



Large Scale Geometric Deep Learning

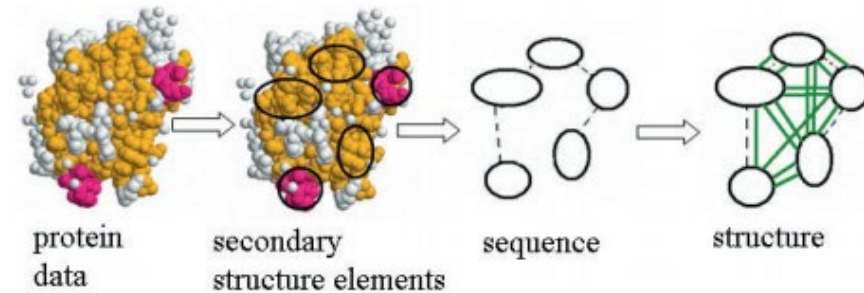
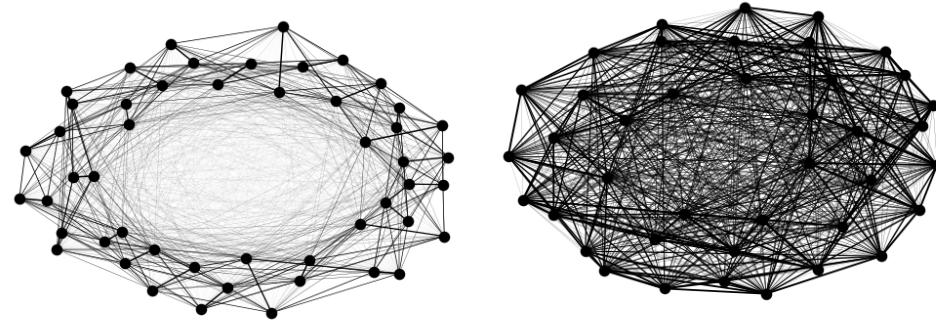
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Going Beyond Grids

- 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



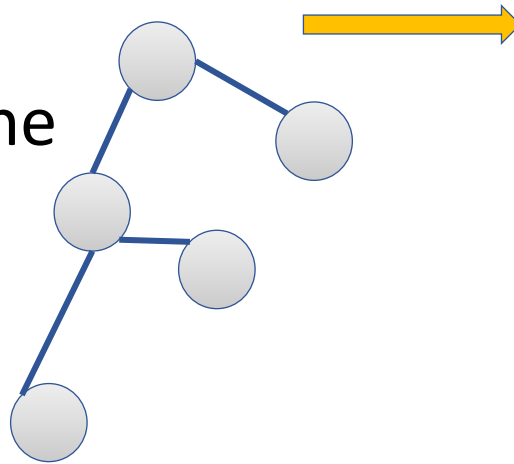
K. M. Borgwardt, C. S. Ong, S. Schoenauer, S. V. N. Vishwanathan, A. J. Smola, and H. P. Kriegel. [Protein function prediction via graph kernels](#). Bioinformatics, 21(Suppl 1):i47–i56, Jun 2005.



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

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



Node Features

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Adjacency Matrix

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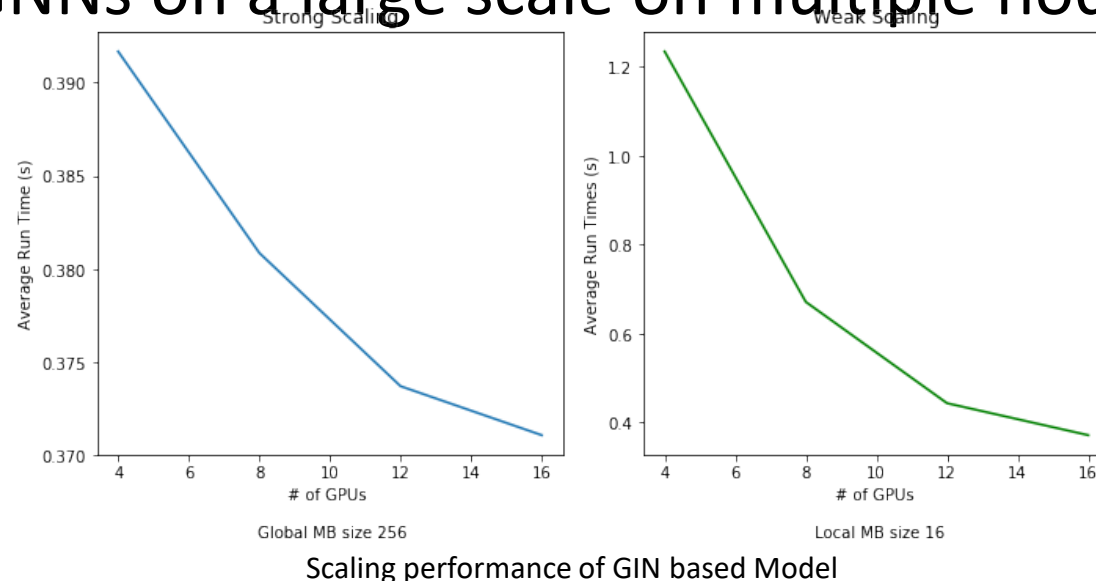
Edge Features

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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





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