Large Scale Geometric Deep Learning

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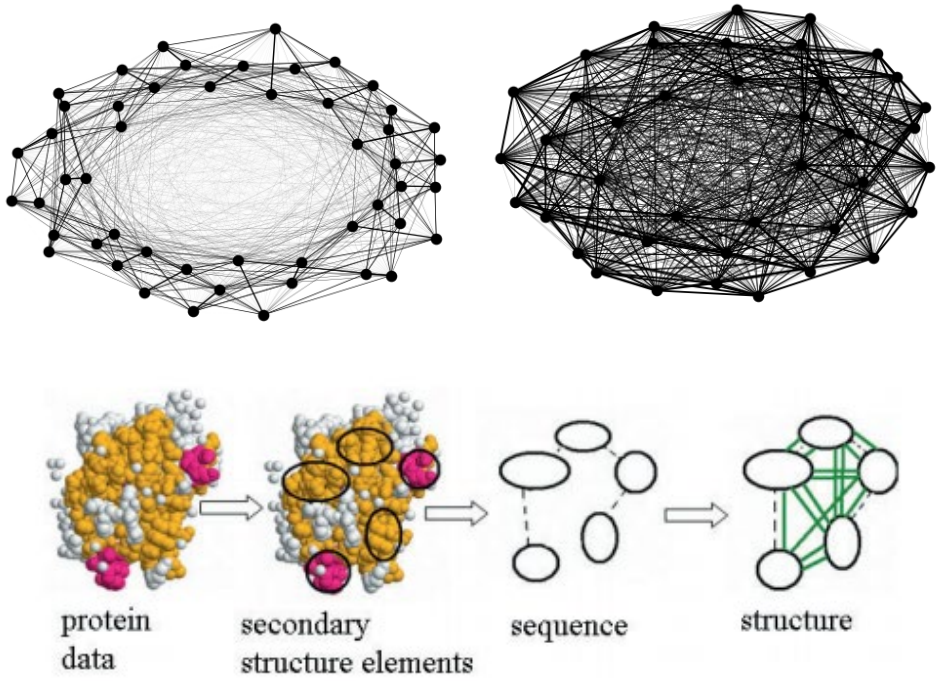
Going Beyond Grids

- 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

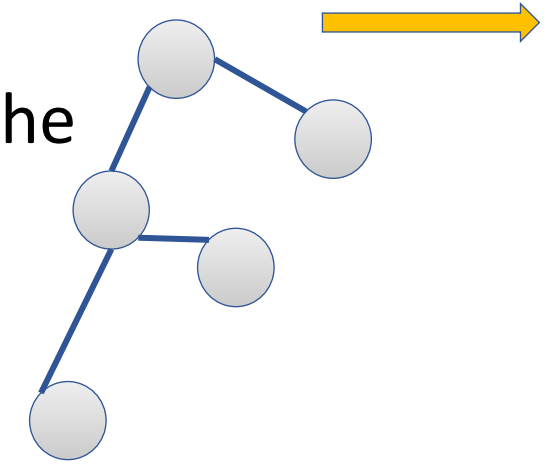


K. M. Borgwardt, C. S. Ong, S. Schoenauer, S. V. N. Vishwanathan, A. J. Smola, and H. P. Kriegel. Protein function prediction via graph kernels. Bioinformatics, 21(Suppl 1):i47–i56, Jun 2005.

Graph Layers on LBANN

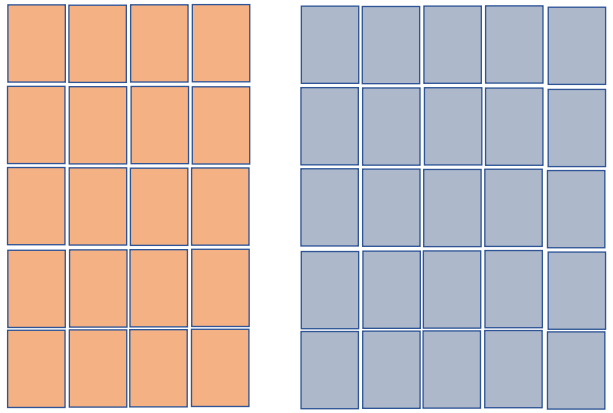
- Matrices to capture the information stored in Graphs
- Use Message Passing over connected nodes and edges to learn embeddings over the graph

$$\grave{x_i} = g_\theta(x_i, \sum_{j \in N_i} h_\theta(x_i, x_j, e_{ij}))$$

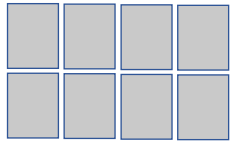


Node Features

Adjacency Matrix

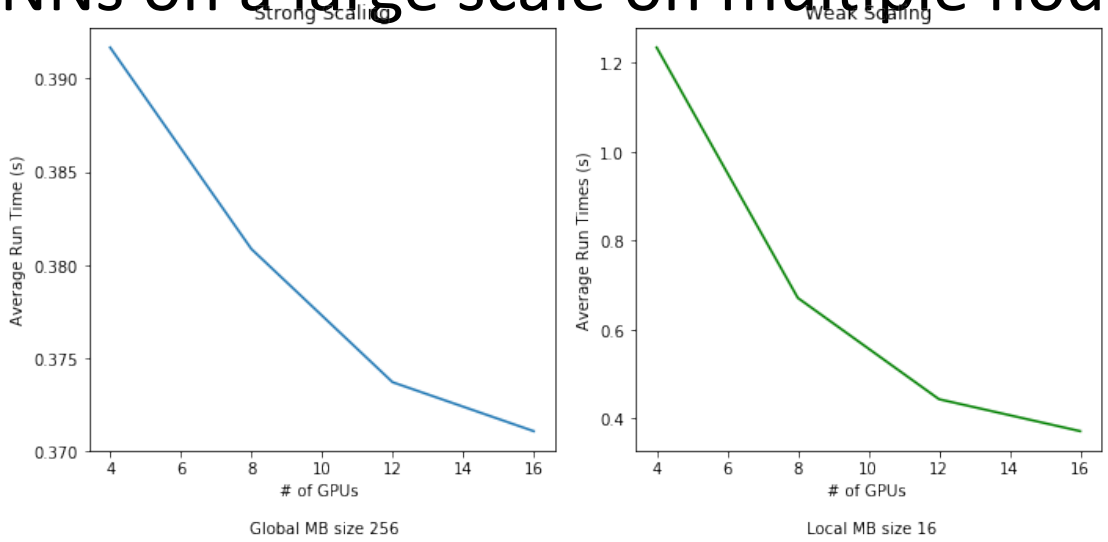


Edge Features



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

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