**[DEEP GEOMETRICAL GRAPH CLASSIFICATION](https://openreview.net/forum?id=Hkes0iR9KX)**

[Mostafa Rahmani](https://openreview.net/profile?email=rahmani.sut%40gmail.com), [Ping Li](https://openreview.net/profile?email=pingli98%40gmail.com)

‎28‎ ‎Sep‎ ‎2018 (modified: ‎21‎ ‎Dec‎ ‎2018) ICLR 2019 Conference Blind Submission Readers: Everyone 10 Replies

[Hide details](https://openreview.net/group?id=ICLR.cc/2019/Conference#Hkes0iR9KX-details-720)

* **Abstract:** Most of the existing Graph Neural Networks (GNNs) are the mere extension of the Convolutional Neural Networks (CNNs) to graphs. Generally, they consist of several steps of message passing between the nodes followed by a global indiscriminate feature pooling function. In many data-sets, however, the nodes are unlabeled or their labels provide no information about the similarity between the nodes and the locations of the nodes in the graph. Accordingly, message passing may not propagate helpful information throughout the graph. We show that this conventional approach can fail to learn to perform even simple graph classification tasks. We alleviate this serious shortcoming of the GNNs by making them a two step method. In the first of the proposed approach, a graph embedding algorithm is utilized to obtain a continuous feature vector for each node of the graph. The embedding algorithm represents the graph as a point-cloud in the embedding space. In the second step, the GNN is applied to the point-cloud representation of the graph provided by the embedding method. The GNN learns to perform the given task by inferring the topological structure of the graph encoded in the spatial distribution of the embedded vectors. In addition, we extend the proposed approach to the graph clustering problem and a new architecture for graph clustering is proposed. Moreover, the spatial representation of the graph is utilized to design a graph pooling algorithm. We turn the problem of graph down-sampling into a column sampling problem, i.e., the sampling algorithm selects a subset of the nodes whose feature vectors preserve the spatial distribution of all the feature vectors. We apply the proposed approach to several popular benchmark data-sets and it is shown that the proposed geometrical approach strongly improves the state-of-the-art result for several data-sets. For instance, for the PTC data-set, we improve the state-of-the-art result for more than 22 %.
* **Keywords:** Graph classification, Deep Learning, Graph pooling, Embedding
* **TL;DR:** The graph analysis problem is transformed into a point cloud analysis problem.

# Mostafa Rahmani

### Baidu

#### Names

Mostafa Rahmani (Preferred)

#### Emails

r\*\*\*\*t@gmail.com

#### Personal Links

#### Education & Career History

**Researcher**

Baidu (baidu.com)

2018 – Present

#### Advisors, Relations & Conflicts

*No relations found*

#### Expertise

*No areas of expertise listed*

# Ping Li

### Baidu

#### Names

Ping Li (Preferred)

#### Emails

p\*\*\*\*8@gmail.com,

l\*\*\*\*1@baidu.com

#### Personal Links

#### Education & Career History

**Researcher**

Baidu (baidu.com)

2018 – Present

#### Advisors, Relations & Conflicts

*No relations found*

#### Expertise

*No areas of expertise listed*