DEMO-Net: Degree-specific Graph Neural Networks for Node and Graph Classification

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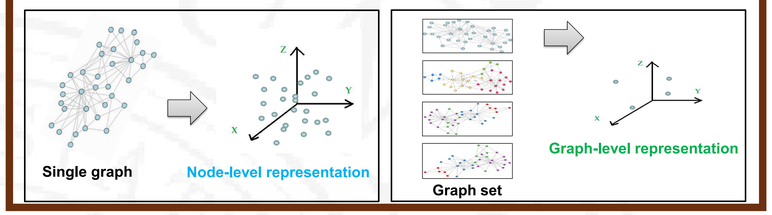
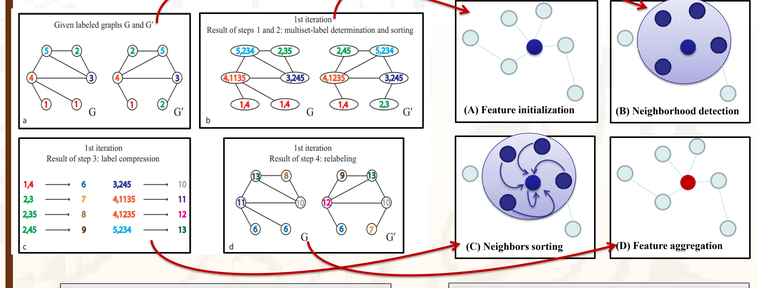
Target Problems:

- ***Node-level representation learning***
  - *Application: In a transaction network, the fraudulent users can be detected using the node (user) representation.*
- ***Graph-level representation learning***
  - *Application: In chemoinformatics, the toxic molecules (represented as graphs) can be classified using the graph (molecule) representation.*

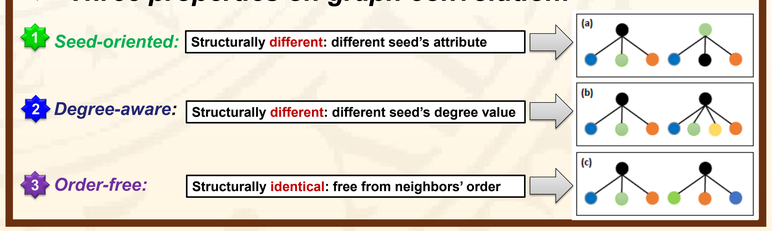


Motivation:

- **Graph convolution in graph neural networks has the similar steps as Weisfeiler-Lehman graph kernel.**



- ***Three properties on graph convolution:***



Proposed Framework:

- ***Multi-task graph convolution:***
  - ***Intuition: nodes with the identical degree value would share the same graph convolution function.***
  - ***Feature update:***

$$h_v^k = f_s\left(h_v^{k-1}\right) \circ f_{\deg(v)}\left(\{h_u^{k-1} | u \in N(v)\}\right) = \sigma\left(W_0^k h_v^{k-1}\right) \circ f_{\deg(v)}\left(h_{N(v)}^{k-1}\right)$$

Degree-specific function

Multi-task convolution

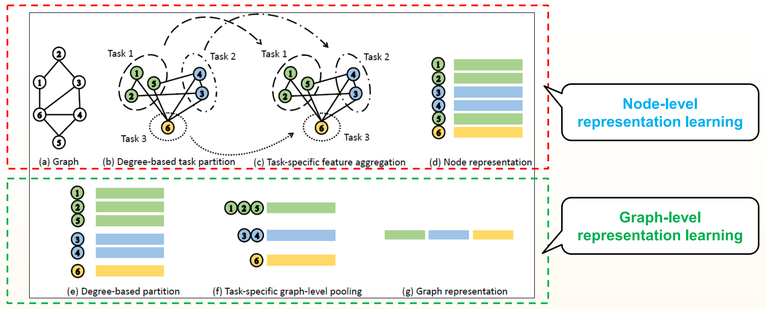
Feature hashing:

$$f_{\deg(v)}\left(h_{N(v)}^{k-1}\right) = \sigma\left(\sum_{u \in N(v)} W^k\left(\phi_g\left(h_u^{k-1}\right) + \phi_{\deg(v)}\left(h_u^{k-1}\right)\right)\right)$$

Weight sharing:

$$f_{\deg(v)}\left(h_{N(v)}^{k-1}\right) = \sigma\left(\sum_{u \in N(v)} \left(W_g^k + W_{\deg(v)}^k\right) h_u^{k-1}\right)$$

- ***DEMO-Net framework:***



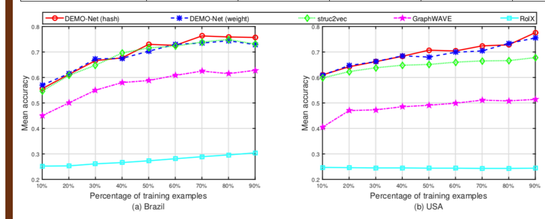
Theoretical Analysis:

- **(*Existence Theorem*) There exist the functions f_s and $\{f_{deg} | deg \in degree(G)\}$ so that for any pair of subtrees, the composite function $f_s \circ f_{deg}$ could map them to different feature vectors if they are not structurally identical.**
- **(*Graph Kernel Space*) The learned graph-level representation lies in a Reproducing Kernel Hilbert Space (RKHS) induced by a degree-specific Weisfeiler-Lehman graph kernel.**

Experimental Results:

- ***Node classification:***

	Social networks				Air-traffic networks		
	Facebook	Wiki-Vote	BlogCatalog	Flickr	Brazil	Europe	USA
GraphSAGE [5]	0.389 ±0.019	0.245 ±0.000	0.828 ±0.007	0.641 ±0.006	0.404 ±0.035	0.272 ±0.022	0.316 ±0.022
GCN [9]	0.575 ±0.013	0.329 ±0.029	0.720 ±0.013	0.546 ±0.019	0.432 ±0.064	0.371 ±0.046	0.432 ±0.022
GCN_cheby [9]	0.646 ±0.012	0.495 ±0.016	0.686 ±0.037	0.479 ±0.023	0.516 ±0.070	0.460 ±0.038	0.526 ±0.045
Union [12]	0.600 ±0.000	0.463 ±0.000	0.730 ±0.000	0.566 ±0.000	0.466 ±0.006	0.418 ±0.002	0.582 ±0.000
Intersection [12]	0.598 ±0.000	0.462 ±0.000	0.725 ±0.000	0.557 ±0.000	0.459 ±0.003	0.443 ±0.002	0.573 ±0.000
GAT [18]	0.570 ±0.036	0.594 ±0.070	0.663 ±0.000	0.359 ±0.000	0.382 ±0.126	0.424 ±0.073	0.585 ±0.021
DEMO-Net(hash)	0.887 ±0.020	0.997 ±0.000	0.849 ±0.006	**0.678 ±0.010**	**0.614 ±0.069**	**0.479 ±0.064**	**0.659 ±0.020**
DEMO-Net(weight)	**0.919 ±0.003**	**0.998 ±0.000**	**0.849 ±0.000**	0.656 ±0.000	0.543 ±0.034	0.459 ±0.025	0.647 ±0.021

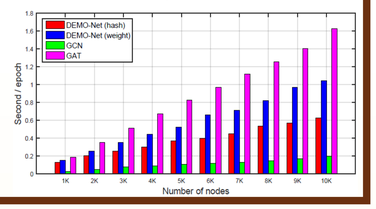


Higher is better

- ***Graph classification:***

	MUTAG	PTC	PROTEINS	ENZYMES
DeepWL [23]	0.733	0.537	0.680	0.210
DCNN [1]	0.670	**0.572**	0.579	0.160
PATCHY-SAN [13]	0.795	0.568	0.714	0.170
DIFFPOOL [24]	0.663	0.251	**0.733**	0.184
*DEMO-Net*_m(hash)	0.760	**0.586**	0.617	0.236
*DEMO-Net*_m(weight)	0.798	0.550	0.616	0.251
DEMO-Net(hash)	0.771	0.563	0.705	0.251
DEMO-Net(weight)	**0.814**	0.572	0.708	**0.272**

- ***Efficiency:***



Conclusion:

- **Association of three key properties for graph convolution with Weisfeiler-Lehman isomorphism test.**
- **A novel degree-specific graph neural network model (DEMO-Net) for encoding the subtree structures from graphs.**
- **Extensive results demonstrating the proposed DEMO-Net method.**

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