Composition-based Multi-Relational Graph Convolutional Networks

Shikhar Vashishth*¹,²
svashish@cs.cmu.edu

Soumya Sanyal*¹
soumyasanyal@iisc.ac.in

Vikram Nitin¹,³
vikram.nitin@columbia.edu

Partha Talukdar¹
ppt@iisc.ac.in

¹Indian Institute of Science, ²Carnegie Mellon University, ³Columbia University
Multi-relational Graphs

- Graphs with **directed-labeled edges**
- Multi-relational graphs are **pervasive**, examples include...

Knowledge Graphs

Proteins

Dependency Parse
Graph Convolutional Networks (GCNs)

Most GCN formulations are for simple undirected graphs

Naive extension of GCNs to Multi-relational graphs using relation-specific filter matrix (W)

- Suffers from overparameterization
Existing Multi-Relational GCN models

<table>
<thead>
<tr>
<th>Methods</th>
<th>Node Embeddings</th>
<th>Directions</th>
<th>Relations</th>
<th>Relation Embeddings</th>
</tr>
</thead>
<tbody>
<tr>
<td>GCN Kipf &amp; Welling (2016)</td>
<td>✓</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Directed-GCN Marcheggiani &amp; Titov (2017)</td>
<td>✓</td>
<td>✓</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Weighted-GCN Shang et al. (2019)</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>Relational-GCN Schlichtkrull et al. (2017)</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
</tbody>
</table>

- **Directed-GCN**: Utilizes direction-specific filter matrix
- **Weighted-GCN**: Learns a scalar weight for each relation
- **Relational-GCN**: Relation-specific filters in terms of basis matrices

Although solve overparameterization to different degrees of granularity, none of them learn relation embeddings
Motivation

● Extensive research done on embedding Knowledge Graphs where representations of both nodes and relations are jointly learned.

● Can we develop a **GCN framework** that can leverage the advances in KGE approaches to:
  ○ Learn both node and relation embeddings
  ○ Solve the issue of overparameterization
Contributions

- We propose **CompGCN**, a novel framework for incorporating multi-relational information in GCNs which leverages a variety of composition operations from KG embedding techniques.

- Unlike previous GCN methods, CompGCN jointly learns to embed both nodes and relations in the graph.

<table>
<thead>
<tr>
<th>Methods</th>
<th>Node Embeddings</th>
<th>Directions</th>
<th>Relations</th>
<th>Relation Embeddings</th>
</tr>
</thead>
<tbody>
<tr>
<td>GCN Kipf &amp; Welling (2016)</td>
<td>✓</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Directed-GCN Marcheggiani &amp; Titov (2017)</td>
<td>✓</td>
<td>✓</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Weighted-GCN Shang et al. (2019)</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>Relational-GCN Schluchtrull et al. (2017)</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>COMPGCN (Proposed Method)</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
</tbody>
</table>
CompGCN: Overview

- London
- United Kingdom
- Christopher Nolan
- The Dark Knight

Relationships:
- Born-in: London to Christopher Nolan
- Citizen-of: United Kingdom to Christopher Nolan
- Directed-by: Christopher Nolan to The Dark Knight
CompGCN: Overview
CompGCN: Overview

Relational Graph with Embeddings
CompGCN: Overview

Relational Graph with Embeddings

CompGCN Update
CompGCN: Update Equation

Node Update:

\[ h_{v}^{k+1} = f \left( \sum_{(u,r) \in N(v)} W_{g(r)}^k \phi(h_{u}^{k}, h_{r}^{k}) \right) \]

Composition Operation:

\[ W_{g(r)} = \begin{cases} W_{O}, & r \in \mathcal{R} \\ W_{I}, & r \in \mathcal{R}_{inv} \\ W_{S}, & r = \top \end{cases} \]

Summation over neighborhood of \( v \)

non-linearity

Original edges
Inverse Edges
Self Loops

Composition Operation:

\[ \phi(h_{u}^{k}, h_{r}^{k}) = \begin{cases} e_s - e_r & \text{Subtraction (TransE)} \\ e_s \times e_r & \text{Multiplication (DistMult)} \\ e_s \star e_r & \text{Circular-correlation (HolE)} \end{cases} \]

Relation Update:

\[ h_{r}^{k+1} = W_{rel}^k h_{r}^k \]
Evaluation Tasks

- **Link Prediction in Knowledge Graph**
  -Michelle Obama
  -Sasha Obama
  -Barack Obama
  -Link Prediction
  -Inferring missing links

- **Node Classification**
  -Michelle Obama
  -Sasha Obama
  -Barack Obama
  -Functional Group Classification

- **Graph Classification**
  -Carcinogenic
  -Molecule Classification
CompGCN: Link Prediction Results

- Effect of different GCN models and composition operators

ConvE + CompGCN(Corr) gives best performance across all settings.
CompGCN: Link Prediction Results

- **Performance on Link Prediction**

<table>
<thead>
<tr>
<th>Model</th>
<th>FB15k-237</th>
<th>WN18RR</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>MRR</td>
<td>H@10</td>
</tr>
<tr>
<td>R-GCN</td>
<td>.248</td>
<td>.417</td>
</tr>
<tr>
<td>ConvE</td>
<td>.325</td>
<td>.501</td>
</tr>
<tr>
<td>SACN</td>
<td>.35</td>
<td>.54</td>
</tr>
<tr>
<td>RotatE</td>
<td>.338</td>
<td>.533</td>
</tr>
<tr>
<td><strong>CompGCN</strong></td>
<td><strong>.355</strong></td>
<td><strong>.535</strong></td>
</tr>
</tbody>
</table>

**CompGCN provides a consistent improvement across all the datasets.**
CompGCN: Results

- Performance on **Node Classification and Graph Classification**

**Node classification Performance**

<table>
<thead>
<tr>
<th>Dataset</th>
<th>RGCN</th>
<th>WGCN</th>
<th>CompGCN</th>
</tr>
</thead>
<tbody>
<tr>
<td>MUTAG (Node)</td>
<td>70</td>
<td>82.5</td>
<td>90</td>
</tr>
<tr>
<td>AM</td>
<td>95</td>
<td>82.5</td>
<td>90</td>
</tr>
</tbody>
</table>

**Graph classification Performance**

<table>
<thead>
<tr>
<th>Dataset</th>
<th>RGCN</th>
<th>WGCN</th>
<th>CompGCN</th>
</tr>
</thead>
<tbody>
<tr>
<td>MUTAG (Graph)</td>
<td>65</td>
<td>77.5</td>
<td>90</td>
</tr>
<tr>
<td>PTC</td>
<td>65</td>
<td>77.5</td>
<td>90</td>
</tr>
</tbody>
</table>

**CompGCN outperforms or performs comparably to existing baselines.**
CompGCN: Scalability

- Effect of number of relation basis vectors and relations on FB15k-237

**COMPGCN** outperforms **RGCN** even with limited parameters.
Multi-relational graphs are prevalent in real-world problems.

Current GCN approaches mainly focus on simple undirected graphs.

We propose CompGCN, a parameter efficient method for embedding both nodes and relation types.

We demonstrate the effectiveness of CompGCN for link prediction, node and graph classification tasks.
Thank you!

Paper Link:
Composition-Based Multi-Relational Graph Convolutional Networks

Source Code:
github.com/malllabiisc/CompGCN

Research Supported by: