

论文学习笔记 (4): 一些公式

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1 图神经网络中的一些测试环境

$$h_{v_i}^{(l+1)} = \sigma \left(\sum_j \frac{1}{c_{ij}} h_{v_j}^{(l)} W^{(l)} \right),$$

Get features $\{h_{v_j}\}$ of neighboring nodes $\{v_j\}$ Update node feature $h_{v_i} \leftarrow \text{hash} \left(\sum_j h_{v_j} \right)$, where $\text{hash}(\cdot)$ is (ideally) an injective hash function

where j indexes the neighboring nodes of v_i . c_{ij} is a normalization constant for the edge (v_i, v_j) which originates from using the symmetrically normalized adjacency matrix $D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$ in our GCN model. We now see that this propagation rule can be interpreted as a differentiable and parameterized (with $W^{(l)}$) variant of the hash function used in the original Weisfeiler-Lehman algorithm. If we now choose an appropriate non-linearity and initialize the random weight matrix such that it is orthogonal (or e.g. using the initialization from Glorot & Bengio, AISTATS 2010), this update rule becomes stable in practice (also thanks to the normalization with c_{ij}). And we make the remarkable observation that we get meaningful smooth embeddings where we can interpret distance as (dis-)similarity of local graph structures!