VS-Graph: Scalable and Efficient Graph Classification Using Hyperdimensional Computing

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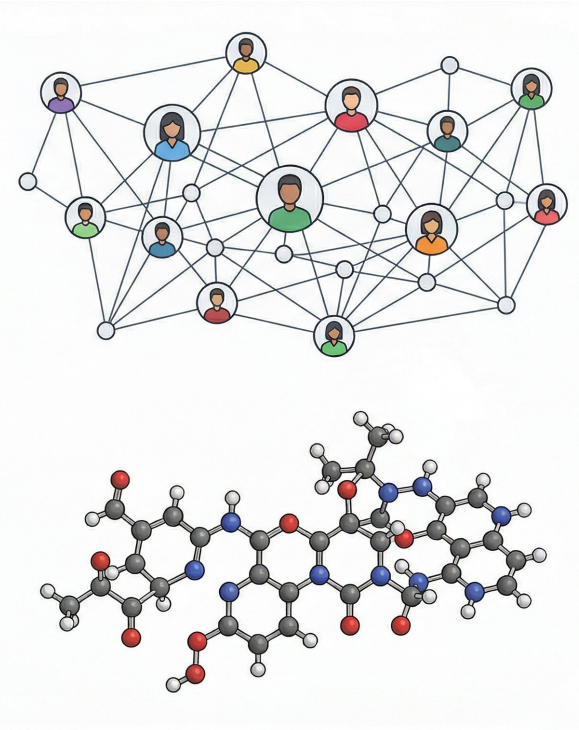
Euclidean vs non-Euclidean Data

Euclidean

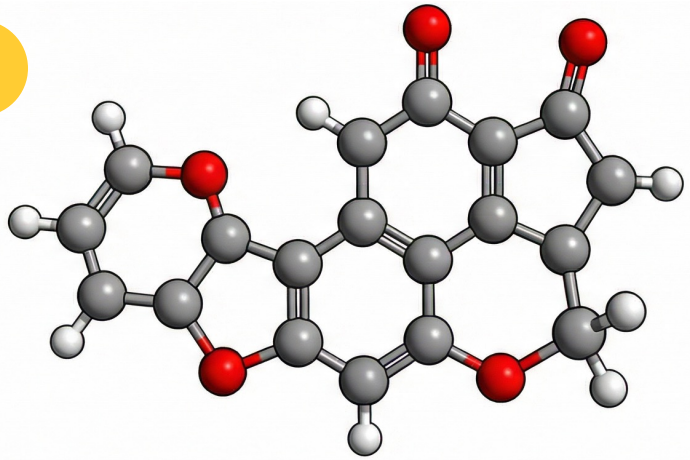
Non-Euclidean



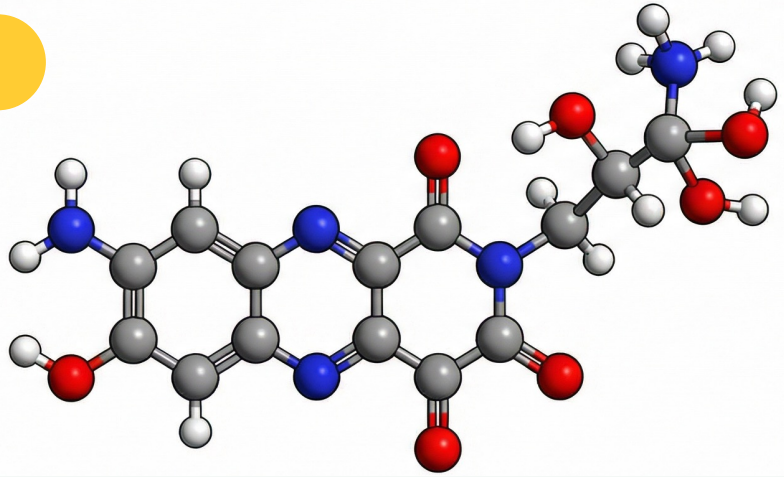
Nature Doesn't Always Live on a Grid!

Graph Classification

Aflatoxin B1



Riboflavin



Drug Discovery

Protein Function

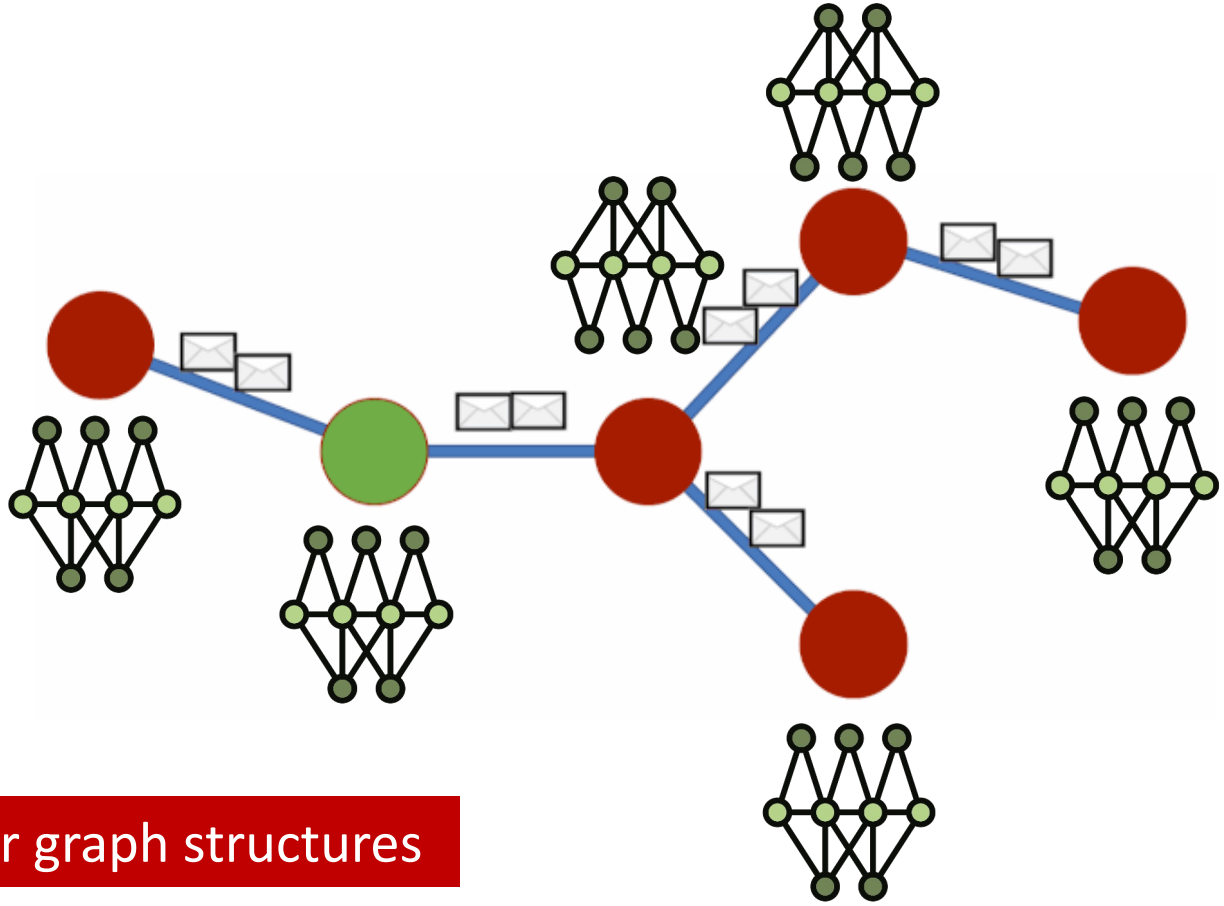
Recommendation Systems

Social Networks

Fraud Detection

Graph Neural Networks (GNN)

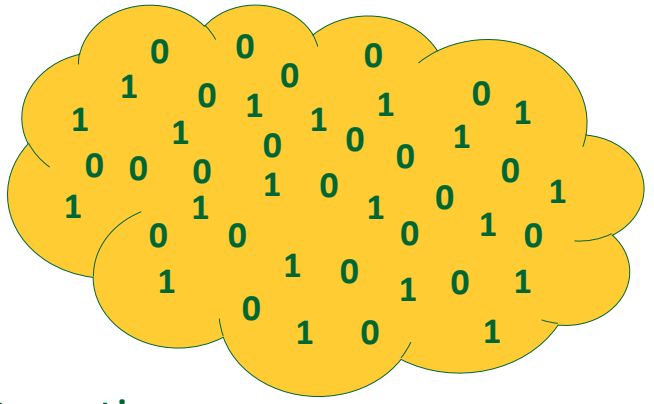
- Message Passing
- Neighborhood Aggregation
- Neural Network Transformation
- Multi-Layer Depth



Backpropagation over sparse and irregular graph structures

Not ideal for deployment on resource-constrained devices

Hyperdimensional Computing (Vector Symbolic Architectures)



- **High-Dimensional Representation**
  - **Atomic basis** → Randomly Generated Hypervectors → Psudo Orthogonal
  - Simple Algebraic Operations:
    - **Bundling** → Combines multiple vectors → Element-wise addition/majority voting
    - **Binding** → Associates two vectors → Element-wise XOR/multiplication
    - **Permutation** → Encodes order or structure → Cyclic shifting of elements
- **Prototype Formation:** Accumulate hypervectors of each class → one prototype per class
- **Similarity-Based Inference**: Encode input → compare with prototypes → choose most similar

GNN vs HDC

GNN

Accuracy

Efficiency

HDC

Accuracy

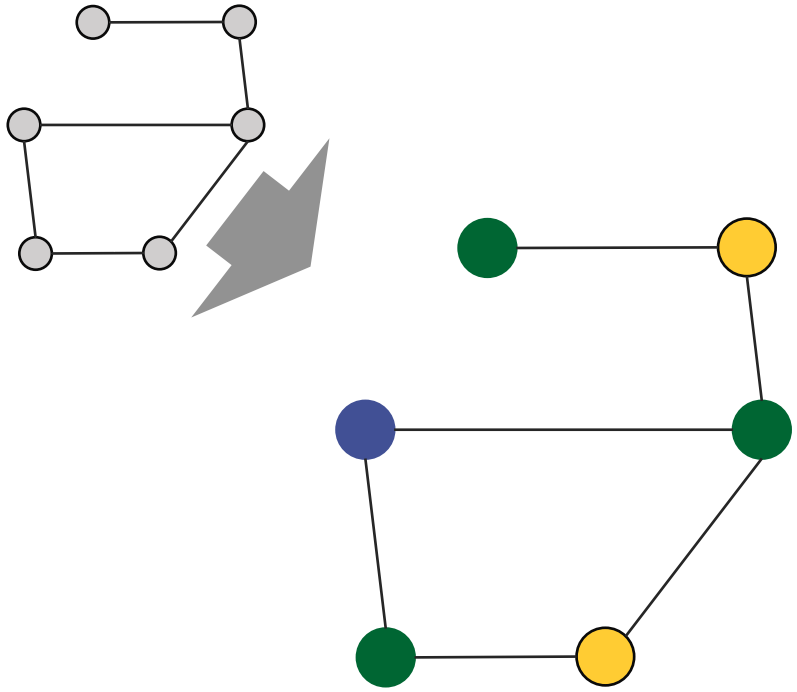
Efficiency

VS-Graph

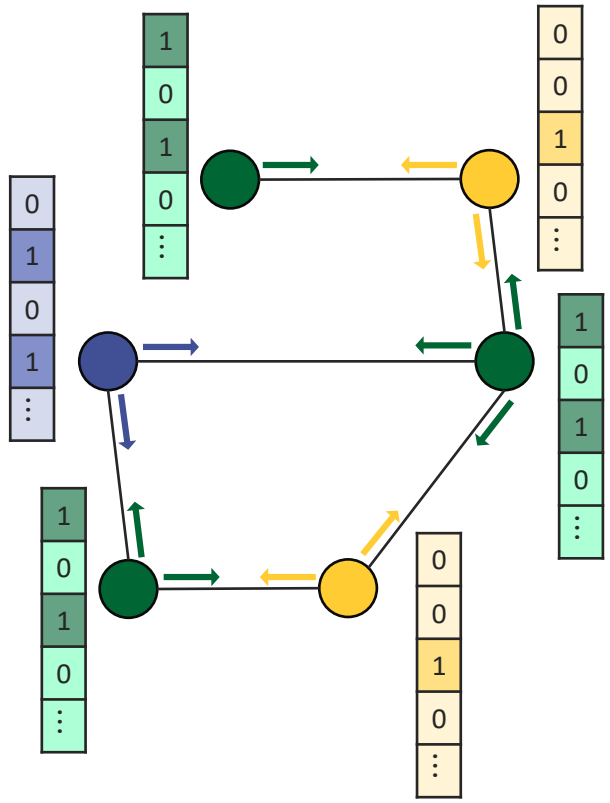
Vector Symbolic Graph Learning

VS-Graph Overview

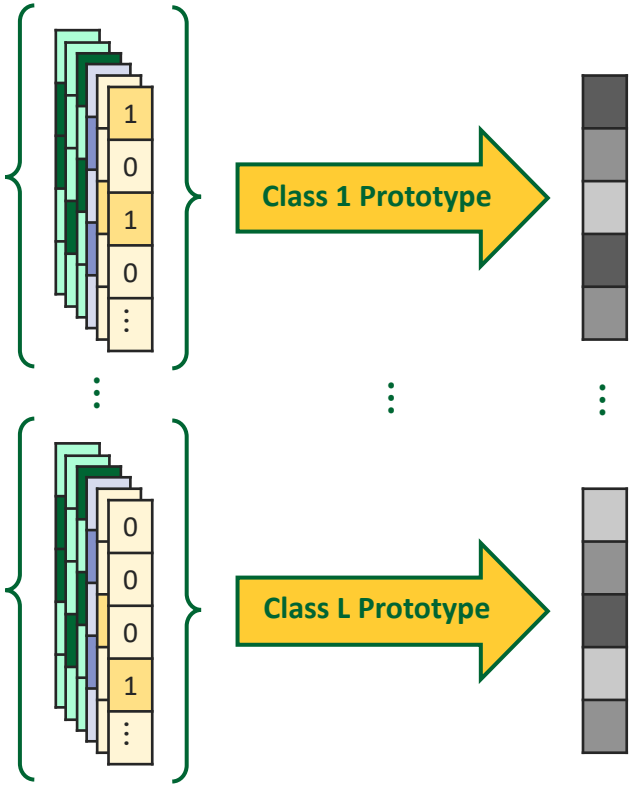
Spike-Diffusion
Node Identification



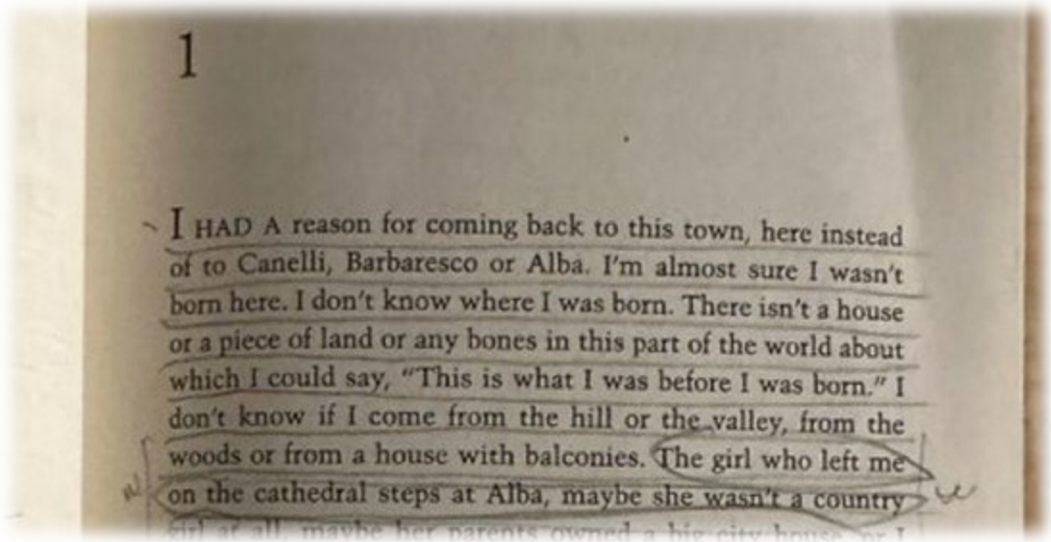
Vector Symbolic Encoding and
Associative Message Passing



Graph-level Readout and
Prototype Classification



Node Identification



1

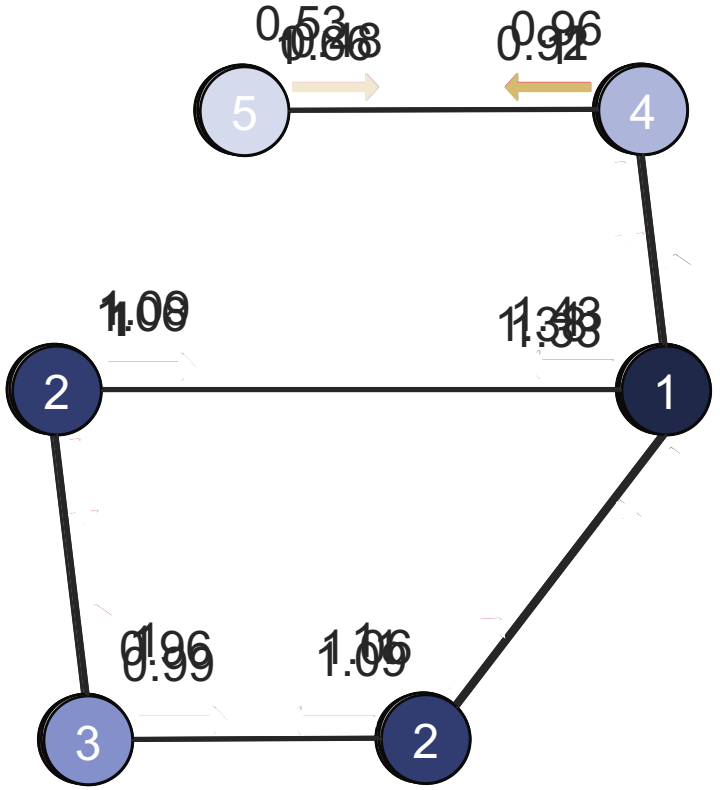
I HAD A reason for coming back to this town, here instead of to Canelli, Barbaresco or Alba. I'm almost sure I wasn't born here. I don't know where I was born. There isn't a house or a piece of land or any bones in this part of the world about which I could say, "This is what I was before I was born." I don't know if I come from the hill or the valley, from the woods or from a house with balconies. The girl who left me on the cathedral steps at Alba, maybe she wasn't a country

What is the first word?

Which one is the first node?

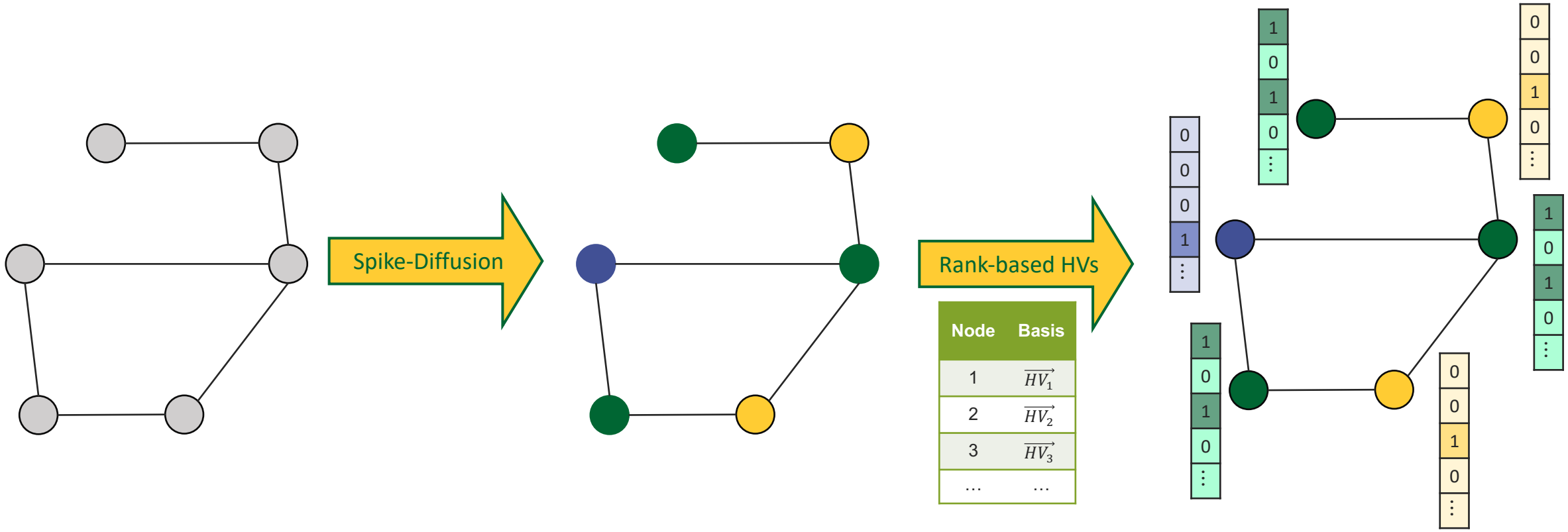
We need a way to consistently identify nodes across different graphs

Spike-Diffusion

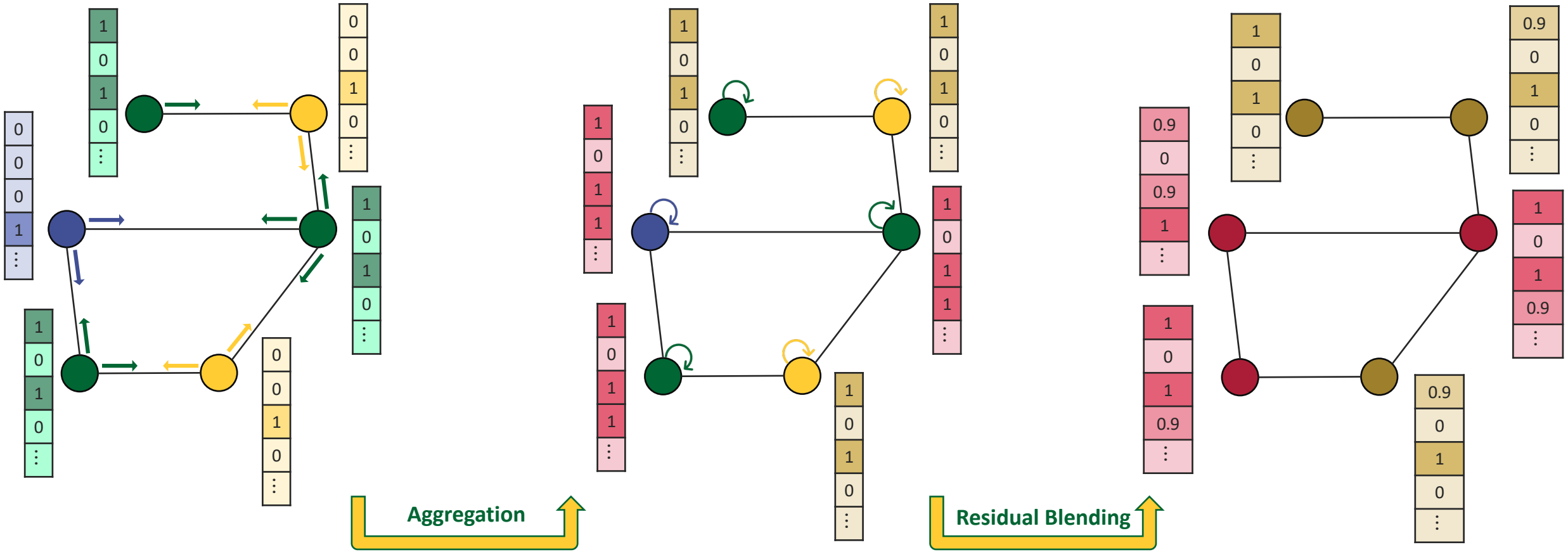


Identifier Assignment

Vector Symbolic Encoding



Associative Message Passing

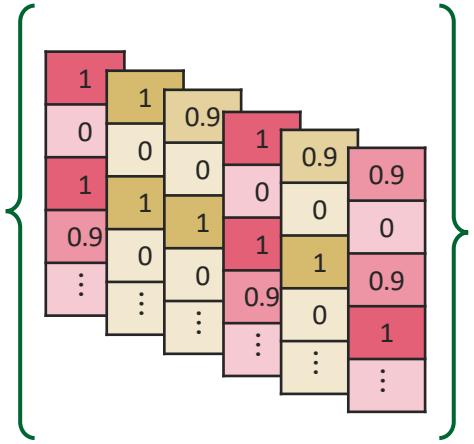


$$m_i^{(l)} = \bigvee_{j \in \mathcal{N}(i)} h_j^{(l)}$$

$$h_i^{(l+1)} = \alpha h_i^{(l)} + (1-\alpha) m_i^{(l)}$$

Graph-level Readout and Prototype Classification

Training



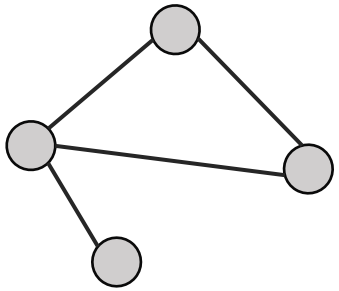
Average and Normalize

Graph HV

Bundle All Graph HVs

Class Prototype

Inference



Spike Diffusion Identification
Vector Symbolic Encoding
Associative Message Passing
Graph-level Readout

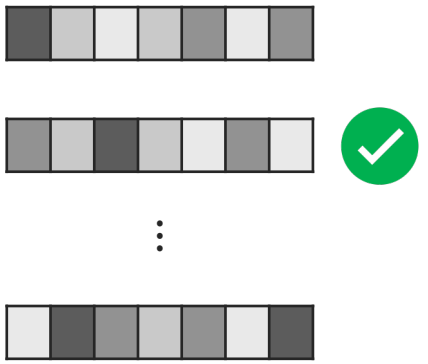
Graph HV

Similarity Check

Similarity Check

Similarity Check

Class Prototypes



Experimental Setup

Datasets

Dataset	Graphs	Classes	Avg. vertices	Avg. edges
MUTAG	188	2	17.93	19.79
PTC_FM	349	2	14.11	14.48
PROTEINS	1113	2	39.06	72.82
DD	1178	2	**284.32**	**715.66**
NCI1	**4110**	2	29.87	32.30

Baselines

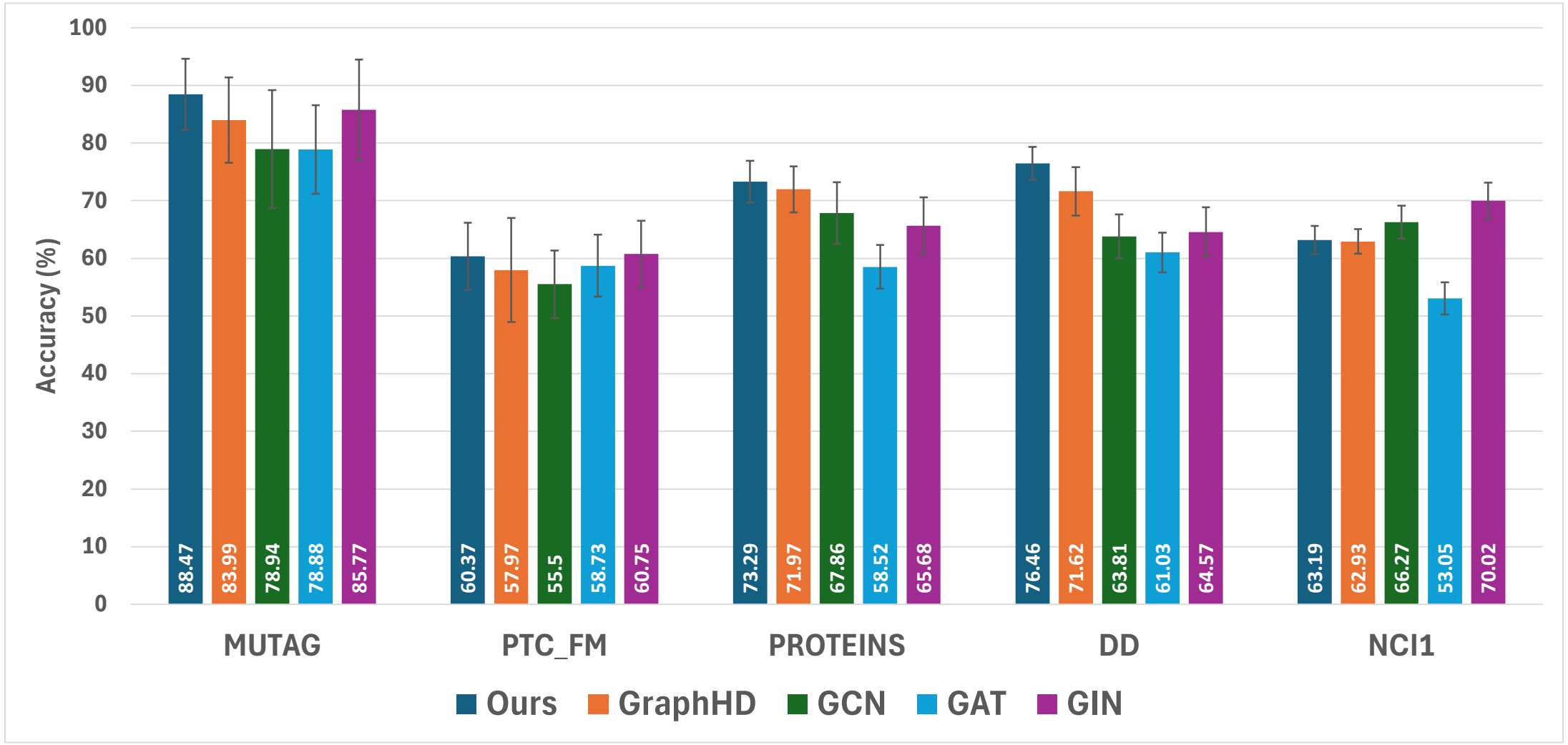
GNN

GCN
GAT
GIN

HDC

GraphHD

Results


100
90
80
70
60
50
40
30
20
10
0
Accuracy (%)
88.47
83.99
78.94
78.88
85.77
60.37
57.97
55.5
58.73
60.75
73.29
71.97
67.86
58.52
65.68
76.46
71.62
63.81
61.03
64.57
63.19
62.93
66.27
53.05
70.02
MUTAG
PTC_FM
PROTEINS
DD
NCI1
Ours
GraphHD
GCN
GAT
GIN

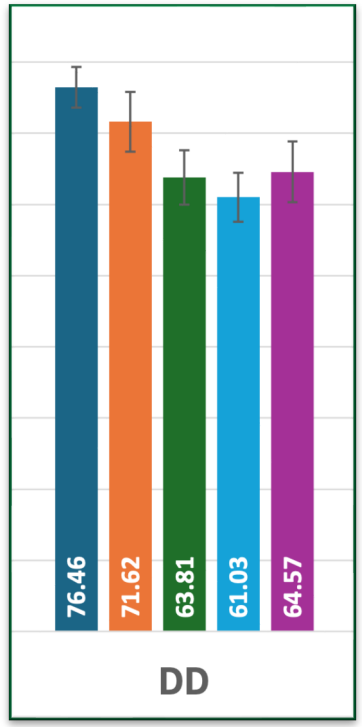
Results

Training Time Per Graph (ms)

	Ours	GraphHD	GCN	GAT	GIN
MUTAG	0.142	0.801	61.21	41.77	47.20
PTC_FM	0.153	0.929	36.71	33.93	37.39
PROTEINS	0.230	0.904	37.76	27.47	49.24
DD	2.120	1.892	41.36	28.85	72.92
NCI1	**0.192**	**0.768**	**56.40**	**20.40**	**85.84**

Inference Latency Per Graph (ms)

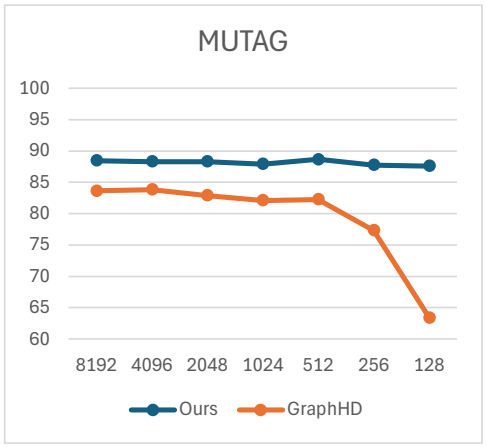
	Ours	GraphHD	GCN	GAT	GIN
MUTAG	0.366	0.980	0.948	0.727	0.641
PTC_FM	**0.368**	**1.143**	**0.572**	**0.492**	**0.552**
PROTEINS	0.418	1.050	0.281	0.368	0.405
DD	2.288	2.028	0.332	0.431	0.521
NCI1	0.328	0.923	0.286	0.394	0.374

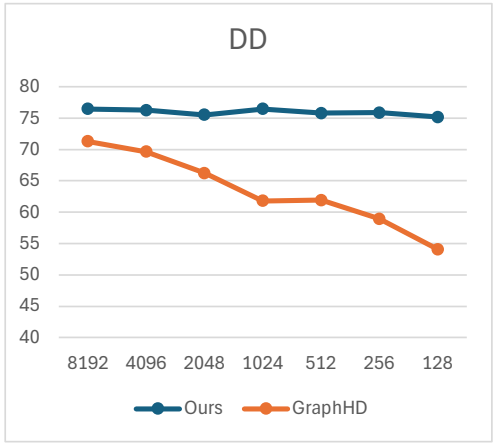


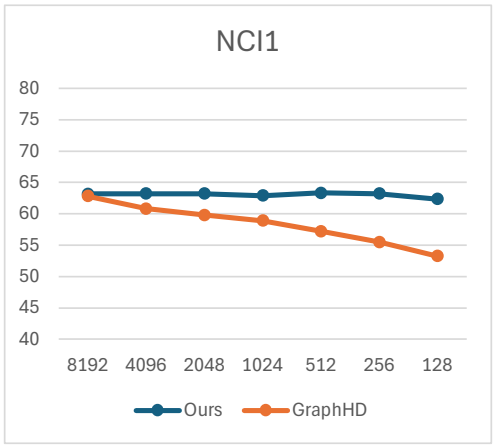
	Avg. vertices	Avg. edges
DD	**284.32**	**715.66**

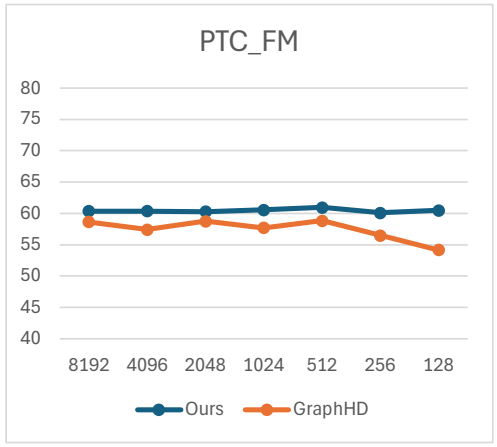
Results

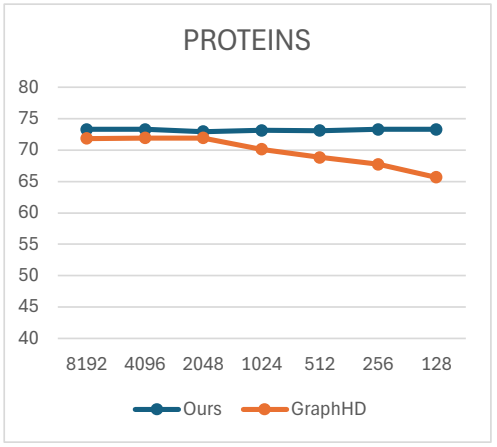
Accuracy vs Dimensionality





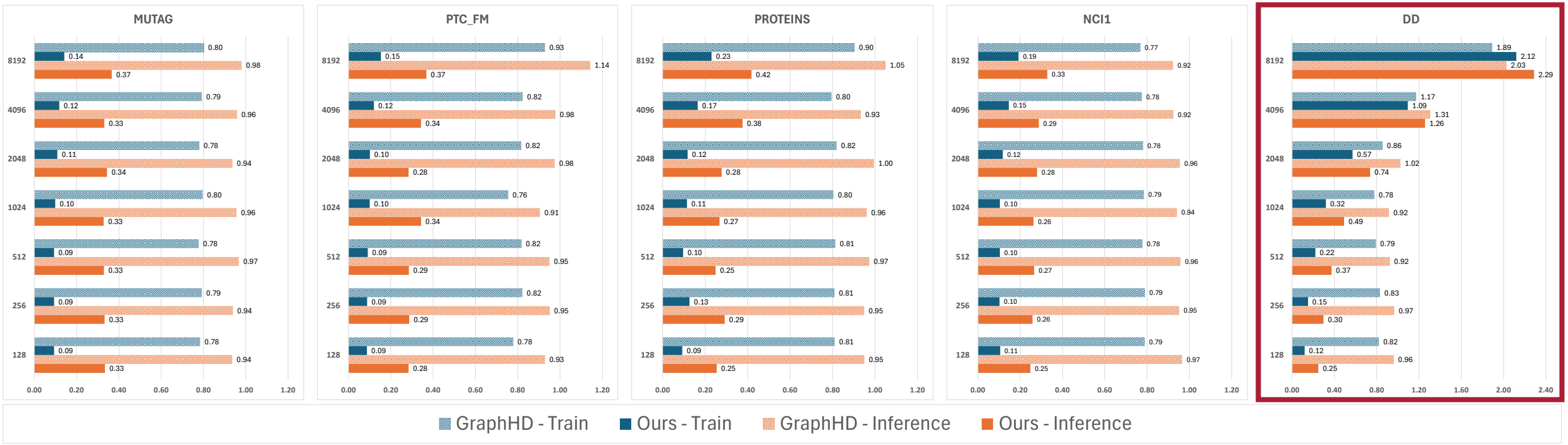




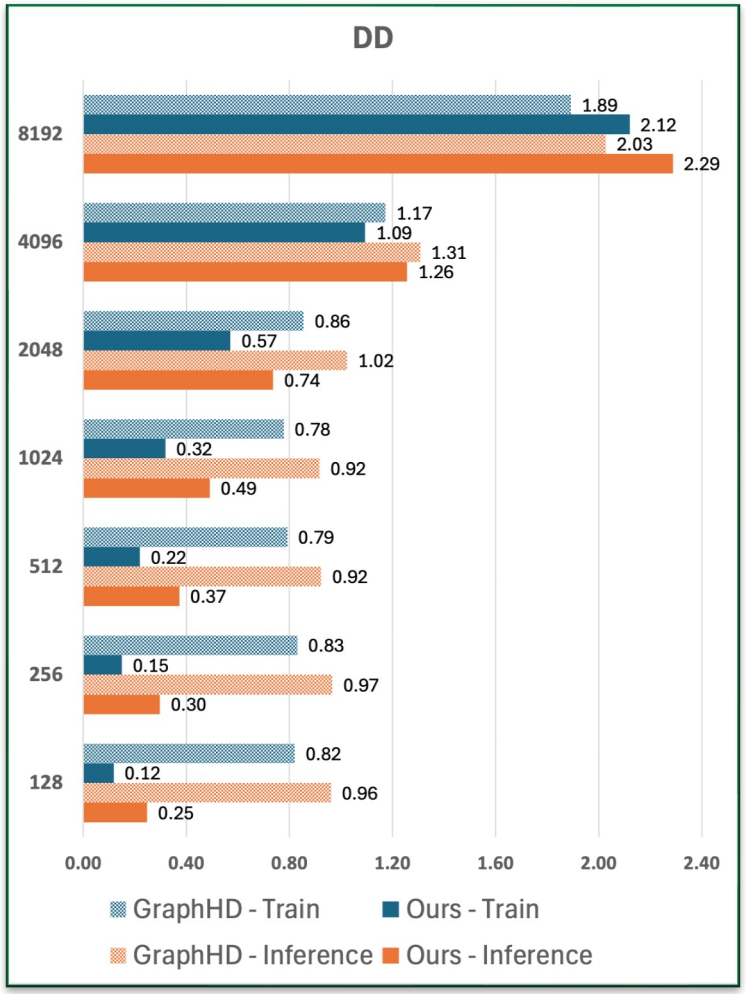


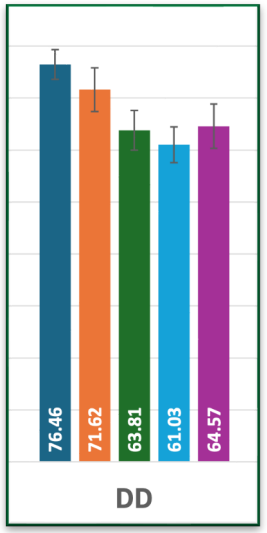
Results

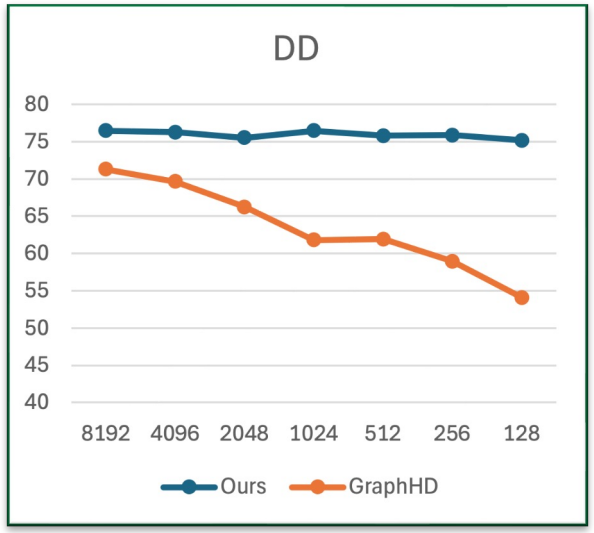
Latency vs Dimensionality



Results







		Ours	GraphHD	GCN	GAT	GIN
8192	Accuracy	**76.46**	71.62	63.81	61.03	64.57
	Training Time	2.120	**1.892**	41.36	28.85	72.92
	Inference Latency	2.288	2.028	**0.332**	0.431	0.521
128	Accuracy	**75.18**	53.65	63.81	61.03	64.57
	Training Time	**0.118**	0.820	41.36	28.85	72.92
	Inference Latency	**0.248**	0.961	0.332	0.431	0.521

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