The background of the slide is a complex, abstract network graph. It features numerous nodes, represented by circles of varying sizes and colors (blue, grey, and white), interconnected by thin, light-colored lines. The overall aesthetic is futuristic and technical, with a color palette dominated by soft blues, greys, and warm oranges. The title text is overlaid on the right side of the image.

G-Mixup: Graph Data Augmentation for Graph Classification

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Presenter: Tanya Djavahepour
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Overview

- Background and Motivation
- Methodology
- Experiments
- Conclusion



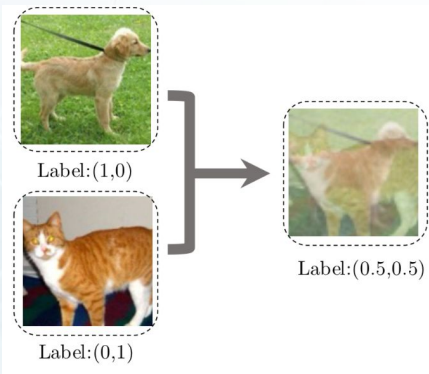
Background and Motivation

The background features a complex network of thin, light-colored lines connecting small, dark nodes. This network is overlaid on a soft, glowing orange sphere that is partially obscured by the network. The overall color palette is a mix of light blues, greys, and warm oranges, creating a futuristic and technological feel.

Mixup

Mixup is a cross-instance data augmentation method, which linearly interpolates random sample pair to generate more synthetic training data.

Mixup have been empirically and theoretically shown to improve the generalization and robustness of deep neural networks.



$$\mathbf{x}_{new} = \lambda \mathbf{x}_i + (1 - \lambda) \mathbf{x}_j,$$

$$\mathbf{y}_{new} = \lambda \mathbf{y}_i + (1 - \lambda) \mathbf{y}_j,$$

Challenges for Graph Mixup

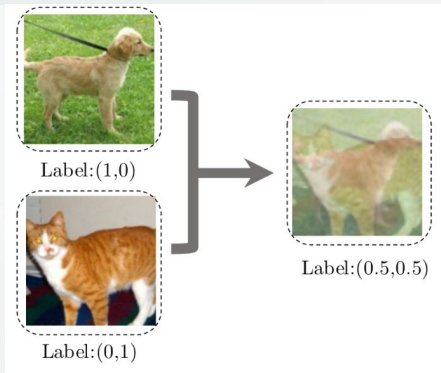
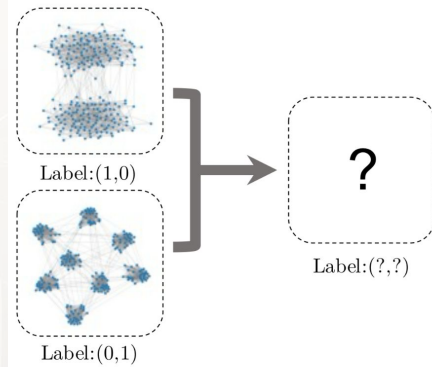


Image data is regular (image can be represented as matrix)

Image data is well-aligned (pixel to pixel correspondence)



Graph data is irregular (the number of nodes)

Graph data is not well-aligned (nodes not naturally ordered)

What are Graphons?

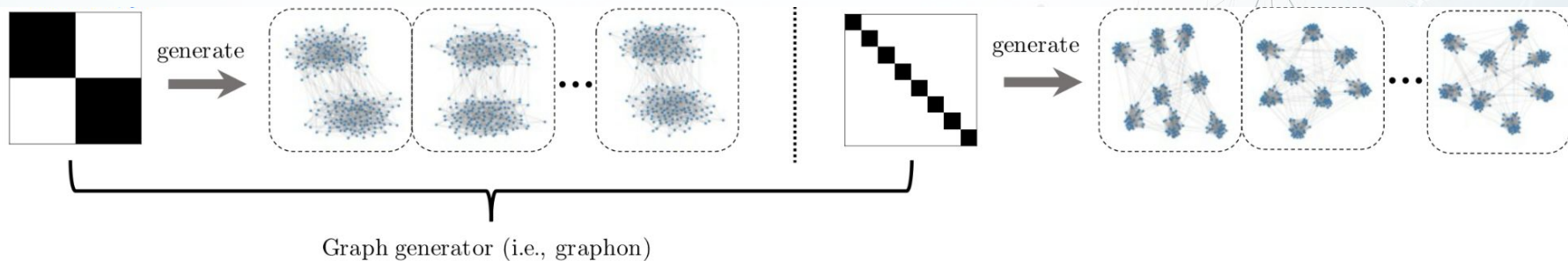
In this study Graphons are used to achieve the input graph mixup.

Graphon serves as a tool in graph theory for approximating large-scale network structures. It works based on the probability of an edge existing between each two nodes.

The graphons of different graphs are regular and well-aligned.

Graph Generator: Graphon

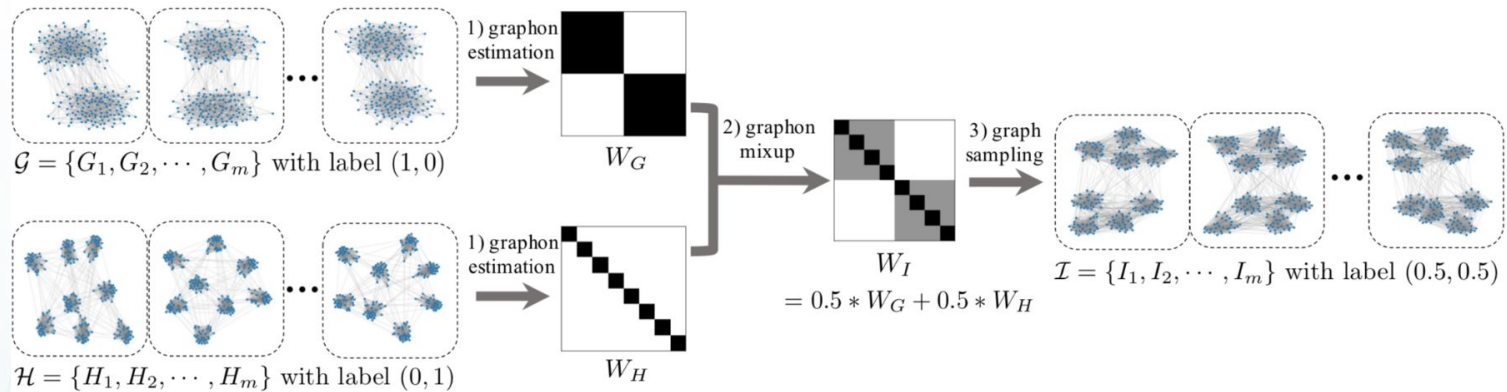
The real-world graphs can be regarded as generated from generator (i.e., graphon). For example,



Methodology

The background features a complex network of thin, light-colored lines connecting small, semi-transparent nodes. The nodes are colored in shades of blue, grey, and orange. The overall color palette transitions from a cool blue on the left to a warm orange on the right, with a bright, hazy light source at the top center. The network structure is dense and interconnected, suggesting a complex system or data flow.

G-Mixup



The formal mathematical expression are as follows:

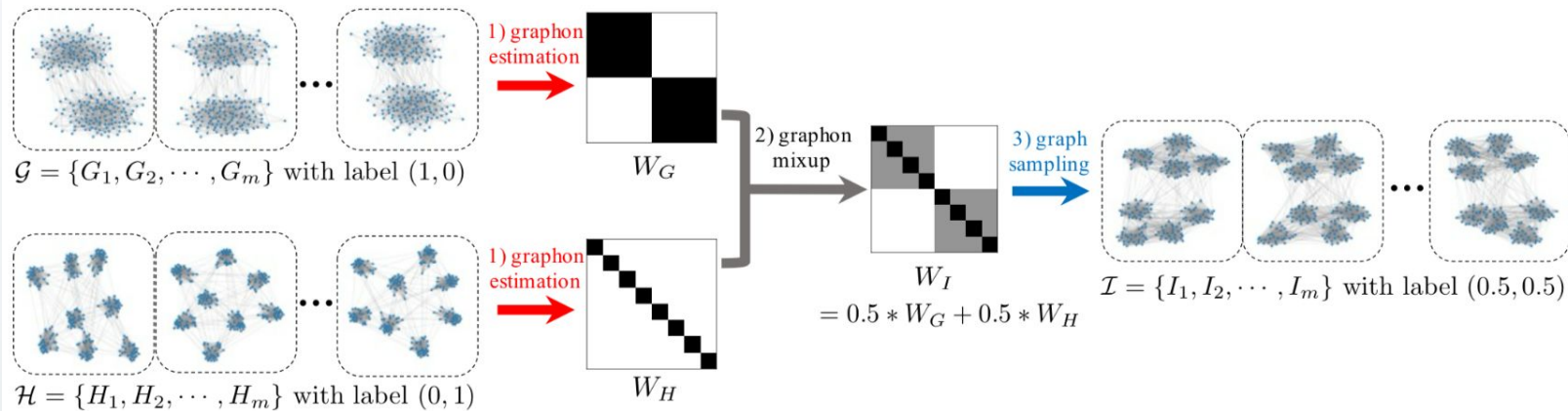
Graphon Estimation: $\mathcal{G} \rightarrow W_G, \mathcal{H} \rightarrow W_H$

Graphon Mixup: $W_I = \lambda W_G + (1 - \lambda) W_H$

Graph Generation: $\{I_1, I_2, \dots, I_m\} \stackrel{\text{i.i.d.}}{\sim} \mathbb{G}(K, W_I)$

Label Mixup: $\mathbf{y}_I = \lambda \mathbf{y}_G + (1 - \lambda) \mathbf{y}_H$

Implementation



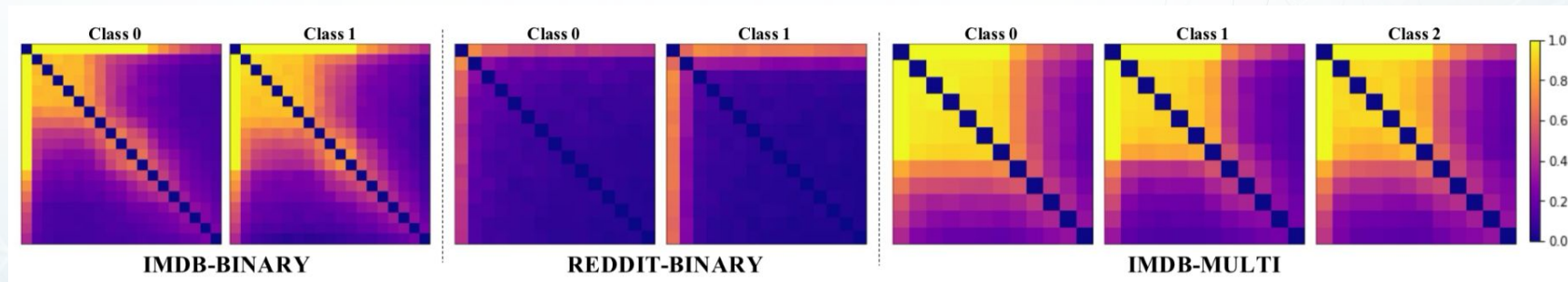
1. Graphon Estimation Using Graphons
2. Synthetic Graphs Generation Using Bernoulli Distributions

Experiments

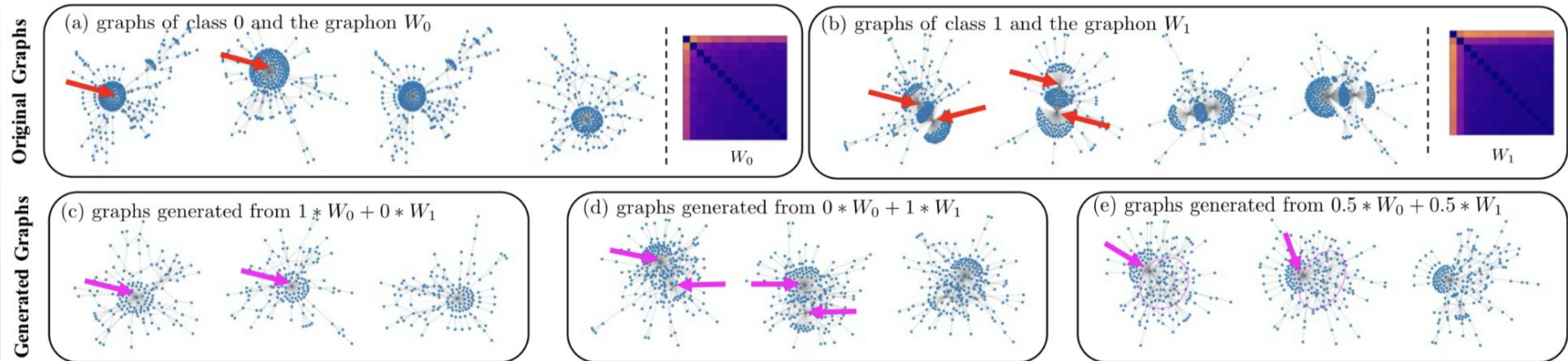
The background features a complex network of thin, light-colored lines connecting small, dark nodes. This network is overlaid on a soft, glowing orange sphere that is partially obscured by the network. The overall color palette is a mix of light blues, greys, and warm oranges, creating a futuristic and scientific atmosphere.

Do different classes of graphs have different graphons?

Visualization the estimated graphons on IMDB-BINARY, REDDIT-BINARY, and IMDB-MULTI:



What is G-Mixup doing? A case study



The class 0 has one high-degree node while class 1 have two (a)(b).

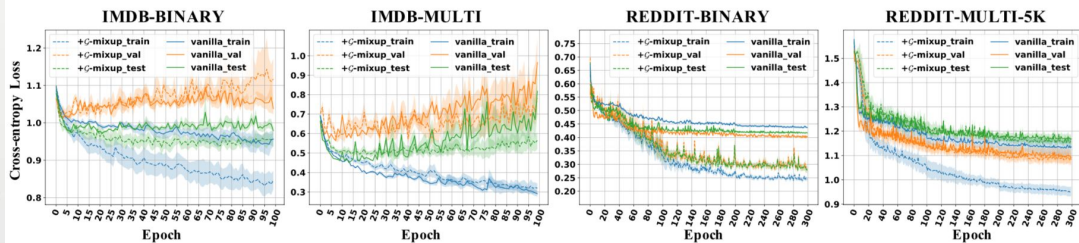
The generated graphs based on

- $(1 * W_0 + 0 * W_1)$ have one high-degree node (c).
- $(0 * W_0 + 1 * W_1)$ have two high-degree nodes (d).
- $(0.5 * W_0 + 0.5 * W_1)$ have a high-degree node and a dense subgraph (e).

Graphs generated by \mathcal{G} -Mixup are the mixture of original graphs.

Can G-Mixup improve the performance of GNNs?

Dataset	IMDB-B	IMDB-M	REDD-B	REDD-M5	REDD-M12	
#graphs	1000	1500	2000	4999	11929	
#classes	2	3	2	5	11	
#avg.nodes	19.77	13.00	429.63	508.52	391.41	
#avg.edges	96.53	65.94	497.75	594.87	456.89	
GCN	vanilla	72.18	48.79	78.82	45.07	46.90
	w/ Dropedge	72.50	49.08	81.25	51.35	47.08
	w/ DropNode	72.00	48.58	79.25	49.35	47.93
	w/ Subgraph	68.50	49.58	74.33	48.70	47.49
	w/ M-Mixup	72.83	49.50	75.75	49.82	46.92
	w/ G-Mixup	72.87	51.30	89.81	51.51	48.06
GIN	vanilla	71.55	48.83	92.59	55.19	50.23
	w/ Dropedge	72.20	48.83	92.00	55.10	49.77
	w/ DropNode	72.16	48.33	90.25	53.26	49.95
	w/ Subgraph	68.50	47.25	90.33	54.60	49.67
	w/ M-Mixup	70.83	49.88	90.75	54.95	49.81
	w/ G-Mixup	71.94	50.46	92.90	55.49	50.50



The loss curves of G-Mixup are lower than the vanilla model.

G-Mixup can improve the generalization of graph neural networks.

Conclusion

The background features a complex network of thin, dark lines connecting various points, resembling a molecular structure or a data network. These points are represented by small, semi-transparent spheres in shades of blue, grey, and orange. The overall aesthetic is futuristic and scientific, with a color gradient transitioning from a cool blue on the left to a warm orange and yellow on the right. Faint, curved lines and scattered glowing particles add to the sense of dynamic movement and connectivity.

Conclusion

G-Mixup Introduction: A new method for graph data augmentation.

Graphon Utilization: Mixing graphons from different classes to generate new graphs.

Improved GNN Performance: Enhanced performance, generalization, and noise robustness.

Innovation in Graph Data Handling: A novel approach to address graph data augmentation challenges.

References

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Zhang, L., Deng, Z., Kawaguchi, K., Ghorbani, A., & Zou, J. (2021). How does mixup help with robustness and generalization? International Conference on Learning Representations.

Thanks for your attention!

The background is a complex, abstract composition. It features a large, semi-transparent globe in the upper right quadrant. Overlaid on and around the globe are numerous thin, light-colored lines that form a network or web-like structure. In the lower half of the image, there are several darker, more prominent lines and dots, some of which are connected by straight lines, suggesting a data visualization or a network diagram. The overall color palette is muted, with shades of beige, light green, and grey, giving it a professional and modern feel.