbf{h}_1^\top \mathbf{s}_1 + \mathbf{h}_2^\top \mathbf{s}_2 \\ \text{s.t.} \quad & \mathbf{s}_1 \geq \alpha \bar{\mathbf{B}}_2^+ \mathbf{s}_2 \\ & \mathbf{s}_1 \in \{0, 1\}^{\bar{N}_1}, \quad \mathbf{s}_2 \in \{0, 1\}^{\bar{N}_2} \\ & \mathbf{1}^\top \mathbf{s}_1 \geq C_1, \quad \mathbf{1}^\top \mathbf{s}_2 \geq C_2. \end{aligned}$$

# Baselines

- Hierarchical Approach [1]:

- First solve for edges 
$$\begin{aligned} \min_{\mathbf{s}_1} \quad & \mathbf{h}_1^\top \mathbf{s}_1 \\ \text{s.t.} \quad & \mathbf{1}^\top \mathbf{s}_1 \geq C_1, \quad \mathbf{s}_1 \in \{0, 1\}^{\bar{N}_1} \end{aligned}$$

- Then, restrict to feasible triangle set  $\mathcal{T}(\hat{\mathbf{s}}_1)$ , and solve

$$\begin{aligned} \min_{\mathbf{s}_2} \quad & \mathbf{h}_2^\top \mathbf{s}_2 \\ \text{s.t.} \quad & [\mathbf{s}_2]_t = 0, \quad \forall t \notin \mathcal{T}(\hat{\mathbf{s}}_1) \\ & \mathbf{1}^\top \mathbf{s}_2 \geq C_2, \quad \mathbf{s}_2 \in \{0, 1\}^{\bar{N}_2}. \end{aligned}$$

# Baselines

Greedy, alternating approach [1]:

$$\begin{aligned} \min_{\mathbf{s}_1, \mathbf{s}_2} \quad & \|\mathbf{s}_1\|_0 + \|\mathbf{s}_2\|_0 + \mathbf{h}_1^\top \mathbf{s}_1 + \mathbf{h}_2^\top \mathbf{s}_2 \\ & + \gamma(\mathbf{1} - \mathbf{s}_1)^\top \bar{\mathbf{B}}_2^+ \mathbf{s}_2 \\ \text{s.t.} \quad & \mathbf{s}_1 \in \{0, 1\}^{\bar{N}_1}, \quad \mathbf{s}_2 \in \{0, 1\}^{\bar{N}_2} \\ & \|\mathbf{s}_1\|_0 \geq C_1, \quad \|\mathbf{s}_2\|_0 \geq C_2. \end{aligned}$$

- Form a cost per edge, choose the edges with the lowest cost.
- Form a cost per triangle, choose the triangles with the lowest cost.
- Alternate.
- Inclusion penalty embedded in cost.

# Simulated Experiments

- Sample an Erdős-Rényi graph with a certain edge probability.
- Smooth node signals are then generated by filtering white noise through the graph Laplacian.
- From the set of feasible triangles, half are randomly chosen.
- Edge signals are generated similarly, using the appropriate Laplacian (associated to either curl or similarity).

# Simulated Experiments

# Real Data Experiments : Co-Authorship Networks

- Nodes: authors, node signals: frequency of keywords used.
- Edges and triangles: co-authors of the same paper.
- Edge signals: element wise minimum of node signals.
- Important property:

Edge signals are not low curl but have high similarity.

# Co-Authorship Experiments

# Conclusion

- Solving jointly captures better structural relationships: allowed by the linear constraint.
- The joint method truly reflects how well the higher simplices adhere to the prior- no reliance on feasibility.

# Going Forward

- Learning weighted simplicial complexes.

Needs special requirement: proposed constraint works only for binary support.

$s_1 \geq \alpha \bar{\mathbf{B}}_2^+ s_2$  imposes the requirement that each edge weight be at least the sum of the weights of its incident triangles

- Tracking time-varying simplicial complexes.

Thanks!  
Questions?

Find the paper on Arxiv



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