Graph Neural Networks go grammatical

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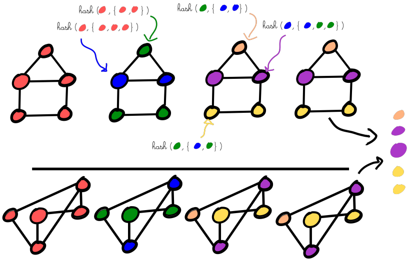
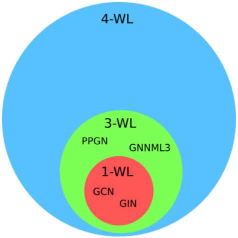
CodeGnn

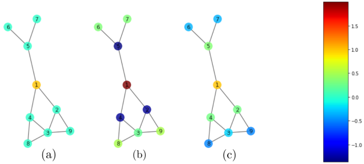
4^{th} april 2023

Weisfeiler-Lehman hierarchy [Xu et al., 2019]

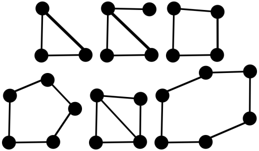




Spectral response [Balcilar et al., 2021b]



Counting power [Chen et al., 2020]



Contributions

New GNN design strategy based on Context Free Grammar (CFG).

Example of 1-WL CFG.

Grammatical Graph Neural Network (G^2N^2) a 3-WL GNN.

G^2N^2 spectral response and counting power.

In [Brijder et al., 2019] they introduced MATLANG a matrix language.

Matlang

$\mathrm{ML}(\mathcal{L})$ is a matrix language with an allowed operation set $\mathcal{L} = \{op_1, \ldots, op_n\}$, where $op_i \in \{\cdot, +, {}^{\mathbf{T}}, \mathrm{diag}, \mathrm{Tr}, 1, \odot, \times, f\}$.

Sentence

$e(X) \in \mathbb{R}$ is a sentence in $\mathrm{ML}(\mathcal{L})$ if it consists of any possible consecutive operations in $\mathcal{L}$, operating on a given matrix X and resulting in a scalar value.

As an exemple, $1^{\mathbf{T}}(X \odot \mathrm{diag}(1))\,1$ is a sentence in $\mathrm{ML}\left({}^{\mathbf{T}}, 1, \odot, \cdot, \mathrm{diag}\right)$ that computes trace of square matrix X.

$\mathrm{ML}(\mathcal{L})$-*equivalent* for matrices

Two matrices A and B in $\mathcal{M}_{m,n}(\mathbb{R})$ are said to be $\mathrm{ML}(\mathcal{L})$-*equivalent*, denoted by $A \equiv_{\mathrm{ML}(\mathcal{L})} B$, if and only if $e(A) = e(B)$ for all sentences in $\mathrm{ML}(\mathcal{L})$.

$\mathrm{ML}(\mathcal{L})$-*equivalent* for graphs

Two graphs $\mathcal{G}$ and $\mathcal{H}$ of the same order are said to be $\mathrm{ML}(\mathcal{L})$-*equivalent*, denoted by $\mathcal{G} \equiv_{\mathrm{ML}(\mathcal{L})} \mathcal{H}$, if and only if their adjacency matrices are $\mathrm{ML}(\mathcal{L})$-*equivalent*.

In [Geerts and Reutter, 2021], they proved the following theorems for the sets of operations $\mathcal{L}_1 = \{\cdot, {}^{\mathbf{T}}, 1, \text{diag}\}$ and $\mathcal{L}_3 = \{\cdot, {}^{\mathbf{T}}, 1, \text{diag}, \odot\}$.

1-WL equivalence

Two adjacency matrices are indistinguishable by the 1-WL test if and only if $e(A_G) = e(A_H)$ for all $e \in \mathcal{L}_1$. Hence, all possible sentences in $\mathcal{L}_1$ are the same for $1-$WL-*equivalent* adjacency matrices. Thus,

$$A_{\mathcal{G}} \equiv_{\text{1-WL}} A_{\mathcal{H}} \iff A_{\mathcal{G}} \equiv_{\text{ML}(\mathcal{L}_1)} A_{\mathcal{H}}$$

3-WL equivalence

Two adjacency matrices are indistinguishable by the 3-WL test if and only if $e(A_G) = e(A_H)$ for all $e \in \mathcal{L}_3$. Hence, all possible sentences in $\mathcal{L}_3$ are the same for $3-$WL-*equivalent* adjacency matrices. Thus,

$$A_{\mathcal{G}} \equiv_{\text{3-WL}} A_{\mathcal{H}} \iff A_{\mathcal{G}} \equiv_{\text{ML}(\mathcal{L}_3)} A_{\mathcal{H}}$$

For $\mathcal{L}_1 = \{\cdot, \ ^{\mathbf{T}}, 1, \text{diag}\}$, define $G_{\mathcal{L}_1} = (V, \Sigma, R, S_t)$.

$$V = \{M, V_c, V_l, S\}$$
$$\Sigma = \{A, \text{diag}, 1, \ ^{\mathbf{T}}, (,)\}$$
$$S_t = S$$

where the rules in R are

$$S \to (V_l)(V_c) \mid \text{diag}\,(S) \mid SS$$
$$M \to MM \mid (M)^{\mathbf{T}} \mid \text{diag}\,(V_c) \mid (V_c)(V_l) \mid A$$
$$V_c \to MV_c \mid (V_l)^{\mathbf{T}} \mid V_cS \mid 1$$
$$V_l \to V_lM \mid (V_c)^{\mathbf{T}} \mid SV_l$$

	Rules applied
S	
$\downarrow$	$S \to V_lV_c$
V_lV_c	
$\swarrow \ \searrow$	$V_l \to (V_c)^T, \quad V_c \to MV_c$
$(V_c)^T MV_c$	
$\swarrow \ \downarrow \ \downarrow$	$V_c \to 1, \quad M \to MM, \quad V_c \to 1$
$(1)^T MM1$	
$\swarrow \ \downarrow$	$M \to A, \quad M \to \text{diag}(V_c)$
$(1)^T A\text{diag}(V_c)1$	
$\downarrow$	$V_c \to MV_c$
$(1)^T A\text{diag}(MV_c)1$	
$\downarrow \ \downarrow$	$M \to A, \quad V_c \to 1$
$(1)^T A\text{diag}(A1)1$	

Theorem ($\mathrm{ML}(\mathcal{L}_1)$ Reduced CFG)

The following CFG denoted by r-$G_{\mathcal{L}_1}$ is as expressive as 1-WL.

$$V_c \rightarrow \mathrm{diag}(V_c)\, V_c \mid AV_c \mid 1$$

Corollary (GNNML1 CFG)

The following CFG, as expressive than $\mathrm{ML}(\mathcal{L}_1)$ represents GNNML1 [Balcilar et al., 2021a].

$$V_c \rightarrow V_c \odot V_c \mid AV_c \mid 1$$

GNNML1 node update:

$$\begin{aligned} H^{(l+1)} = \sigma(&H^{(l)} \cdot W^{(l,1)} + A \cdot H^{(l)} \cdot W^{(l,2)} \\ &+ H^{(l)} \cdot W^{(l,3)} \odot H^{(l)} \cdot W^{(l,4)}) \end{aligned}$$

Proposition (GCN CFG)

The following CFG is strictly less expressive than $\mathrm{ML}(\mathcal{L}_1)$.

$$V_c \to C_1 V_c \mid \cdots \mid C_k V_c \mid 1$$

When C_s *is include in* $\mathrm{ML}(\mathcal{L}_1)$.

As an example, the following CFG, strictly less expressive than $\mathrm{ML}(\mathcal{L}_1)$ represents GCN [Kipf and Welling, 2017].

$$V_c \to C V_c \mid 1$$

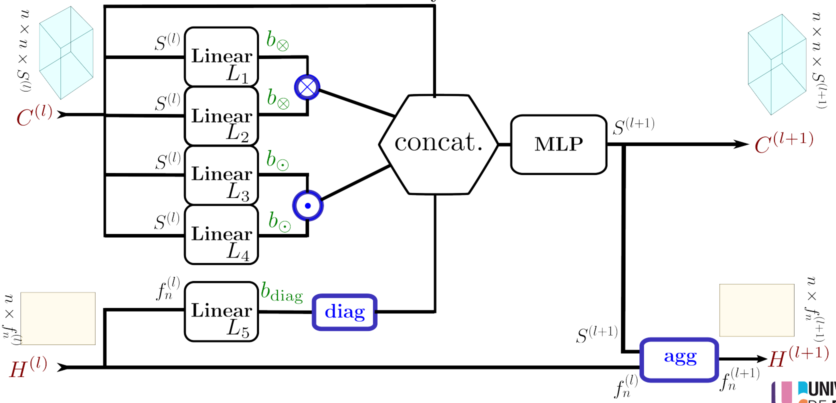
Where $C = \mathrm{diag}\left((A + \mathrm{I})1\right)^{-\frac{1}{2}} (A + \mathrm{I}) \mathrm{diag}\left((A + \mathrm{I})1\right)^{-\frac{1}{2}}$

Theorem (ML ($\mathcal{L}_3$) Reduced CFG)

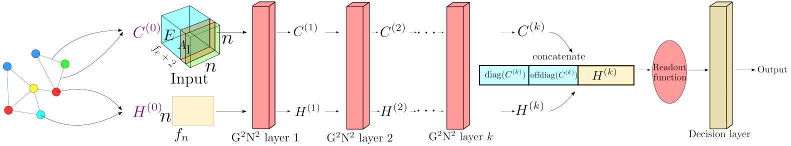
The following CFG denoted by r-$G_{\mathcal{L}_3}$ is as expressive as 3-WL.

$$V_c \to MV_c \mid 1$$
$$M \to (M \odot M) \mid MM \mid \mathrm{diag}(V_c) \mid A$$

G^2N^2 layer :



G^{2}N^2 architecture :



G^{2}N^2 update equation

$$\mathcal{C}^{(l+1)} = mlp(\mathcal{C}^{(l)}|L_1(\mathcal{C}^{(l)})\odot L_2(\mathcal{C}^{(l)})| L_3(\mathcal{C}^{(l)})\cdot L_4(\mathcal{C}^{(l)})|\mathrm{diag}(L_5(H^{(l)}))),$$

$$H^{(l+1)} = \sum_{i=1}^{S^{(l+1)}} \mathcal{C}_i^{(l+1)} H^{(l)} W^{(l,i)}.$$

Theorem (G^2N^2 in the WL hierarchy)

G^2N^2 is as expressive as 3-WL.

Table: The accuracy on EXP and SR25 datasets denotes the ratio of pairs of non isomorphic respectively 1-WL equivalent and 3-WL equivalent graphs that are separate by the model.

Method	EXP	SR25
1-WL-bounded GNN	0%	0%
CHEBNET	87%	0%
3-WL-bounded GNN	**100%**	0%
PPGN	**100%**	0%
G^2N^2	**100%**	0%
I^2-GNN	**100%**	**100%**

Theorem (G^2N^2 counting power)

G^2N^2 can count chordal cycle and cycle up to lenght 6 at edge level.

Table: G^2N^2 normalised MAE on counting substructures at edge level.

triangle	4-cycle	5-cycle	6-cycle	chordal cycle
3.99e-04	4.55e-04	2.93e-03	3.58e-03	1.56e-04

Theorem (G^{2}N^2 spectral response)

G^{2}N^2 can approximate low-pass, high-pass and band-pass filter in the spectral domain.

Table: R^2 score on spectral filtering node regression problems. Results are median of 10 different runs.

Method	Low-pass	High-pass	Band-pass
MLP	0.9749	0.0167	0.0027
GCN	0.9858	0.0863	0.0051
GAT	0.9811	0.0879	0.0044
GIN	0.9824	0.2934	0.0629
CHEBNET	**0.9995**	0.9901	**0.8217**
PPGN	0.9991	**0.9925**	0.1041
GNNML1	0.9994	0.9833	0.3802
GNNML3	**0.9995**	**0.9909**	**0.8189**
G^{2}N^2	**0.9996**	**0.9994**	**0.8206**

On the left G^{2}N^2's prediction, on the center the input and on the right, the target

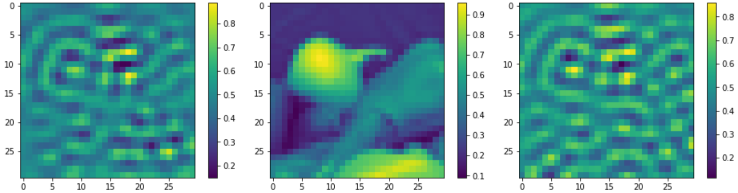


Table: Results on QM9 dataset focusing on the best methods. The metric is MAE, the lower, the better.

Target	I^2 GNN	PPGN(12)	PPGN(1)	G^2N^2(12)
μ	0.428	0.231	0.0934	**0.0973**
α	0.230	0.382	0.318	**0.183**
ϵ_{homo}	0.00261	0.00276	0.00174	**0.0022**
ϵ_{lumo}	0.00267	0.00287	0.0021	**0.00215**
$\Delta\epsilon$	0.0038	0.00406	0.0029	**0.00296**
R^2	18.64	16.07	3.78	**1.12**
ZPVE	0.00014	0.00064	0.000399	**0.000166**
U_0	0.211	0.234	0.022	**0.0513**
U	0.206	0.234	0.0504	**0.0513**
H	0.269	0.229	0.0294	**0.0513**
G	0.261	0.238	0.024	**0.0513**
C_v	0.0730	0.184	0.144	**0.0702**

Table: Results of G^2N^2 on TUD dataset compared to the best competitor. The metric is accuracy, the higher, the better.

Dataset	G^2N^2	rank	Best GNN competitor
MUTAG	92.0±4.3	2	92.2±7.5
PTC	71.8±6.7	1	68.2±7.2
Proteins	77.8±3.2	1	77.4±4.9
NCI1	80.2±2.1	8	83.5±2.0
IMDB-B	76.8±2.8	2	77.8±3.3
IMDB-M	54.0±2.93	2	54.3±3.3

G^2N^2 assets

3-WL equivalent
Large spectral response
Counting power at **edge level**
Direct from CFG

G^2N^2 drawbacks

Time complexity $O\left(n^3\right)$
Memory complexity $O\left(n^2\right)$

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Thank you for your attention.

Our paper is available here.

Graph Neural Network go Grammatical

https://arxiv.org/abs/2303.01590