Graph Neural Networks

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1 Graph Neural Networks

Graph Neural Networks (GNN) are a recent subfield of machine learning for processing data that can be represented as graphs. More generally, graph neural network belongs to the class of "Geometric Neural Networks".

Graph neural networks can be used for data without order preference, and can be applied to irregular non-Euclidean data structures such as chemical molecules, social networks, meshes, etc.

2 GNN Layer Architectures

There are 3 main architectures for GNNs: Permutation equivariant, local pooling, and global pooling (permutation invariant).

2.1 Permutation Equivariant Layer

Permutation equivariant layer maps a representation of the graph into an updated representation of the same graph.

2.2 Local Pooling Layer

Local pooling layer 'coarsens' the given graph structure by convoluting a local structure of nodes into a smaller set of nodes.

2.3 Global Pooling (permutation invariant) Layer

Global pooling layer aggregates the given graph structure into a single output. The layer is "permutation invariant" as the output of the layer shouldn't be dependent on the ordering of the node aggregation.

3 Graph Convolutional Network

Graph Convolutional Network is a convolutional layer that generalizes over all toplogies unlike traditional convolutional layer which only operates on grid-like Euclidean data.

Given a graph as an input, the output will return a set of updated node features that have aggregated the local nodes' features and of itself.

A single pass into the grah convolutional layer will have a receptive field of 1-hop, meaning the update will aggregate features of nodes that are 1 away from the node being updated. k number of graph convolutional layer will correspond to the nodes having a receptive field of k hops.

4 Manifold Learning

Manifold learning, also referred to as nonlinear dimensionality reduction refers to techniques that attempt to reduce high-dimensional data into lower-dimensional data.

GNNs although not explicitly a dimensionality reductino methodology, can be designed to exploit the local dynamics throughout the graph. As a result, given a high-dimensional data that is known to have dynamics defined locally, can be broken up into subsets of local interactions.

5 Speculations of GNNs in building science

Many layers of the operations and dynamics within buildings can be understood as graph structured data.

For instance, the thermal interactions between building components will have high-dimensionality due to the complexity of the buildings, the heat-exchange interactions are dominated by the spatially local building compo-

nents, and a GNN trained on the local heat exchange dynamics can potential be used to infer about the entire building heat exchange data.