GraphNorm:

A Principled Approach to Accelerating Graph Neural Network Training

ICML 2021

Tianle Cai*, Shengjie Luo*, Keyulu Xu, Di He, Tie-Yan Liu, Liwei Wang

PRINCETON UNIVERSITY

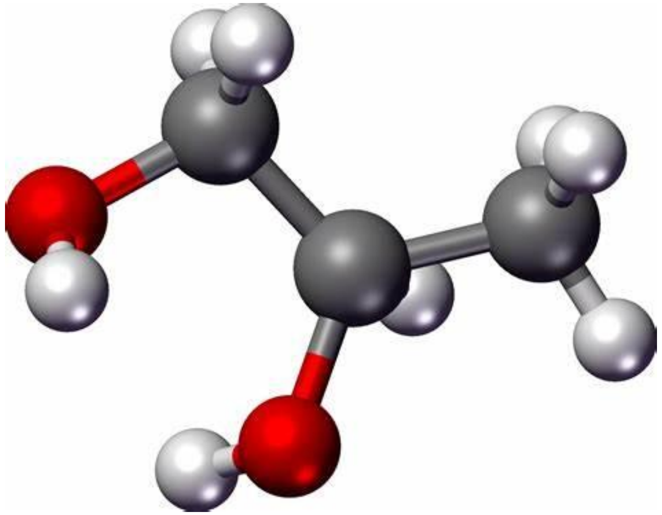
北京大學 PEKING UNIVERSITY

Massachusetts Institute of Technology

中关村 | 海华 | 信息技术前沿研究院
Haihua Institute For Frontier Information Technology

Microsoft

Learning with graph – a general form of data

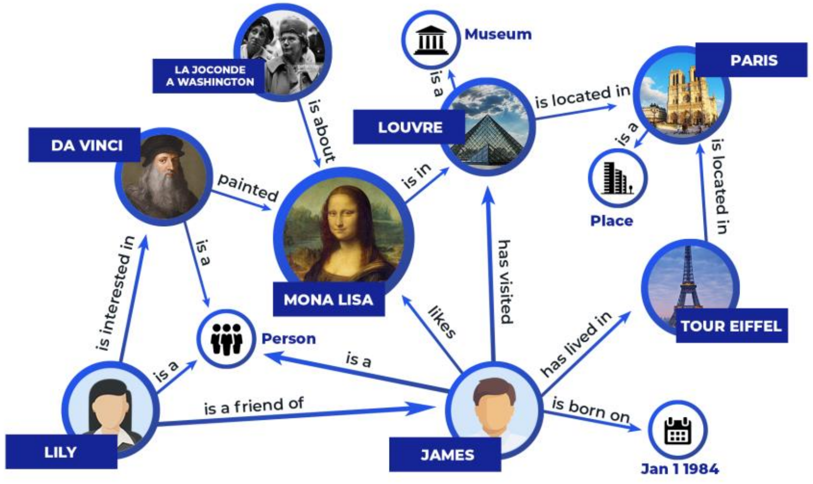


Drug Discovery

(phys.org)

Social Networks

(acwits)



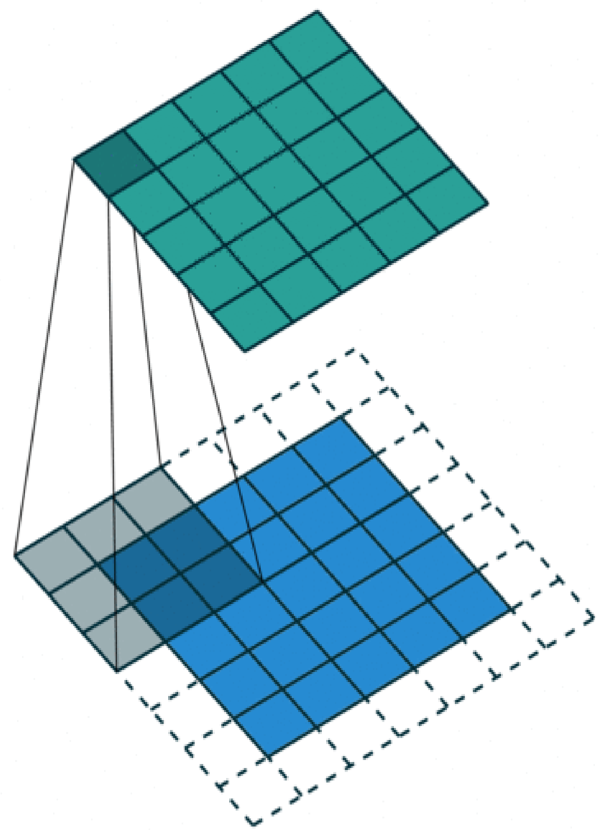
Knowledge Graph

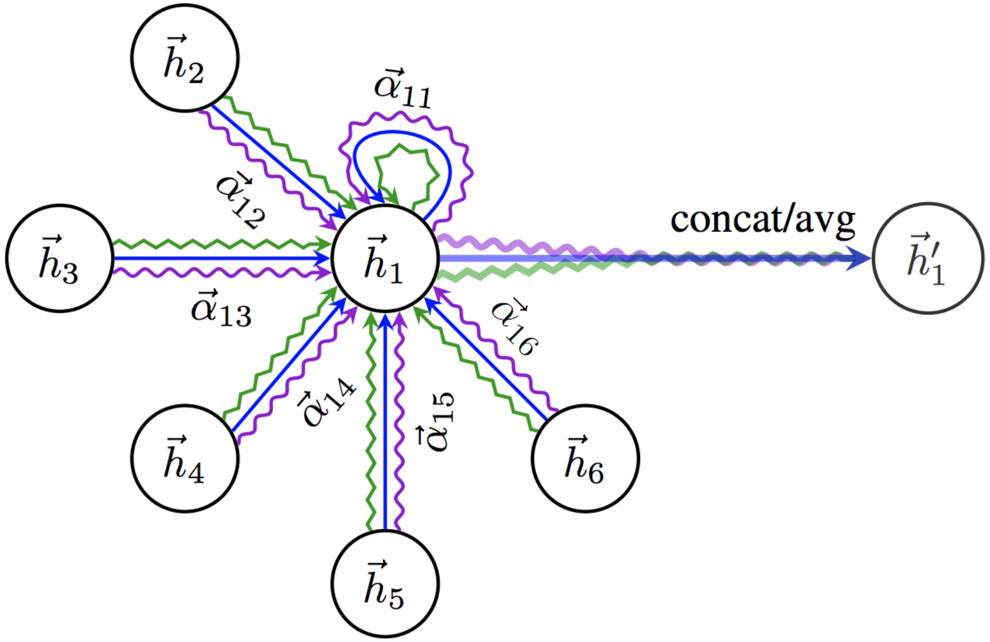
(yashuseth.blog)

Graph Neural Networks

Neighborhood Aggregation a.k.a. Message Passing or Graph Convolution

Aggregate neighbor features with permutation invariance functions





Graph Neural Networks

Neighborhood Aggregation

$$h_i^{(k)} = AGGREGATE^{(k)}\left(h_i^{(k-1)}, \left\{h_j^{(k-1)} : v_j \in \mathcal{N}(v_i)\right\}\right)$$

Feature of node v_j in layer k-1.

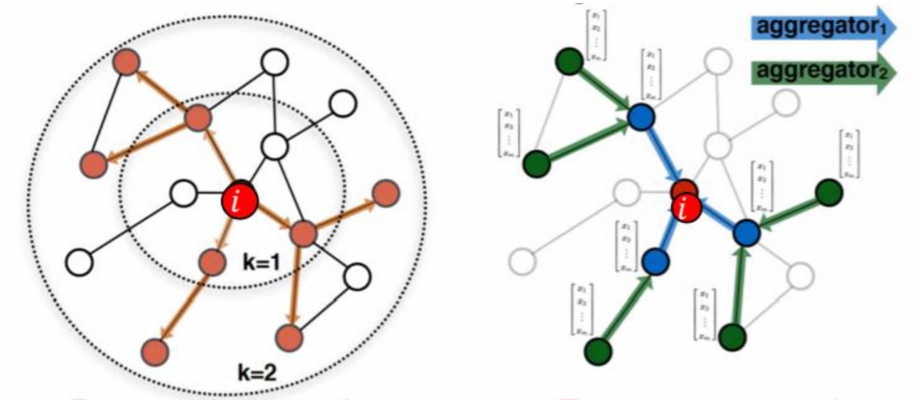
Example -- GIN

$$h_i^{(k)} = MLP^{(k)}\left(\left(1+\epsilon^{(k)}\right)\cdot h_i^{(k-1)} + \sum_{j\in\mathcal{N}(v_i)} h_j^{(k-1)}\right)$$

$\epsilon^{(k)}$ is a learnable parameter

Readout Function

$$h_G = READOUT(\{h_i^{(K)} | v_i \in V\})$$

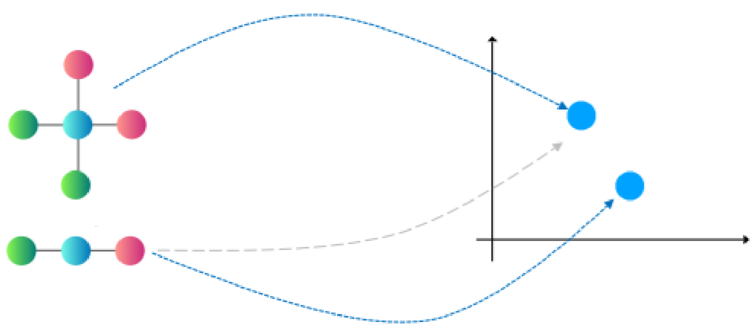


Determine node computation graph

Propagate and transform information

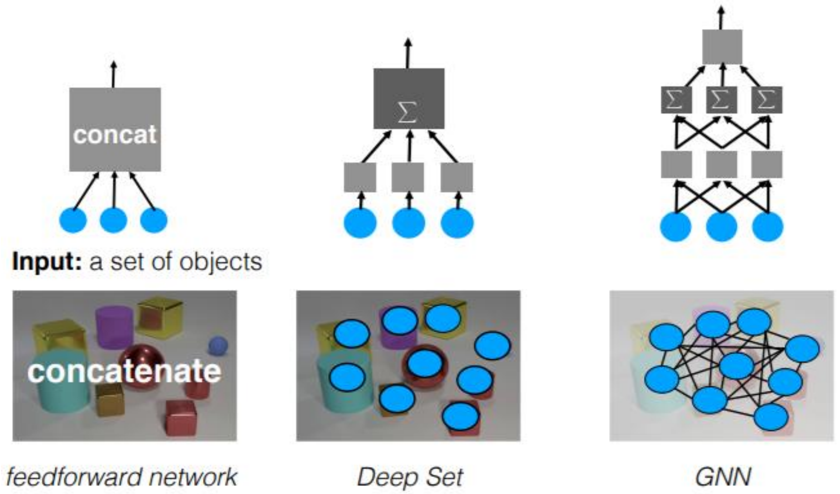
Investigations on Graph Neural Network

Expressive Power



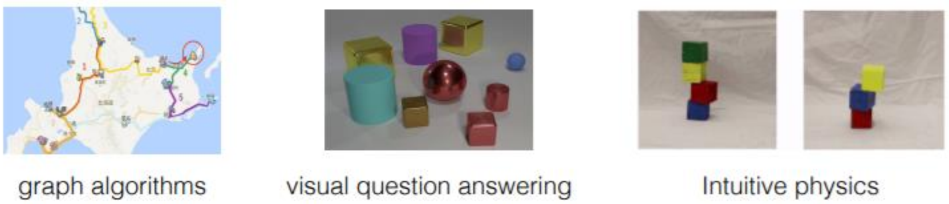
Which graphs can a GNN distinguish?

Generalization

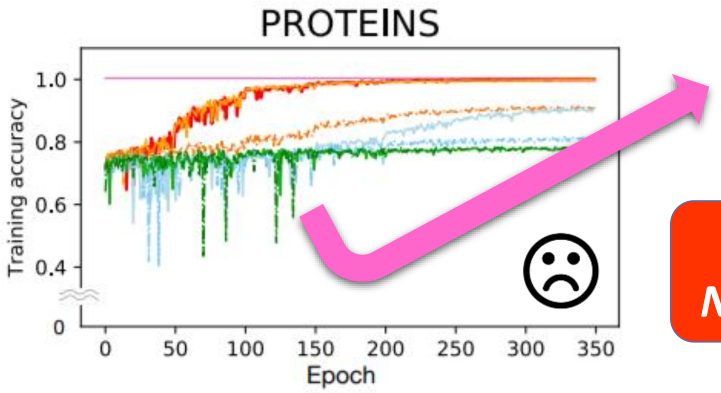


Reasoning

Reasoning tasks as dynamic programming (DP):



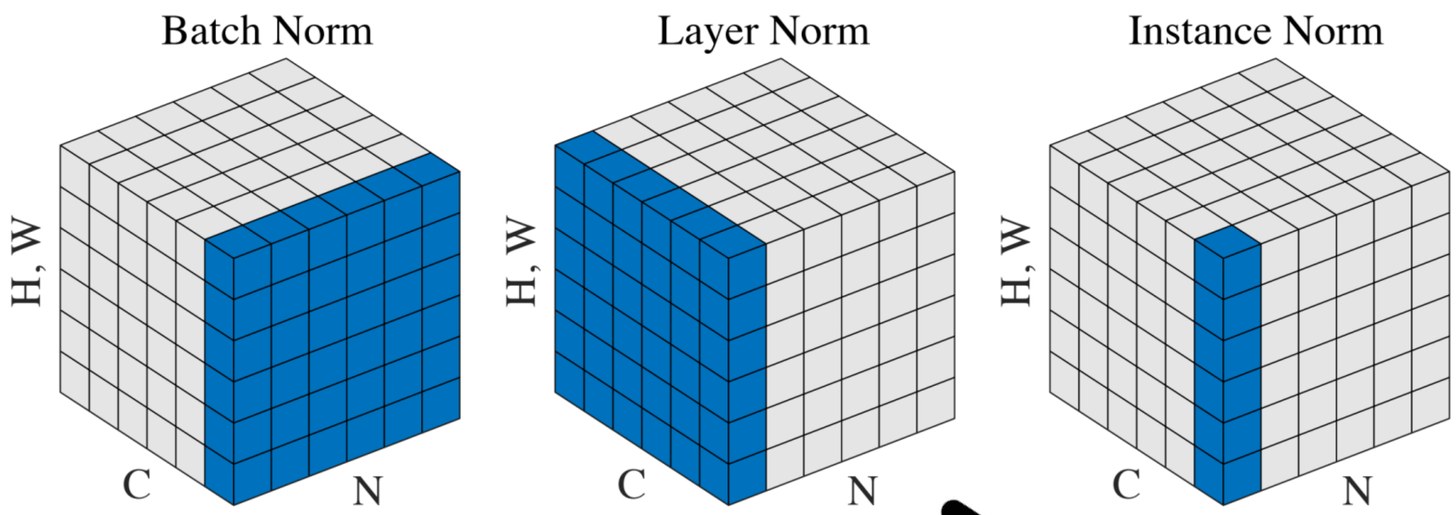
Optimization?

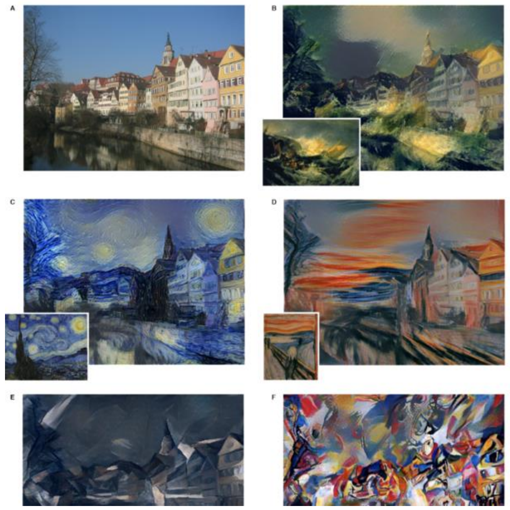


- Training instability
- Slow convergence

Even with Normalization methods.

Normalization for Neural Networks





Style Transfer

IMAGENET

Image Classification

NLP Tasks

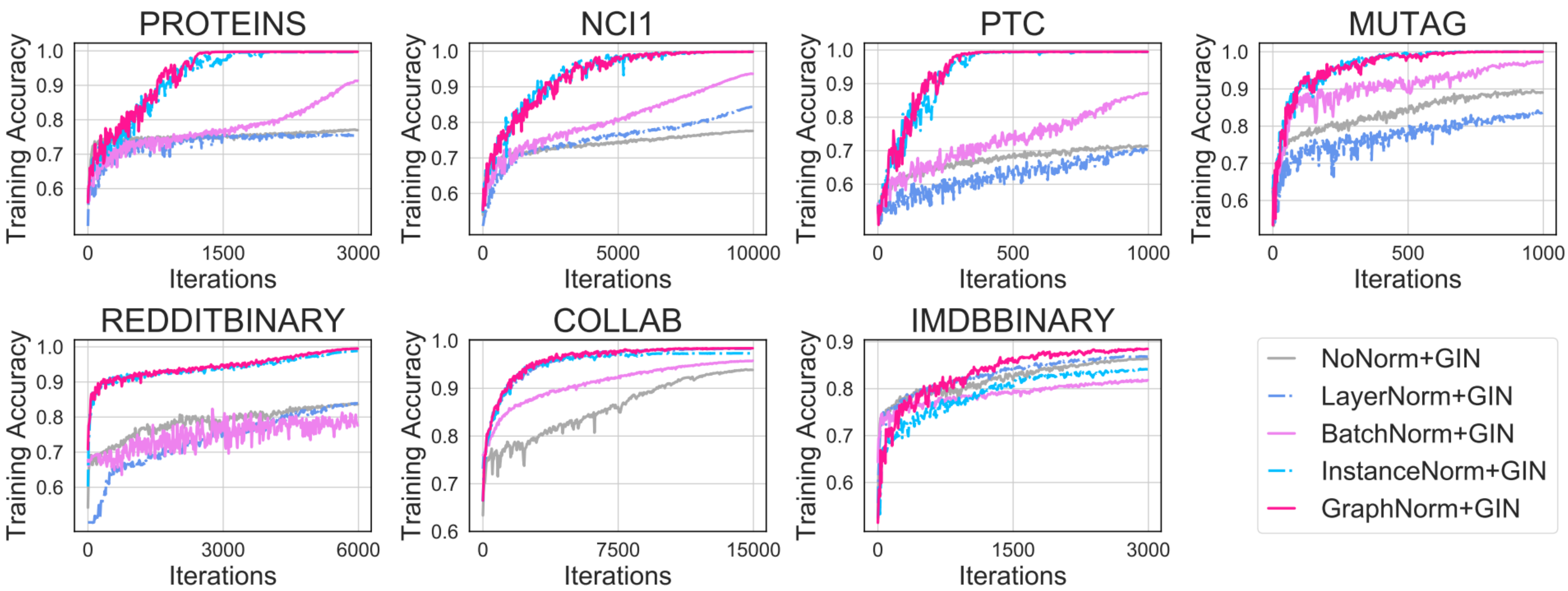
For GNNs, BN and LN are simply adopted without further investigations.

What normalization methods are effective for Graph Neural Networks?

This paper

- Adapting and evaluating existing normalization methods to GNNs.
- Explaining the effectiveness of InstanceNorm over BatchNorm.
- Identifying an expressiveness degradation of InstanceNorm.
- Proposing GraphNorm which addresses the issue and converges faster.

Evaluation of existing normalization methods



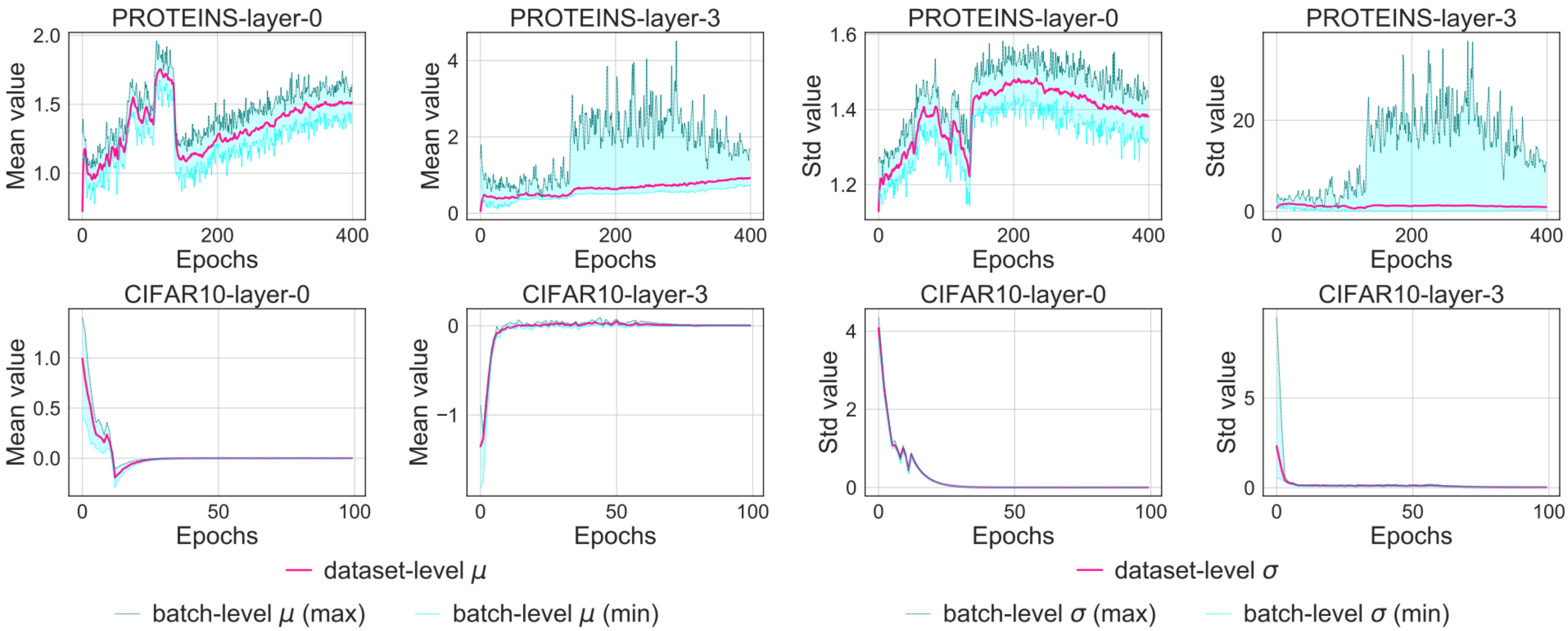
Preconditioning effect of InstanceNorm

Theorem 3.1 (Shift Serves as a Preconditioner of Q). *Let Q, N be defined as in Eq. (6), $0 \leq \lambda_1 \leq \cdots \leq \lambda_n$ be the singular values of Q. We have $\mu_n = 0$ is one of the singular values of QN, and let other singular values of QN be $0 \leq \mu_1 \leq \mu_2 \leq \cdots \leq \mu_{n-1}$. Then we have*

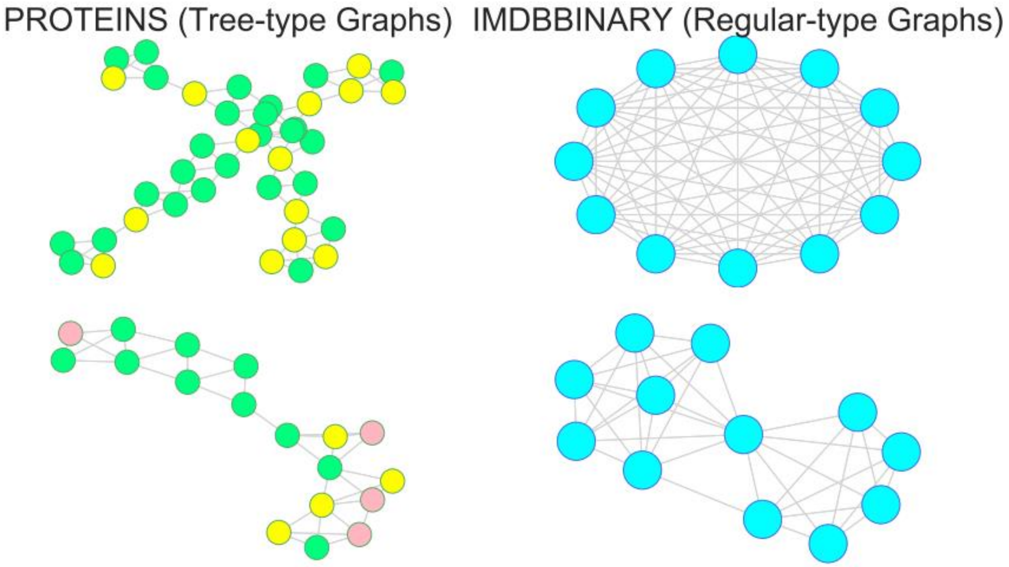
$$\lambda_1 \leq \mu_1 \leq \lambda_2 \leq \cdots \leq \lambda_{n-1} \leq \mu_{n-1} \leq \lambda_n, \tag{7}$$

where $\lambda_i = \mu_i$ or $\lambda_i = \mu_{i-1}$ only if there exists one of the right singular vectors α_i of Q associated with λ_i satisfying $\mathbf{1}^\top \alpha_i = 0$.

Heavy batch noise in graphs



Expressiveness degradation of InstanceNorm



Proposition 4.1. *For a r-regular graph with one-hot encodings as its features described above, we have for GIN,* $\text{Norm}\left(W^{(1)}H^{(0)}Q_{\text{GIN}}\right) = S\left(W^{(1)}H^{(0)}Q_{\text{GIN}}\right)N = 0$, *i.e., the output of normalization layer is a zero matrix without any information of the graph structure.*

Proposition 4.2. *For a complete graph ($r = n - 1$), we have for GIN, $Q_{\text{GIN}}N = \xi^{(k)}N$, i.e., graph structural information in Q will be removed after multiplying N.*

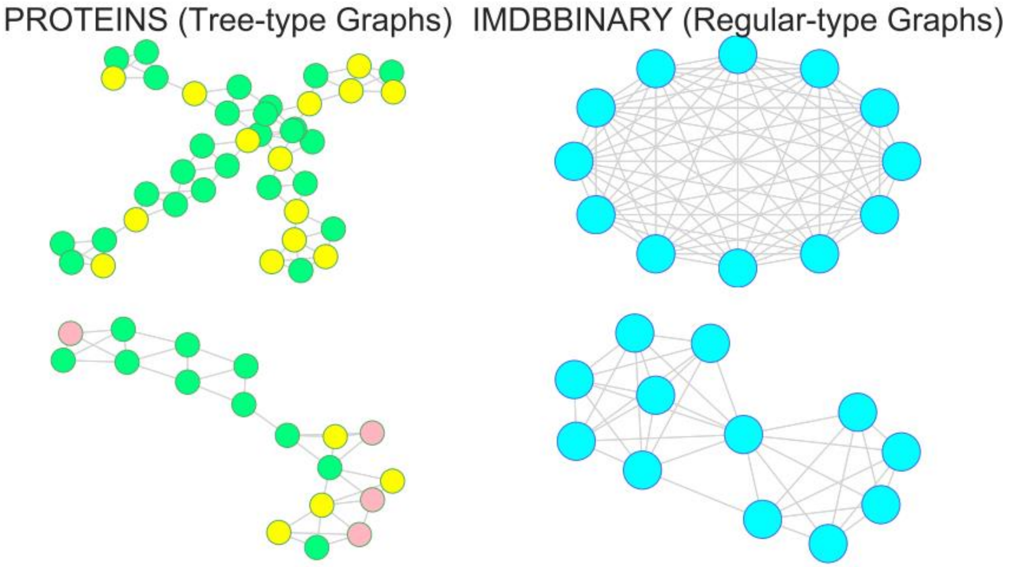
Proposed method: **GraphNorm**

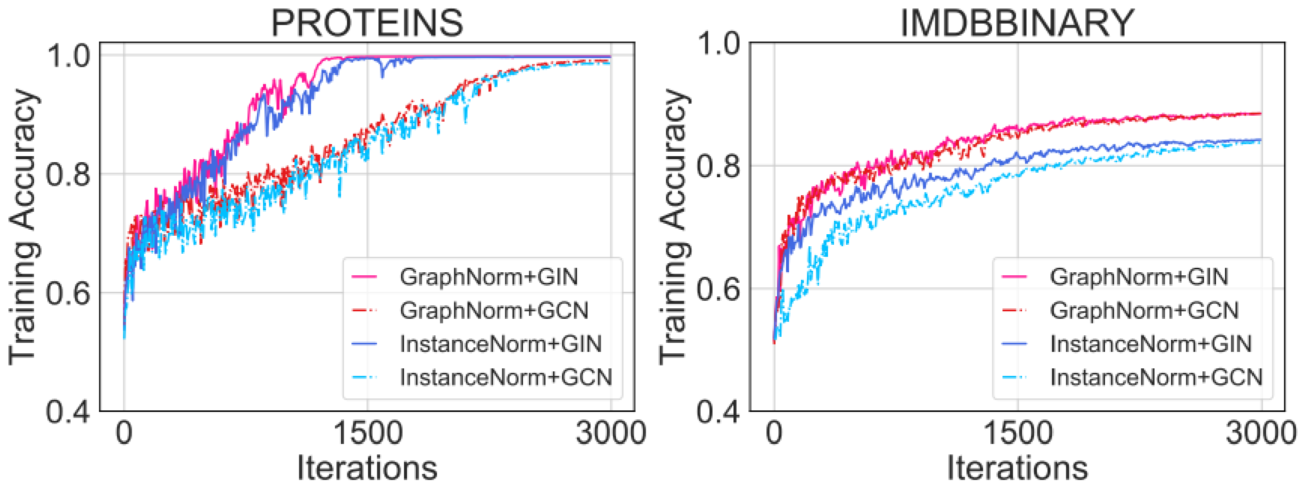
Key: learnable parameter to control how much information we need to keep in the mean

$$\mathrm{GraphNorm}\left(\hat{h}_{i,j}\right) = \gamma_j \cdot \frac{\hat{h}_{i,j} - \boxed{\alpha_j} \cdot \mu_j}{\hat{\sigma}_j} + \beta_j,$$

- Inheriting the merit of InstanceNorm
- Solving the expressiveness degradation problem

GraphNorm addresses the issue of InstanceNorm





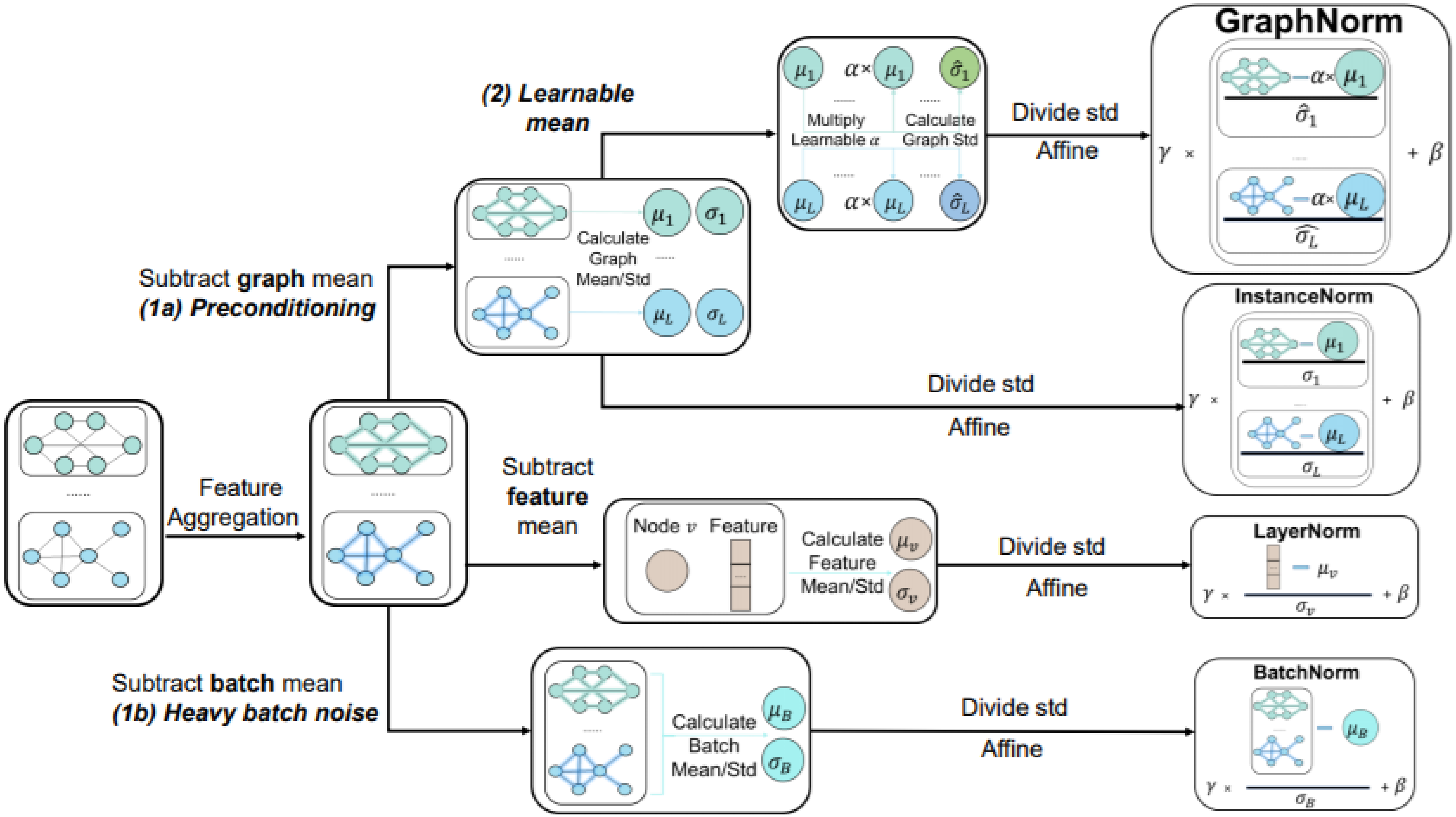
GraphNorm achieves good performance

Datasets	MUTAG	PTC	PROTEINS	NCI1	IMDB-B	RDT-B	COLLAB
# graphs	188	344	1113	4110	1000	2000	5000
# classes	2	2	2	2	2	2	2
Avg # nodes	17.9	25.5	39.1	29.8	19.8	429.6	74.5
WL SUBTREE (SHERVASHIDZE ET AL., 2011)	90.4 ± 5.7	59.9 ± 4.3	75.0 ± 3.1	**86.0 ± 1.8**	73.8 ± 3.9	81.0 ± 3.1	78.9 ± 1.9
DCNN (ATWOOD & TOWSLEY, 2016)	67.0	56.6	61.3	62.6	49.1	-	52.1
DGCNN (ZHANG ET AL., 2018)	85.8	58.6	75.5	74.4	70.0	-	73.7
AWL (IVANOV & BURNAEV, 2018)	87.9 ± 9.8	-	-	-	74.5 ± 5.9	87.9 ± 2.5	73.9 ± 1.9
GIN+LAYERNORM	82.4 ± 6.4	62.8 ± 9.3	76.2 ± 3.0	$78.3 \pm 1,7$	$74.5 \pm 4,4$	82.8 ± 7.7	80.1 ± 0.8
GIN+BATCHNORM ((XU ET AL., 2019))	89.4 ± 5.6	64.6 ± 7.0	76.2 ± 2.8	82.7 ± 1.7	75.1 ± 5.1	92.4 ± 2.5	**80.2 ± 1.9**
GIN+INSTANCENORM	90.5 ± 7.8	64.7 ± 5.9	76.5 ± 3.9	81.2 ± 1.8	74.8 ± 5.0	93.2 ± 1.7	80.0 ± 2.1
GIN+GraphNorm	**91.6 ± 6.5**	**64.9 ± 7.5**	**77.4 ± 4.9**	81.4 ± 2.4	**76.0 ± 3.7**	**93.5 ± 2.1**	**80.2 ± 1.0**

Table 2. **Test performance** on OGB.

Datasets	OGBG-MOLHIV
# graphs	41,127
# classes	2
Avg # nodes	25.5
GCN (Hu et al., 2020)	76.06 ± 0.97
GIN (Hu et al., 2020)	75.58 ± 1.40
GCN+LayerNorm	75.04 ± 0.48
GCN+BatchNorm	76.22 ± 0.95
GCN+InstanceNorm	78.18 ± 0.42
GCN+GraphNorm	**78.30 ± 0.69**
GIN+LayerNorm	74.79 ± 0.92
GIN+BatchNorm	76.61 ± 0.97
GIN+InstanceNorm	77.54 ± 1.27
GIN+GraphNorm	**77.73 ± 1.29**

Thank you :)



GraphNorm
InstanceNorm
LayerNorm
BatchNorm
(2) Learnable mean
Multiply Learnable α
Calculate Graph Std
Divide std
Affine
Subtract graph mean
(1a) Preconditioning
Calculate Graph Mean/Std
Divide std
Affine
Feature Aggregation
Subtract feature mean
Node v
Feature
Calculate Feature Mean/Std
Divide std
Affine
Subtract batch mean
(1b) Heavy batch noise
Calculate Batch Mean/Std
Divide std
Affine