Graph Attention Networks

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Networks are the backbone of modern society, including transportation networks, biological networks, and social networks. The surging demand for tackling graph-structured data motivates the development of Graph Neural Networks (GNNs), which is a generalization of recursive neural networks and can directly deal with a general class of graphs. GNNs consist of an iterative process, where each node in the graph aggregates its one-hop neighbors' states until equilibrium. Over the past few years, there is an increasing interest in devising a more efficient aggregator over the network. In this paper, the authors develop the graph attention networks (GATs), incorporating GNN architectures with the self-attention mechanisms. In GATs, each node learns how to automatically distribute different attentions over its neighbors. Specifically, a network of nodes share an attentional mechanism to compute the attention coefficients. The coefficients of each node indicate the importance of the information given by each of its neighbors to the node itself. Compared to the prior approaches modeling graph-structured data with neural networks, this attention-based architecture has several appealing properties. First, the self-attention operation is more computationally efficient, since it can be parallelized across all edges without requiring any additional costly matrix operations. Further, the proposed attention mechanism allows each node to assign different importances to the nodes in its neighborhood. Also, since GAT does not depend on knowing the global graph structure upfront , it is readily applicable to inductive as well as transductive learning problems, including tasks where the graphs are completely unseen during the training.