Large Scale Geometric Deep Learning

Shehtab Zaman
DSSI / Computing
Brian Van Essen, Tom Benson, Tim Moon, Same Ade Jacobs, and LBANN Team
Going Beyond Grids

- Deep Learning has been focused on Euclidean Domains
  - Image analysis, CV
- Graphs are ubiquitous in Biology, Physics, and Social Sciences
- We want Large Neural Networks to operate on Graph Structured Data
  - Large Graphs
  - Large Datasets

Graph Layers on LBANN

- Matrices to capture the information stored in Graphs
- Use Message Passing over connected nodes and edges to learn embeddings over the graph

\[ x'_i = g_\theta(x_i, \sum_{j \in N_i} h_\theta(x_i, x_j, e_{ij})) \]
Enabling Large Scale GNNs

- Livermore Big Artificial Neural Network (LBANN) toolkit is scalable deep learning toolkit
  - Optimized for distributed large-scale systems
- We can run GNNs on a large scale on multiple nodes

Scaling performance of GIN based Model

---

LLNL-PRES-813007