M.Sc Defence Thesis Presentation

Empowering Graph Wavelet Convolution for Node Classification: A Novel Approach with Local Lifting Scheme

RME 5401: Thesis

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Overview

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- Homophilic and Heterophilic graphs
- Problem Statement
- Related Works
- Proposed Generalized Adaptive Graph Wavelet Neural Network (GA-GWNN)
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Part 2

- Simple and Effective Graph Wavelet Neural Network (SEA-GWNN)
- Experimental Analysis
- Conclusion

Motivation for Node Classification



Homophilic and Heterophilic Graphs





Due to similar neighbours, homophilic graphs are suitable for low pass filtering

Heterophilic Graph





high pass filter

Due to dissimilar neighbour, it is necessary to recognise high frequency pattern via



Problem Statement



[1]Mallat et. al., A wavelet Tour of Signal Processing", Elsevier, 1999

[2]Xu et. al., "Graph wavelet neural network," ICLR, 2018

[3]Zheng et. al., "How framelets enhance graph neural networks," ICLR, 2021

[4] Zheng et. al., "Mathnet: Haarlike wavelet multiresolution analysis for graph representation learning," Knowledge-Based Systems, 2023.

[5]Li et. al., "Fast haar transforms for graph neural networks," Neural Networks, 2020.

[6]Xu et. al., "Graph neural networks with lifting-based adaptive graph wavelets," IEEE Transactions on Signal and Information Processing over Networks, 2022

Related Work

Input Graph



[7]Shen et. al., "Optimized distributed 2d transforms for irregularly sampled sensor network grids using wavelet lifting," in IEEE ICASS, 2008 [8]Narang et. al., Lifting based wavelet transforms on graphs," APSIPA, 2009.

Related Works: Adaptive Wavelet based Approach



Undesirable Wavelet: A Filter produced over a disrupted graph structure

Proposed Generalized Adaptive Graph Wavelet Neural Network (GA-GWN)



Our Contributions

- Limitations of existing wavelet based methods
 - Predefined wavelet filter based methods consider only homophily assumption.
 - Predefined wavelet filter based methods require domain specific knowledge.
 - Adaptive wavelet filter based methods produces undesirable filters.

- Contributions
 - Our Proposed GA-GWNN can generalize to both homophilic and heterophilic graphs.
 - Since proposed GA-GWNN is adaptive wavelet based approach thus does not require domain specific knowledge.
 - GA-GWNN is able to produce desirable wavelet filters.
 - Also proposed further simple and effective version SEA-GWNN.
 - No need of inverse transform.
 - Attention detachment.
 - Multiscale information.



Fusion Module/Operation

 Fuses both the low and high frequency information to enhance representation



Dataset and Evaluation Metrics

- Homophilic dataset
 - Citation graph[24] (Cora, Citeseer, PubMed)
- Heterophilic dataset
 - Webpage graph[13] (Cornell, Texas, Wisconsin)
 - Film industry graph[13] (Film)
- Large scale graphs
 - Ogbn-Arxiv[19]

- Evaluation Metrics
 - Accuracy
 - Percentage correct prediction
 - Precision
 - Recall
 - F1-Score
 - Harmonic mean of precision and recall

• Oghn-Products[10]	Dataset	Classes	Nodes	Edges	Features	Hom. Ratio
	Cora	7	2,708	5,429	1,433	0.81
	Citeseer	6	3,327	4,732	3,703	0.74
	Pubmed	3	19,717	44,338	500	0.80
	Film	5	7,600	33,544	931	0.22
	Cornell	5	183	295	1,703	0.30
	Texas	5	183	309	1,703	0.11
	Wisconsin	5	251	499	1,703	0.21
	Ogbn-Arxiv	40	169,343	1,166,243	128	0.66
	Ogbn-Products	47	2,449,029	61,859,140	100	0.81

Dataset Statistics

Overall Results

Mean accuracy on semi supervised node classification. Best results are heighted in bold



Overall Results(3)

Mean Precision, Recall, F1-score on Semi supervised node classification

	Precision				Recall		F1 Score		
Method	Cora	Citeseer	Pubmed	Cora	Citeseer	PubMed	Cora	Citeseer	PubMed
GRAPHSAGE[9]	$75.77{\pm}0.1$	60.68 ± 0.2	77.13 ± 0.6	79.78 ± 1.5	62.70 ± 0.5	75.16 ± 0.6	78.88 ± 0.7	61.44 ±0.6	76.44 ± 0.6
GAT[10]	$75.79{\scriptstyle \pm 0.1}$	$63.68{\scriptstyle \pm 0.2}$	$79.13{\pm}0.6$	$79.78{\scriptstyle\pm1.5}$	$64.70{\scriptstyle \pm 0.5}$	$75.16 {\pm} 0.6$	79.88 ± 0.7	$63.44 {\scriptstyle \pm 0.6}$	74.44 ± 0.6
HANET[5]	$75.77{\scriptstyle\pm0.1}$	60.68 ± 0.2	77.13 ± 0.6	79.78 ± 1.5	62.70 ± 0.5	75.16 ± 0.6	78.88 ± 0.7	61.44 ± 0.6	76.44 ± 0.6
GWNN[2]	77.31 ± 0.2	$66.93 {\scriptstyle \pm 0.1}$	76.14 ± 0.1	79.62 ± 1.4	$61.89{\scriptstyle~\pm 0.6}$	79.00 ± 0.5	78.04 ± 0.7	63.41 ± 0.5	77.41 ± 0.5
UFGCONVS[3]	$79.08{\scriptstyle\pm1.8}$	$67.59{\scriptstyle \pm 2.6}$	80.04 ± 0.5	$78.74{\pm}0.6$	68.12 ± 9.1	78.19 ± 3.4	66.51 ± 5.1	$66.99{\scriptstyle \pm 5.1}$	79.75 ± 5.1
UFGCONVR[3]	80.01 ± 1.1	67.16 ± 1.9	79.41 ± 0.6	$78.39{\scriptstyle\pm1.5}$	$68.30{\pm}8.4$	77.22 ± 6.7	$80.55{\scriptstyle \pm 5.2}$	66.47 ± 3.6	79.47 ± 3.6
LGWNN[6]	80.21 ± 1.3	67.01 ± 1.9	$78.78{\scriptstyle \pm 0.6}$	$78.60{\scriptstyle\pm1.1}$	$68.38{\scriptstyle \pm 4.9}$	$77.00{\scriptstyle \pm 7.2}$	$80.45{\scriptstyle \pm 4.9}$	66.51 ± 3.1	$79.40{\pm}3.1$
GA-GWNN	80.32+0.2	68.30+01	80.25+01	83.00+1.8	68.16 ± 4.6	79.45 ± 3.5	81.43+33	67.08+1 9	80.08+1 9

Overall Results(2)

Mean accuracy on full supervised node classification. Best results are in bold

Method/	homoph	nilic graph	datasets	hete	rophilic g	graph data	asets				
Acc.(%)	Cora	Cite.	Pubm.	Film	Corn.	Texa.	Wisc.	Avg.	Acc.		
GCN[11]	$85.77{\pm}0.1$	73.68 ± 0.2	88.13 ± 0.6	28.78 ± 1.5	52.70 ± 0.5	52.16 ± 0.6	$45.88{\scriptstyle \pm 0.7}$	61.44	±0.6	۱ I	
GAT[10]	$86.37{\scriptstyle \pm 0.2}$	74.32 ± 0.2	87.62 ± 0.4	28.99 ± 1.4	54.32 ± 0.3	58.38 ± 0.5	49.41 ± 0.9	62.77	± 0.5		Homophilic Graph
APPNP[11]	$87.87{\scriptstyle \pm 0.2}$	$76.53{\scriptstyle \pm 0.2}$	89.40 ± 1.4	34.86 ± 1.1	73.51 ± 1.1	65.41 ± 0.1	$69.02{\scriptstyle\pm1.6}$	70.94	± 0.8	\leq	Neural Network
GWNN[2]	85.31 ± 0.2	73.93 ± 0.1	88.14 ± 0.1	26.62 ± 1.4	61.89 ± 0.6	60.00 ± 0.5	48.04 ± 0.7	63.41	± 0.5	L L	
DEEPWALK[12]	80.08 ± 1.8	53.59 ± 2.6	81.14 ± 0.5	23.74 ± 0.6	44.12 ± 9.1	49.19 ± 3.4	53.51 ± 5.1	55.05	5±5.1	7	
- G-GCN[13]	84.91 ± 1.1	75.16 ± 1.9	88.41 ± 0.6	32.39 ± 1.5	55.68 ± 8.4	66.22 ± 6.7	62.55 ± 5.2	66.47	±3.6	\	
MIXHOP[14]	87.61 ± 0.8	76.26 ± 1.3	85.31 ± 0.6	32.22 ± 2.3	73.51 ± 6.3	77.84 ± 7.7	75.88 ± 4.9	72.66	3 ± 3.4		Heterophilic Graph
H2GCN[15]	87.69 ± 1.3	75.95 ± 2.1	88.78 ± 0.5	36.71 ± 1.4	78.92 ± 5.2	82.16 ± 8.2	82.57 ± 3.2	76.11	± 3.1	\leq	Neural Network
CPGNN[16]	87.18±1.1	75.52 ± 1.8	89.08 ± 0.6	35.51 ± 1.8	63.51 ± 5.8	74.32 ± 7.3	81.76 ± 6.7	72.44	1 ± 3.6	į L	
GPR-GNN[17]	86.70 ± 1.1	75.12 ± 1.9	87.38 ± 0.6	36.47 ± 1.3	82.97 ± 5.6	84.59 ± 4.3	83.92 ± 3.1	76.73	3 ± 2.5	1	
<u>AM-GCN[18]</u>	86.66 ± 1.3	76.01 ± 1.9	86.78 ± 0.6	33.60 ± 1.1	78.38 ± 4.9	78.38 ± 7.2	81.76 ± 4.9	74.51	±3.1	1	Adaptive wavelet
GA-GWNN	$88.32{\scriptstyle\pm0.1}$	76.61 ± 0.2	$89.70{\scriptstyle \pm 0.1}$	$37.16_{\pm 1.8}$	85.16 ± 4.6	84.45 ± 3.5	85.43 ± 3.3	78.08	8 ± 1.9	;<	filters

Overall Results(3)

Mean accuracy on large scale graphs (full supervised). Best results are highlighted in bold. OOM denotes *Out of Memory*

	Method/	Ogbn-Arxiv Ogbn-P		roducts			
	Acc.(%)	Test Acc.	Val. Acc.	Test Acc.	Val. Acc.		Only utilize
	MLP[19]	55.50 ± 0.23	57.65 ± 0.12	61.06 ± 0.08	$75.54 {\pm} 0.02$	\leq	graph signal
Only utilize –	NODE2VEC[20]	70.07 ± 0.13	71.29 ± 0.13	72.49 ± 0.10	90.32 ± 0.06		0 1 0
graph structure	GRAPHZOOM[21]	71.18 ± 0.18	72.20 ± 0.07	74.06 ± 0.26	90.66 ± 0.11		
3 ¹ 1 ¹ 1	GRAPHSAGE[9]	71.49 ± 0.27	72.77 ± 0.17	78.29 ± 0.16	92.24 ± 0.07		
	GCN[11]	71.74 ± 0.29	73.00 ± 0.17	75.64 ± 0.21	92.00 ± 0.03		More depth
	DEEPERGCN[12]	71.92 ± 0.17	72.62 ± 0.14	80.98 ± 0.20	92.38 ± 0.09		More the cost
	SIGN[13]	71.95 ± 0.11	$73.23{\scriptstyle \pm 0.06}$	80.52 ± 0.16	$92.99{\scriptstyle \pm 0.04}$		
	UFGCONV-S[3]	70.04 ± 0.22	71.04 ± 0.11	OOM	OOM		
	UFGCONV-R[3]	$71.97 {\pm} 0.12$	73.21 ± 0.05	OOM	OOM		
	GA-GWNN	72.27 ± 0.21	$73.64{\scriptstyle \pm 0.35}$	80.91 ± 0.18	92.30 ± 0.15		

Computational Cost



GA-GWNN Time Complexity: O(L|N|d_in d_out + L |E| d_out)

Ablation Studies

Performance of GA-GWNN with deeper layer in supervised task

Detect			#La	yers				
Dataset	2	4	6	8	12	16	20	26
Cora	88.32	88.49	88.61	88.63	88.29	88.43	88.40	88.53
Citeseer	77.08	76.92	76.87	77.10	76.37	76.76	77.02	76.87
Film	37.16	36.87	37.11	36.94	37.25	36.92	36.75	36.88
Cornell	85.16	84.60	81.35	81.76	80.94	79.86	79.80	79.70
Texas	84.15	84.83	84.16	84.30	82.38	83.65	82.23	83.00
Wisconsin	85.43	85.32	85.29	85.49	85.29	84.71	83.53	83.33

Semi supervised performance with deeper



(a) TA-GWNN

(b) GWNN

Simple and Effective GWNN (SEA-GWNN)

GA-GWNN



SEA-GWNN

Algorithm 2: Implementation of the proposed SEA-GWNN model	
Input: Graph (\mathcal{G}) adjacency matrix \mathcal{A} , node feature matrix $\mathbf{X} \in \mathbb{R}^{N \times N}$ set of ground truth \mathcal{Y} , max layer L	$^{\langle d}$,
Output: Predicted class label: Y.	
1 Initialize model parameters	
2 for $epoch \leftarrow 1 \dots m$ do	
$\mathbf{H}_0, \tilde{\mathbf{H}}_0 \leftarrow \mathbf{X};$	
4 /* Structure aware lifting operators	*/
$\mathcal{U} \leftarrow \operatorname{ATT}_{gat}(\mathcal{G}, \mathbf{X})$	
$\mathcal{P} \leftarrow \frac{1}{2}\mathcal{U}$	
7 for layers, $l \leftarrow 1 \dots L$ do	
8 $H_{\ell} \leftarrow \mathcal{A} H_{\ell-1}$	
9 $ ilde{\mathrm{H}}_\ell \leftarrow ilde{\mathcal{U}} ilde{\mathrm{H}}_{\ell-1}$	
10 7* Decompose signal in the wavelet domain	*/
11 $\mathbf{Z}_{\ell} \leftarrow \alpha \mathbf{H}_{\ell} + \tilde{\mathbf{H}}_{\ell} \circledast \boldsymbol{\xi}$	
12 $\mathbf{Z} += \gamma_{\ell} \mathbf{Z}_{\ell}$	
13 end	
14 $Y \leftarrow Softmax(Z)$; /* Outputs the softmax probability	*/
15 $\mathcal{L} = \text{Loss}(\mathbf{Y}, \mathcal{Y})$; /* Compute loss	*/
16 Backpropagation and update parameters	
17 end	

SEA-GWNN(2)



Overall Results

Method/	homopl	nilic graph d	latasets	heterophilic graph datasets						
Acc.(%)	Cora	Cite.	Pubm.	Film	Cham.	Squi.	Corn.	Texa.	Wisc.	
GCN[11]	85.77 ± 0.1	73.68 ± 0.2	88.13 ± 0.6	28.78 ± 1.5	28.18 ± 0.78	36.89±1.34	52.70 ± 0.5	52.16 ± 0.6	45.88 ± 0.7	
GAT[10]	86.37 ± 0.2	74.32 ± 0.2	87.62 ± 0.4	28.99 ± 1.4	42.93 ± 0.46	30.62 ± 2.11	54.32 ± 0.3	58.38 ± 0.5	49.41 ± 0.9	
APPNP[11]	87.87 ± 0.2	76.53 ± 0.2	89.40 ± 1.4	34.86 ± 1.1	54.30 ± 0.56	34.77 ± 0.34	73.51 ± 1.1	65.41 ± 0.1	69.02 ± 1.6	
GWNN[2]	85.31 ± 0.2	73.93 ± 0.1	88.14 ± 0.1	26.62 ± 1.4	-	-	61.89 ± 0.6	60.00 ± 0.5	48.04 ± 0.7	
G-GCN[13]	84.91±1.1	75.16±1.9	88.41 ± 0.6	$32.39 {\pm} 1.5$	61.06 ± 0.49	38.28 ± 0.27	55.68 ± 8.4	66.22 ± 6.7	62.55 ± 5.2	
MIXHOP[14]	87.61 ± 0.8	76.26 ± 1.3	$85.31 {\pm} 0.6$	32.22 ± 2.3	60.50 ± 2.53	43.80 ± 1.48	73.51 ± 6.3	77.84±7.7	75.88 ± 4.9	
H2GCN[15]	87.69 ± 1.3	75.95 ± 2.1	88.78 ± 0.5	36.71 ± 1.4	58.38 ± 1.76	37.90 ± 2.02	78.92 ± 5.2	82.16 ± 8.2	82.57 ± 3.2	
CPGNN[16]	87.18±1.1	75.52 ± 1.8	89.08 ± 0.6	35.51 ± 1.8	65.24 ± 0.87	45.00 ± 1.40	63.51 ± 5.8	74.32 ± 7.3	81.76 ± 6.7	
GPR-GNN[17]	86.70 ± 1.1	75.12 ± 1.9	87.38 ± 0.6	36.47 ± 1.3	65.42 ± 2.04	49.93 ± 0.53	82.97 ± 5.6	84.59 ± 4.3	83.92 ± 3.1	
AM-GCN[18]	86.66 ± 1.3	76.01 ± 1.9	$86.78{\scriptstyle \pm 0.6}$	33.60 ± 1.1	68.46 ± 1.70	40.02 ± 0.96	78.38 ± 4.9	78.38 ± 7.2	81.76 ± 4.9	
SEA-GWNN	88.72 ± 0.1	$\textbf{76.08} \pm 0.2$	$89.70{\scriptstyle\pm0.1}$	$37.16{\pm}1.8$	71.67 ± 0.18	54.02 ± 0.17	85.16 ± 4.6	$84.45{\pm}3.5$	85.16 ± 3.3	

Mean accuracy on full supervised node classification. Best results are highlighted in bold

Mean accuracy on semi supervised node classification with best results are highlighted in bold

Methods	Cora	Citeseer	\mathbf{PubMed}
GraphSAGE[9]	74.5 ± 0.8	67.2 ± 1.0	76.8 ± 0.6
GAT[10]	$83.0 \ \pm 0.7$	$72.5 \ \pm 0.7$	79.0 ± 0.3
HANET[5]	81.9	70.1	79.3
GWNN[2]	$81.6 \ \pm 0.7$	$70.5{\scriptstyle~\pm 0.6}$	78.6 ± 0.3
UFGCONVS[3]	$83.0{\scriptstyle~\pm 0.5}$	$71.0{\scriptstyle~\pm 0.6}$	79.4 ± 0.4
UFGCONVR[3]	83.6 ± 0.6	$72.7{\scriptstyle~\pm 0.6}$	79.9 ± 0.1
LGWNN[6]	83.4 ± 0.6	$71.1{\scriptstyle~\pm 0.4}$	79.5 ± 0.5
SEA-GWNN	84.4 ± 0.3	72.8 ± 0.3	80.7 ± 0.2

Overall Results(2)

Mean accuracy on large scale graphs node classification. Best results are highlighted in bold

Methods	Penn94	Arxiv-Year	Genius	Arxiv
MLP[19]	73.61 ± 0.40	36.70 ± 0.21	86.68 ± 0.09	55.00 ± 0.025
LABEL PROP.[19]	74.13 ± 0.46	46.07 ± 0.15	67.04 ± 0.20	68.32 ± 0.00
GCN[11]	82.47 ± 0.27	46.02 ± 0.26	87.42 ± 0.37	71.74 ± 0.29
CHEBNET[20]	82.51 ± 0.31	46.76 ± 0.24	89.36 ± 0.31	71.72 ± 0.22
GAT[11]	81.53 ± 0.55	46.05 ± 0.51	55.80 ± 0.87	71.95 ± 0.11
GCNJK[20]	81.63 ± 0.54	46.28 ± 0.29	89.30 ± 0.19	72.19 ± 0.21
GCNII[21]	82.92 ± 0.59	47.21 ± 0.28	90.24 ± 0.09	72.74 ± 0.16
H2GCN[15]	81.31 ± 0.60	OOM	OOM	OOM
GPRGNN[17]	81.38 ± 0.16	45.97 ± 0.26	90.05 ± 0.31	71.78 ± 0.18
UFGCONV[3]	OOM	OOM	OOM	71.97 ± 0.12
SEA-GWNN	$84.35{\scriptstyle~\pm 0.35}$	$49.70{\scriptstyle~\pm 0.41}$	90.53 ± 0.14	$\textbf{72.85} \pm 0.51$

Overall Results(3)

Graph level classification and prediction

Datasets	PROTEINS	Mutagenicity	D&D	NCI1	QM7
TopKPool	73.48 ±3.57	79.84 ± 2.46	74.87 ± 4.12	75.11 ± 3.45	175.41 ± 3.16
ATTENTION	73.93 ± 5.37	80.25 ± 2.22	77.48 ± 2.65	74.04 ± 1.27	177.99 ± 2.22
SAGPOOL	75.89 ± 2.91	79.86 ± 2.36	74.96 ± 3.60	76.30 ± 1.53	41.93 ± 1.14
SUM	74.91 ± 4.08	80.69 ± 3.26	78.91 ± 3.37	76.96 ± 1.70	42.09 ± 0.91
MAX	73.57 ± 3.94	78.83 ± 1.70	75.80 ± 4.11	75.96 ± 1.82	177.48 ± 4.70
MEAN	73.13 ± 3.18	80.37 ± 2.44	76.89 ± 2.23	73.70 ± 2.55	177.49 ± 4.69
UFGPOOL	77.77 ± 2.60	81.59 ± 1.40	80.92 ± 1.68	77.88 ± 1.24	41.74 ± 0.84
GWNN [31]	73.35 ± 3.71	74.26 ± 2.29	75.04 ± 4.55	69.79 ± 1.67	-
LGWNN [33]	74.02 ± 5.23	82.47 ± 1.90	78.72 ± 4.33	78.97 ± 2.07	
OURS	$80.23{\scriptstyle\pm0.51}$	80.29 ± 1.62	$80.39{\scriptstyle \pm 0.49}$	0.57	$40.95{\scriptstyle \pm 0.83}$

Model Analysis

Computational Cost O(|N|d_in d_out + L|E|d_out)



Model performance on deeper architecture

Datasets/	The n	umber o	of graph	convolu	itional la	yers k	
Accuracy (%)	2	4	6	8	16	28	32
Cora	82.46	84.04	84.38	84.34	82.52	82.86	80.86
PubMed	79.90	79.44	79.84	80.34	80.74	79.94	79.92

Conclusion

- Proposed a novel class of algorithm namely GA-GWNN that produces desirable wavelet filters.
- Proposed a novel lifting scheme namely tree lifting scheme that preserve the original graph structure.
- Our proposed GA-GWNN can learn wavelet filters on arbitrary graphs.
- Experimental results demonstrate the superiority of our proposed algorithm.
- Further proposed a simple and more scalable version of GA-GWNN namely SEA-GWNN

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