NeurIPS 2025

Disentangling Hyperedges through the Lens of Category Theory

Yoonho Lee, Junseok Lee, Sangwoo Seo, Sungwon Kim, Yeongmin Kim and Chanyoung Park

Dec. 2025

Presenter : Yoonho Lee

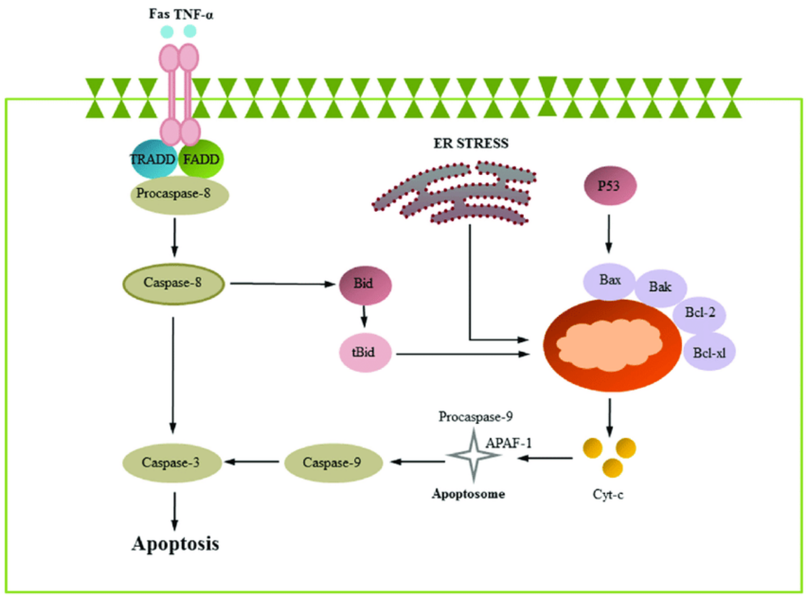
NeurIPS

KAIST

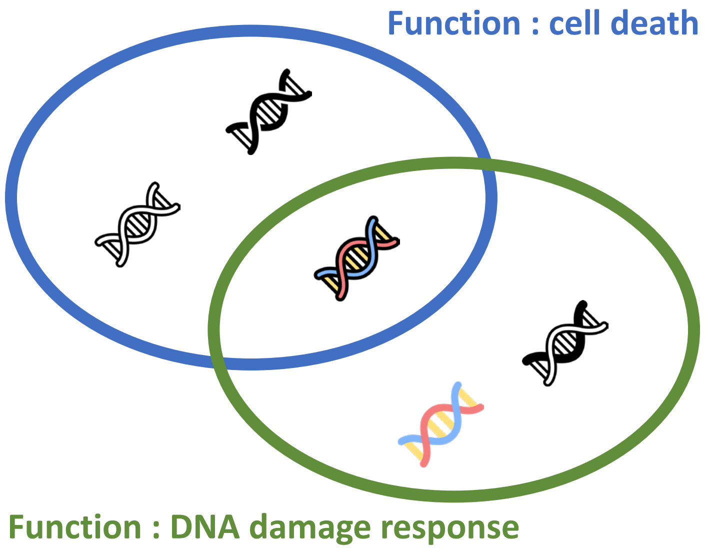
BACKGROUND

- Hypergraph is used to express multiway interactions using hyperedges.
- These multiway interactions (hyperedges) can have hidden semantics.
- Example : **Genetic pathway is a set of genes** that collaborate to perform a **specific biological function**.

Hyperedge **Context behind interaction**



Apoptosis Pathway (example)

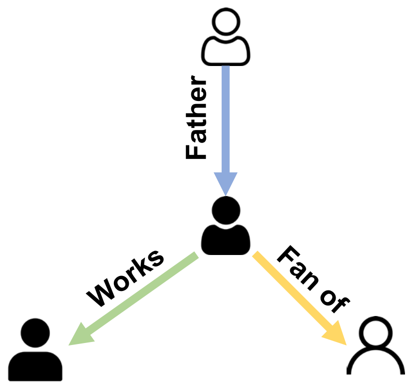


Genetic pathways expressed as hypergraph

Figure: Programmed cell death: The battlefield between the host and alpha-herpesviruses and a potential avenue for cancer treatment

BACKGROUND

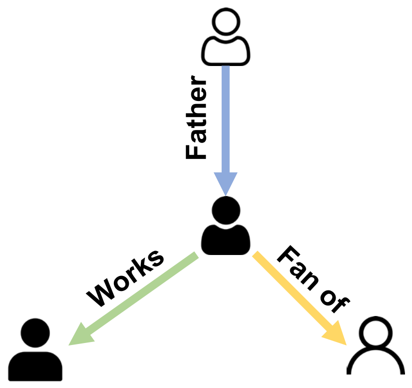
- Disentangled representation learning (DRL) aims to identify **factors** behind observed data
  - Ex) In social network graph, there can be **hidden relations** (family, friend) between individuals
- Usually rely on **factor representation similarity** to identify the most relevant factor
  - Assumption : nodes are connected because they share commonalities (i.e. similarities)



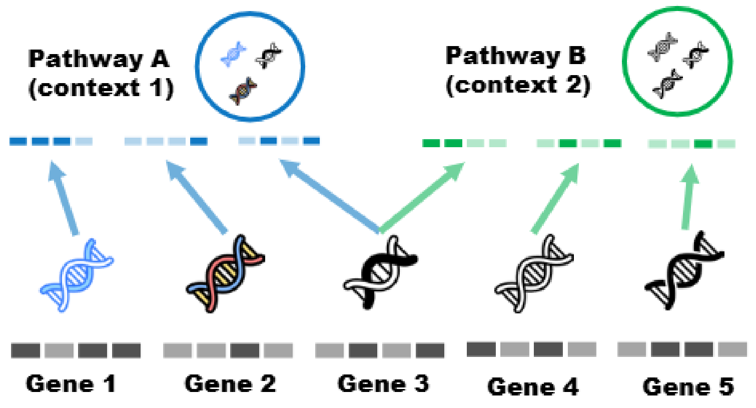
Example of factor in social network

MOTIVATION

- Assumptions can mislead disentanglement and limit applicability of DRL.
  - Ex) Genetic pathway : genes in a pathway do not necessarily have similar properties or gene expression (feature).



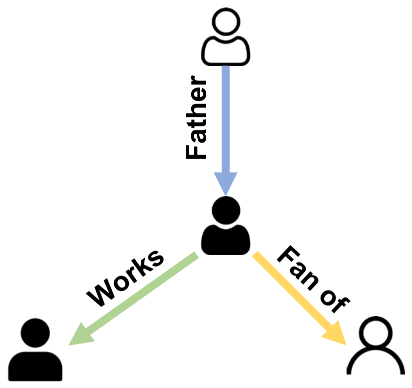
Example of factor in social network



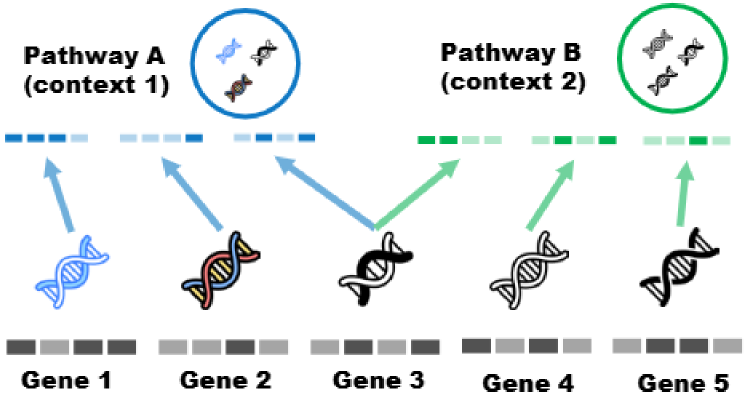
Each pathway has their own functional context.

MOTIVATION

- Assumptions can mislead disentanglement and limit applicability of DRL.
  - Ex) Genetic pathway : genes in a pathway do not necessarily have similar properties or gene expression.
- We aim to design **hyperedge disentanglement criterion**, that does **not rely on assumptions** about data.
  - We need to find a characteristic that is related to the definition of 'hyperedge disentanglement'
  - Since **hyperedge semantics are abstract concepts**, it is difficult to discover characteristics



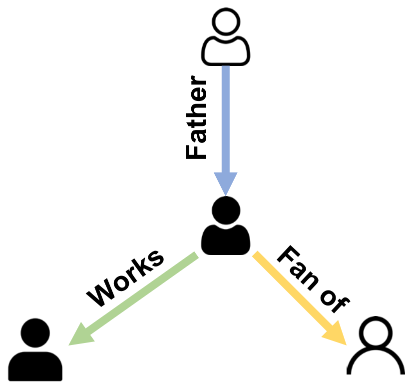
Example of factor in social network



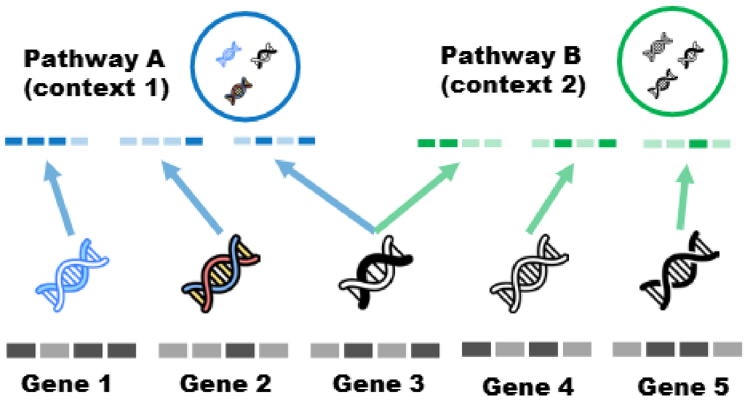
Each pathway has their own functional context.

MOTIVATION

- We use **category theory**, the abstract language of mathematics, to discover characteristics
  - Category theory express a complex system as **compositional structure**
  - We analyze hyperedge disentanglement and semantics with category theory
  - Through analysis, we discovered a criterion (characteristics) that holds **regardless of data**.



Example of factor in social network



Each pathway has their own functional context.

CATEGORY THEORY : INTRODUCTION

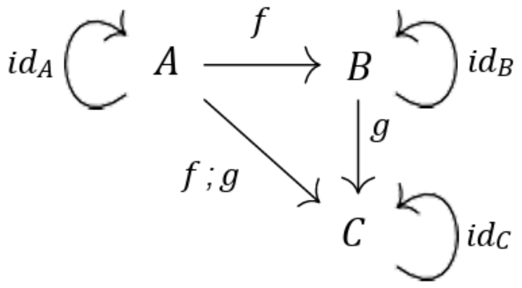
- Quote from [1]. Aim to see global, compositional structure of a system, instead of focusing on each component.

Category theory takes a bird' s eye view of mathematics.
From high in the sky, details become invisible, but we can spot patterns that were impossible to detect from ground level.

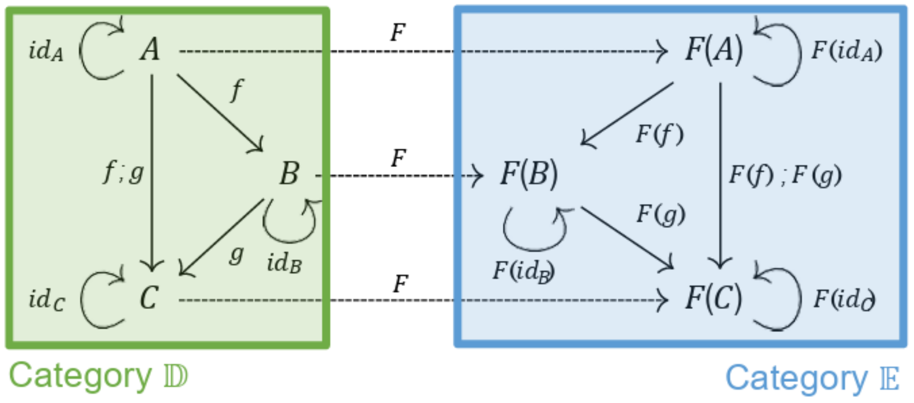
[1] Leinster, Tom. Basic category theory. Vol. 143. Cambridge University Press, 2014.

CATEGORY THEORY : CATEGORY & FUNCTOR

- Category
  - Collection of objects and morphisms between them.
  - Must have identity morphism for each object, and morphisms are composable.
  - Ex) objects are sets, and morphisms are functions
- Functor
  - Structure preserving maps between two categories.



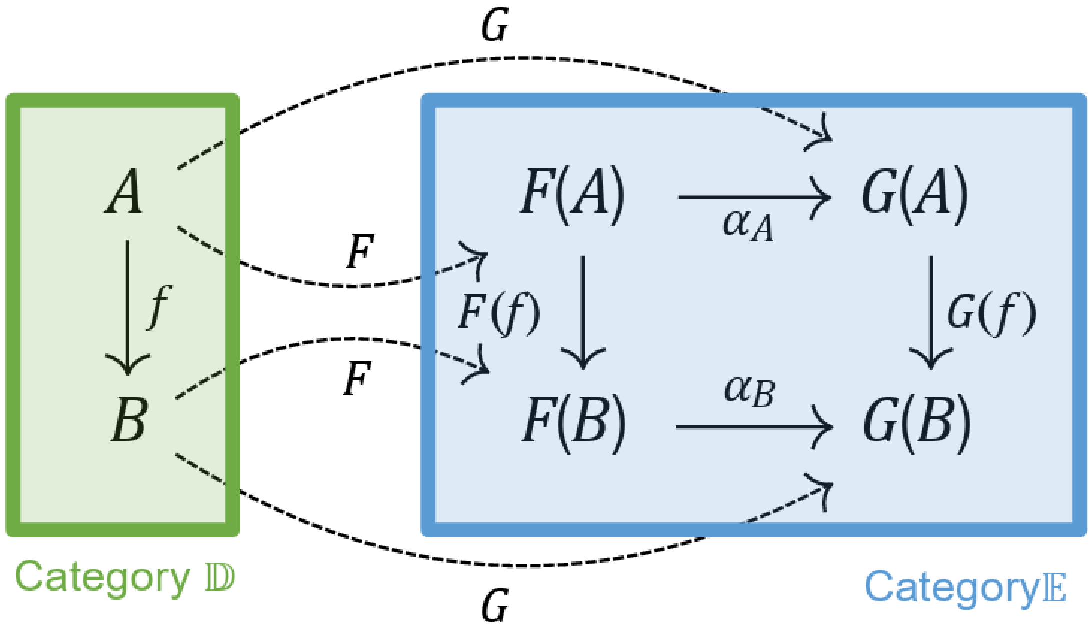
(a) Category



(b) Functor

CATEGORY THEORY : NATURAL TRANSFORMATION

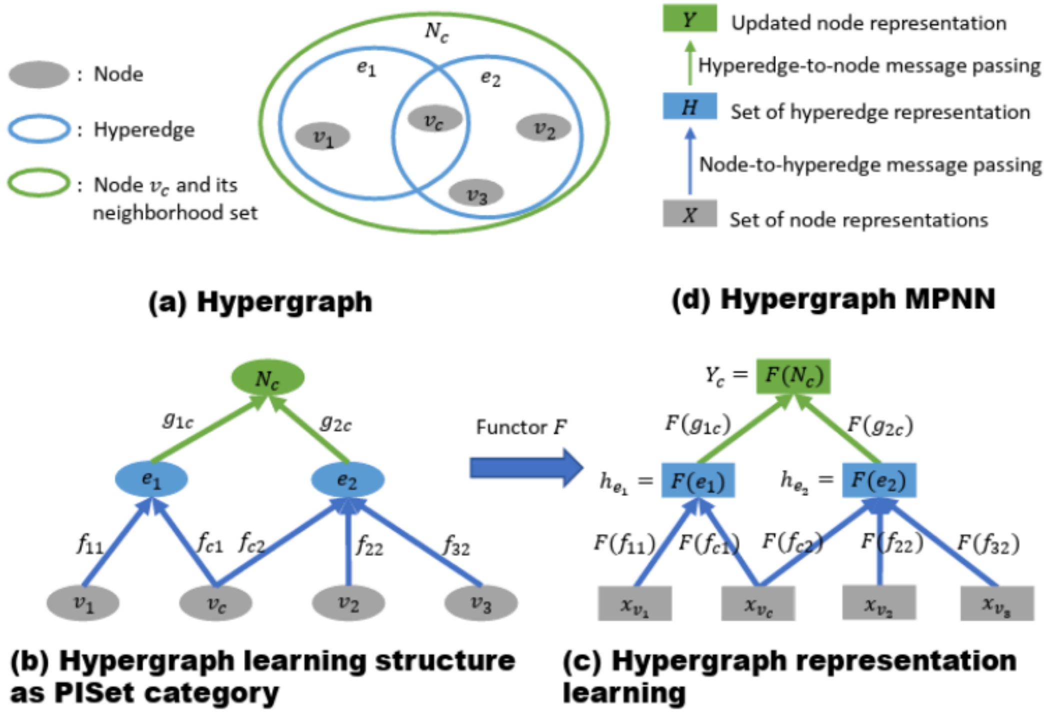
- Natural transformation
  - Assume two functors $F, G : \mathbb{D} \rightarrow \mathbb{E}$. For object $A \in \mathbb{D}$, $\alpha_A : F(A) \rightarrow G(A)$ is natural transformation.
  - This results commutative diagram below, which is often called a 'naturality condition'.



ANALYZING HYPERGRAPH NEURAL NETWORK

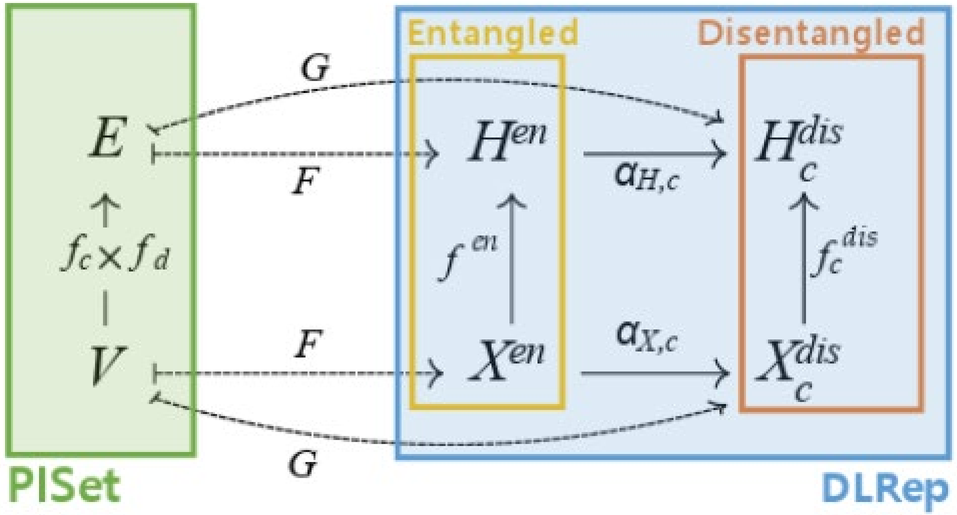
- Hypergraph
  - Consider each node as a set, each hyperedge as larger set that contains some nodes.
  - It induces poset structure with inclusion maps (denoted PISet)

- Hypergraph Neural Network
  - Can be considered as a result of functor that maps PISet to category for representations (denoted DLRep)



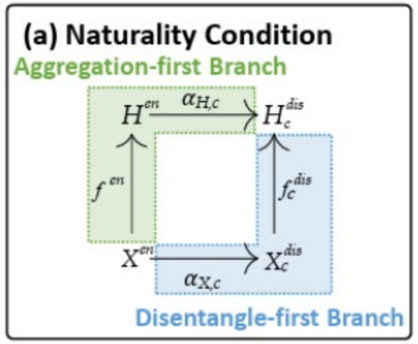
METHOD : CRITERION FOR DISENTANGLEMENT

- For DRL, there are two type of representations
  - Entangled representation and disentangled (factor specific) representation
  - We can consider them as a result of two different functors (entangled, disentangled)
  - Thus we have naturality condition (Commutative diagram) for relevant factor.
- Criterion : If naturality condition holds, then the factor is relevant to hyperedge.

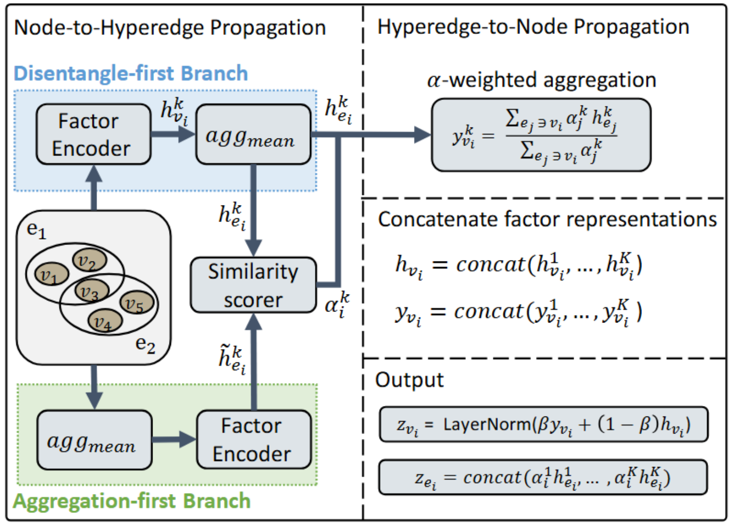


METHOD : IMPLEMENTATION (NATURAL-HNN)

- Node-to-Hyperedge Propagation
  - As relevant factor needs to satisfy commutative diagram (naturality condition), we get two representations
    - Factor representations are learned by projection (1 MLP for each factor)
    - Aggregation-first branch : $\tilde{h}^k_{e_j} = \mathrm{MLP}_k(\mathrm{mean}(\{x_{v_i} | v_i \in e_j\}))$
    - Disentangle-first branch : $h^k_{e_j} = \mathrm{mean}(\{\mathrm{MLP}_k(x_{v_i}) | v_i \in e_j\})$



  - By calculating similarity of two representation, we can check whether naturality condition holds.
    - Relevance of a factor 'k' for hyperedge 'e_i' : $\alpha^k_i = \sigma\left(\frac{h^k_{e_i}}{\|h^k_{e_i}\|_2} W_k \frac{\tilde{h}^{kT}_{e_i}}{\|\tilde{h}^k_{e_i}\|_2}\right)$



- Hyperedge-to-Node propagation
  - For each factor, propagate back to nodes, with hyperedge weights proportional to α^k_i

EXPERIMENT : CANCER SUBTYPE CLASSIFICATION

- Metric : Macro F1
- Task : cancer subtype classification for each patient (hypergraph)
- Patients have same hyperedges (pathways), but node features (gene expression) are different

Table 2: Statistics of 6 cancer datasets used for cancer subtype classification task.

dataset	summary	class distribution(counts)
BRCA	5 class, 769 hypergraphs	Normal-like 33, Her2 44, Basal-like 134, LumB 143, LumA 415
STAD	5 class, 341 hypergraphs	CIN 200, EBV 29, GS 46, MSI 59, HM-SNV 7
SARC	4 class, 257 hypergraphs	LMS 104, MFS/UPS 75, DDLPS 57, Other 21
LGG	2 class, 503 hypergraphs	G2 242, G3 261
HNSC	2 class, 507 hypergraphs	HPV- 411, HPV+ 96
CESC	2 class, 280 hypergraphs	AdenoCarcinoma 46, SquamousCarcinoma 234

Table 1: Model performance on cancer subtype classification task (Macro F1). Top two models are colored by **First**, **Second**. † : the variant of the model using multihead attention. ⋆ : $\mathcal{L}_{dis}$ is not used.

Method	BRCA	STAD	SARC	LGG	HNSC	CESC
HGNN	0.726 ± 0.053	0.563 ± 0.040	0.684 ± 0.067	0.694 ± 0.033	0.799 ± 0.053	0.835 ± 0.052
HCHA	0.704 ± 0.051	0.558 ± 0.044	0.675 ± 0.068	0.682 ± 0.041	0.783 ± 0.055	0.844 ± 0.054
HNHN	0.697 ± 0.046	0.573 ± 0.072	0.688 ± 0.075	0.674 ± 0.038	0.791 ± 0.035	0.837 ± 0.059
UniGCNII	0.697 ± 0.052	0.617 ± 0.059	**0.728** ± 0.066	0.663 ± 0.039	0.830 ± 0.030	0.841 ± 0.046
AllDeepSets	0.716 ± 0.058	0.557 ± 0.044	0.599 ± 0.058	0.665 ± 0.046	0.801 ± 0.058	0.870 ± 0.044
AllSetTransformer	0.743 ± 0.057	0.553 ± 0.046	0.719 ± 0.052	0.653 ± 0.038	0.814 ± 0.036	0.847 ± 0.046
HyperGAT	0.637 ± 0.121	0.534 ± 0.063	0.574 ± 0.153	0.665 ± 0.054	0.789 ± 0.061	0.832 ± 0.046
HyperGAT†	0.641 ± 0.115	0.502 ± 0.087	0.584 ± 0.150	0.646 ± 0.043	0.791 ± 0.079	0.827 ± 0.041
SHINE	0.446 ± 0.155	0.371 ± 0.135	0.529 ± 0.160	0.628 ± 0.104	0.718 ± 0.055	0.745 ± 0.159
SHINE†	0.651 ± 0.053	0.532 ± 0.064	0.673 ± 0.059	0.650 ± 0.046	0.770 ± 0.040	0.837 ± 0.061
HSDN	**0.757** ± 0.044	**0.629** ± 0.045	0.726 ± 0.063	0.692 ± 0.038	0.811 ± 0.044	0.867 ± 0.033
ED-HNN	0.735 ± 0.047	0.615 ± 0.050	0.718 ± 0.071	**0.700** ± 0.030	0.835 ± 0.047	0.875 ± 0.053
ED-HNNII	0.722 ± 0.045	0.536 ± 0.057	0.650 ± 0.087	0.695 ± 0.039	**0.845** ± 0.025	**0.895** ± 0.044
Natural-HNN⋆ (Ours)	**0.804** ± 0.036	**0.659** ± 0.049	**0.745** ± 0.045	**0.707** ± 0.035	**0.862** ± 0.045	**0.881** ± 0.042

EXPERIMENT : CAPTURING HYPEREDGE SEMANTICS

- We selected Top-15 pathways that were relevant to task with SHAP value.
- After clustering pathways with CliXO algorithm, we calculated functional similarity between clusters from the result of our model
  - Measured relevance distribution ($[\alpha_i^1, \ldots, \alpha_i^k]$) similarity between clusters
- (Figure 5) When compared with ground truth, our model (Natural-HNN) could capture functional context while HSDN could not.
- (Figure 6) Each factor captures different context, as each factor has small Pearson correlation with other factors.

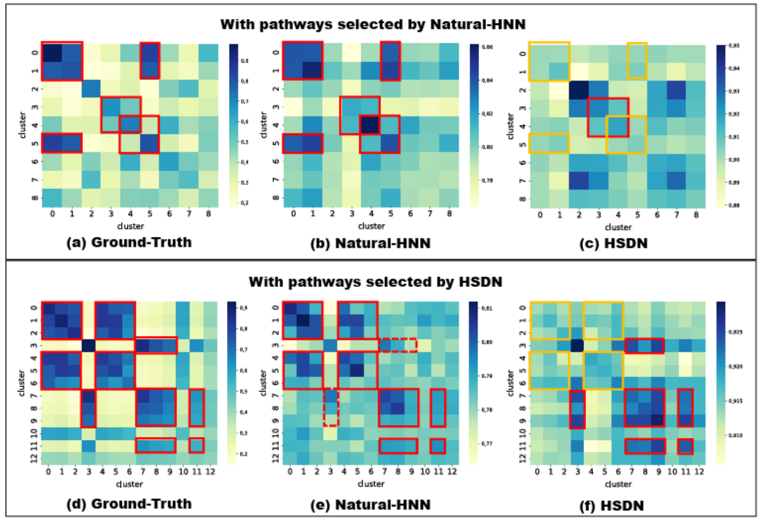


Figure 5: Captured interaction context. Captured patterns are shown in red boxes and not captured patterns are shown with orange boxes. Weakly captured cases are marked as dotted red block.

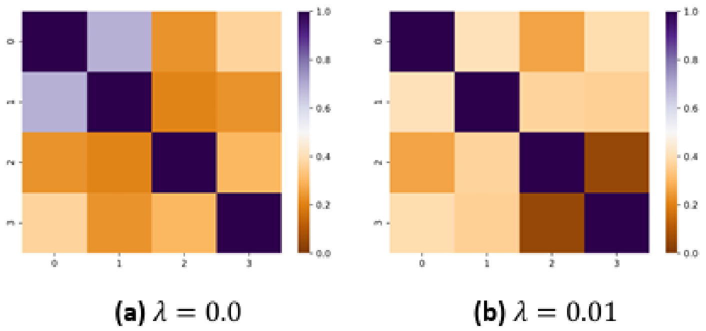


Figure 6: Pearson correlation between hyperedge factors.

EXPERIMENT : CAPTURING HYPEREDGE SEMANTICS

- We tested generalizability of our model by measuring performances with different training ratio (Figure 7)
  - Natural-HNN performs better than convolution-based methods (a) and attention/equivariance based methods (b).
- We checked whether our model captures hyperedge semantics regardless of hyperparameters (Figure 8)
  - (a) For different training ratio, Natural-HNN still captures functional context (hyperedge semantics)
  - (b) For different hyperparameters (e.g. hidden dimension, number of factors, λ), Natural-HNN still captures functional context.

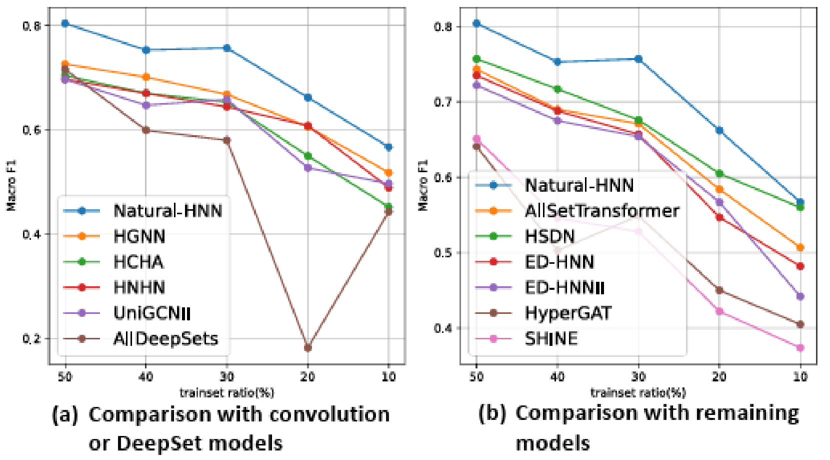


Figure 7: Marcro F1 scores with different training set ratio.

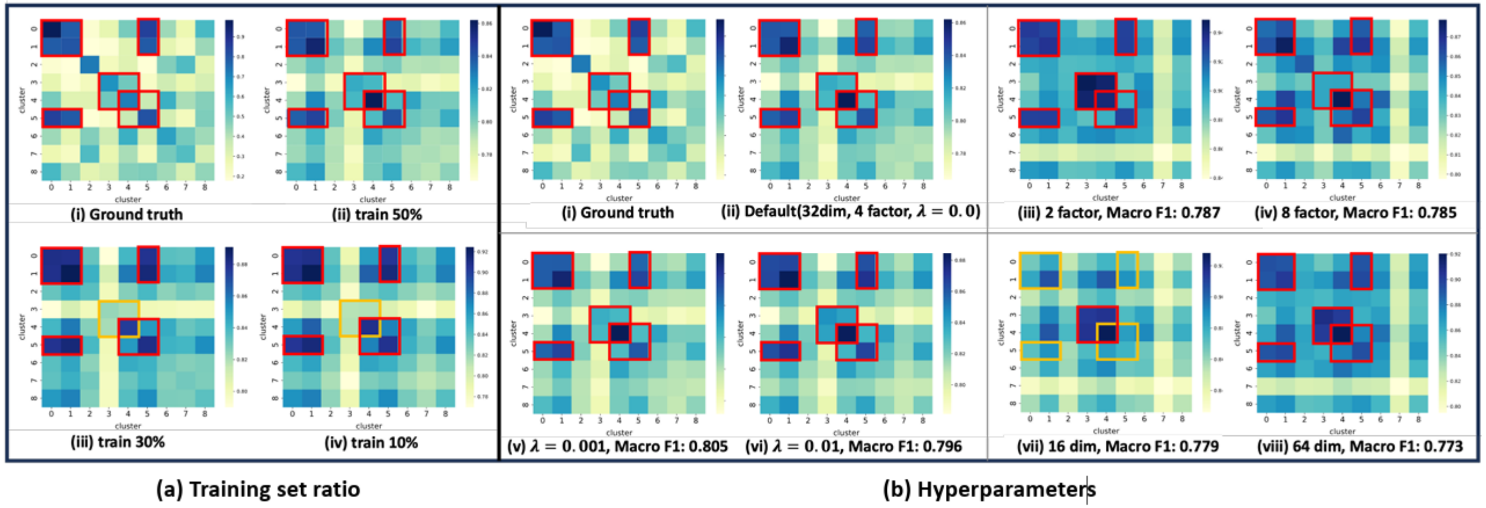


Figure 8: Captured functional context with different (a) Training set ratio and (b) Hyperparameters. Patterns that are well-captured are shown in red and those that are not captured are shown in orange.

CONCLUSION

- Through the lens of category theory, we analyzed hyperedge disentanglement and proposed naturality condition-based criterion for disentanglement
- We experimentally showed that our model (Natural-HNN) with our own criterion could capture functional context of genetic pathways.
- Our model outperforms most of the baselines in cancer subtype classification task by reflecting functional context of genetic pathways.