GRAPH CONVOLUTIONAL NETWORKS

Primary Texts:

Graph Representation Learning - William L. Hamilton (2020)
Semi-Supervised Classification with Graph Convolutional Networks - Kipf & Welling (2017)

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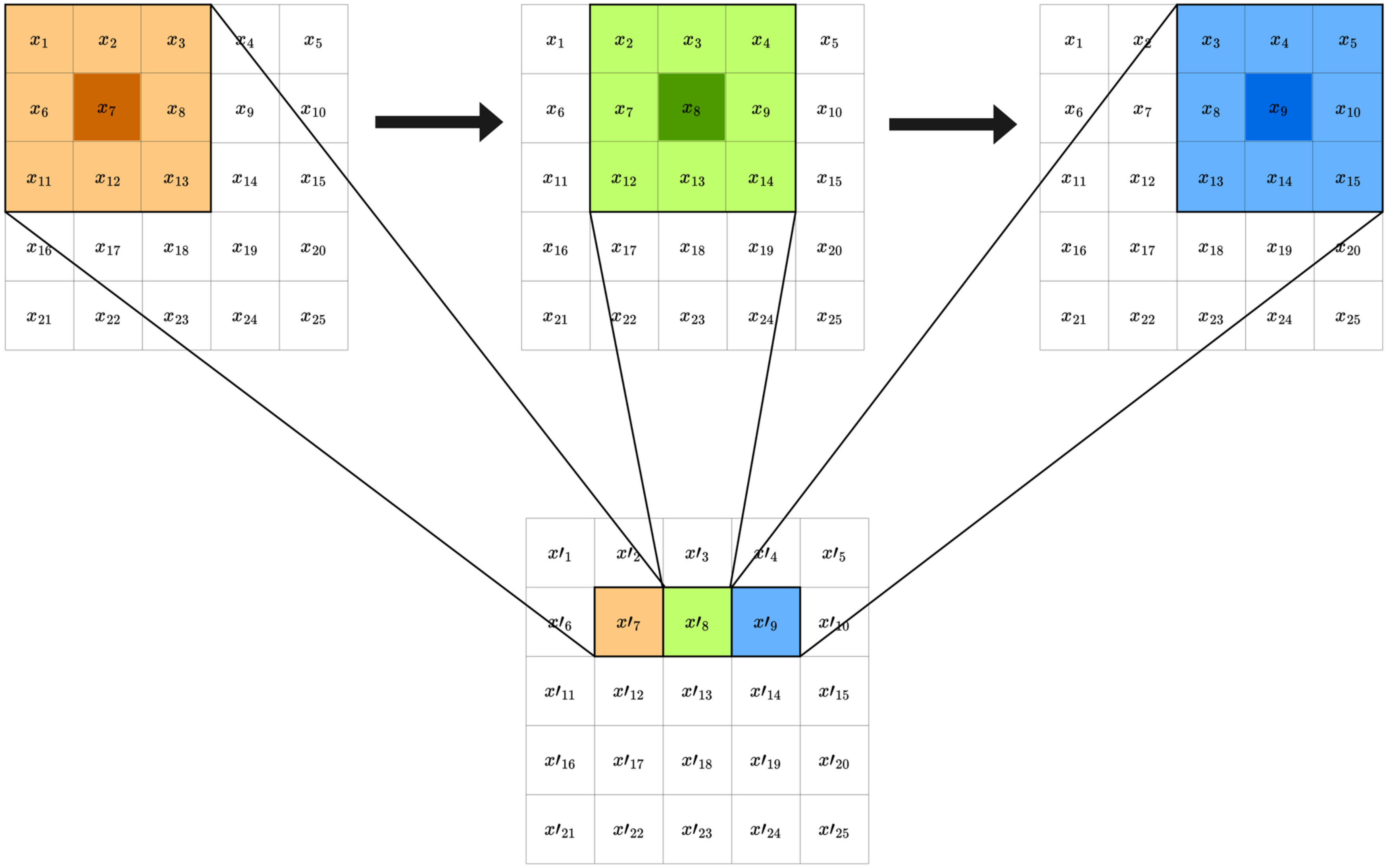
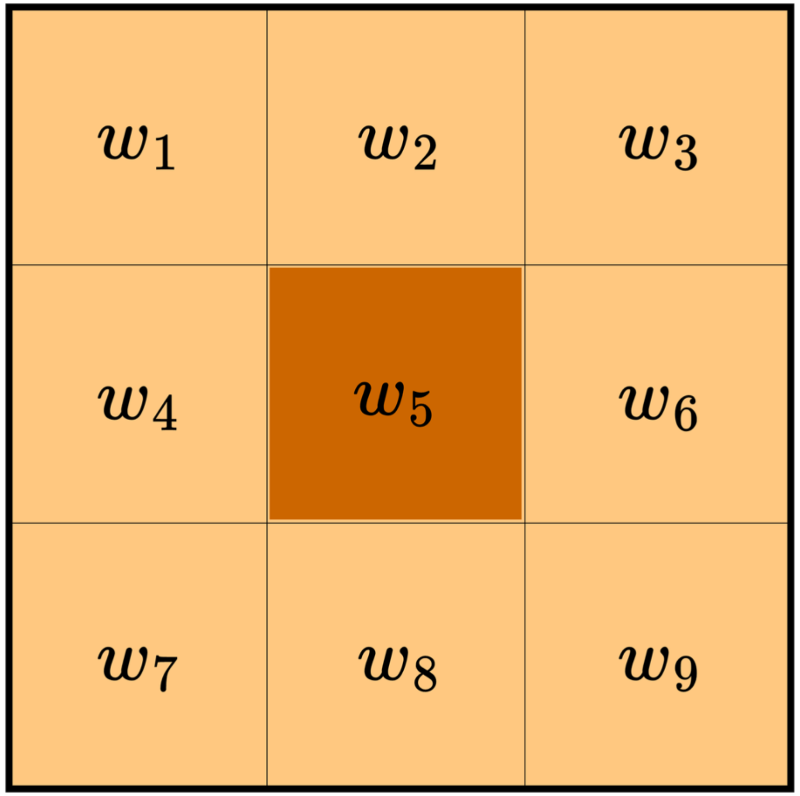
Mentored by **Jennifer Vaccaro**

Convolution on Grid Structured Data



Kernel in Grid Convolution



$$x'_5 = \sum_{i=1}^{9} w_i x_i$$

Convolutional Neural Network Connectivity Defined by Kernel

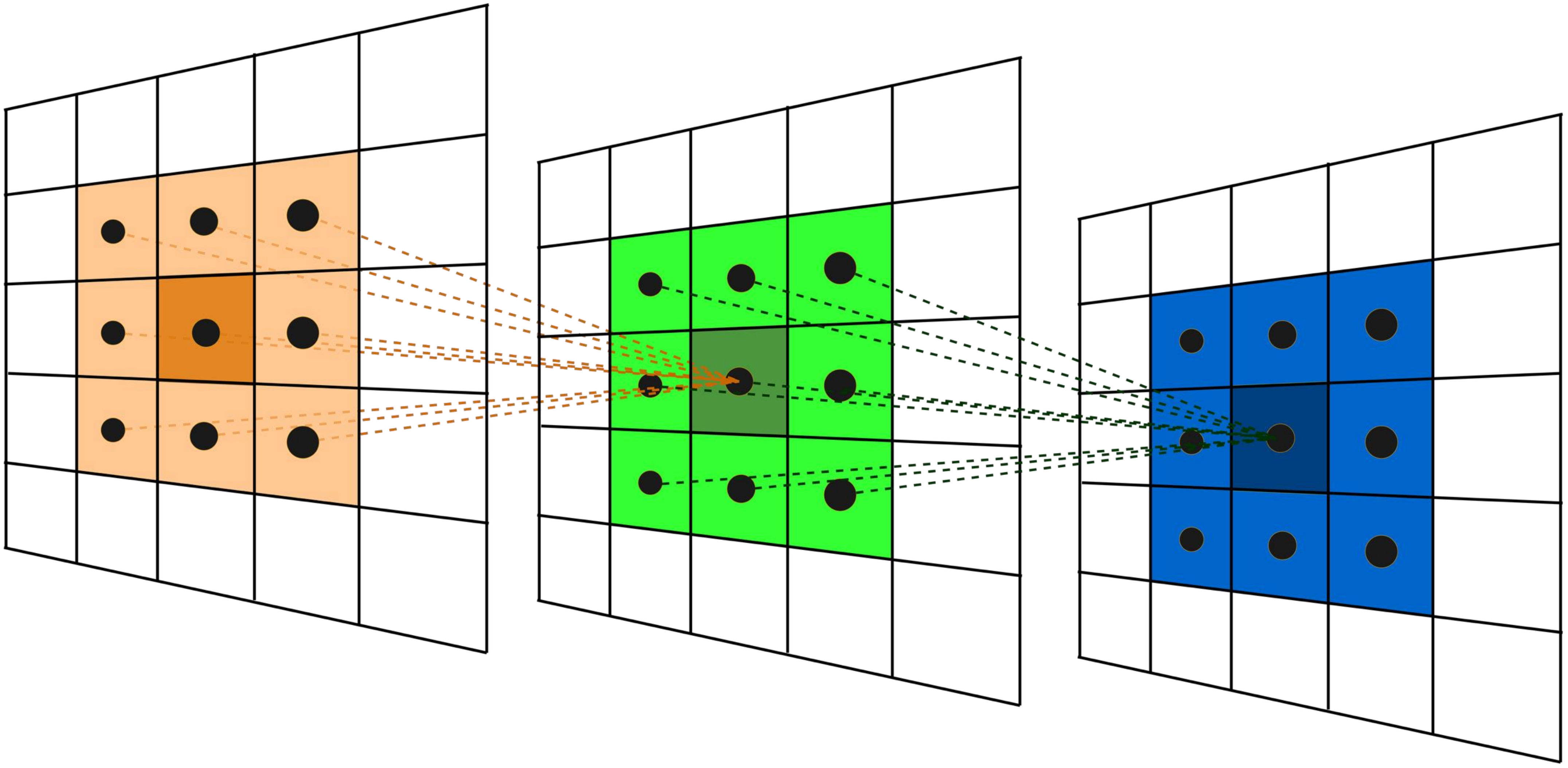
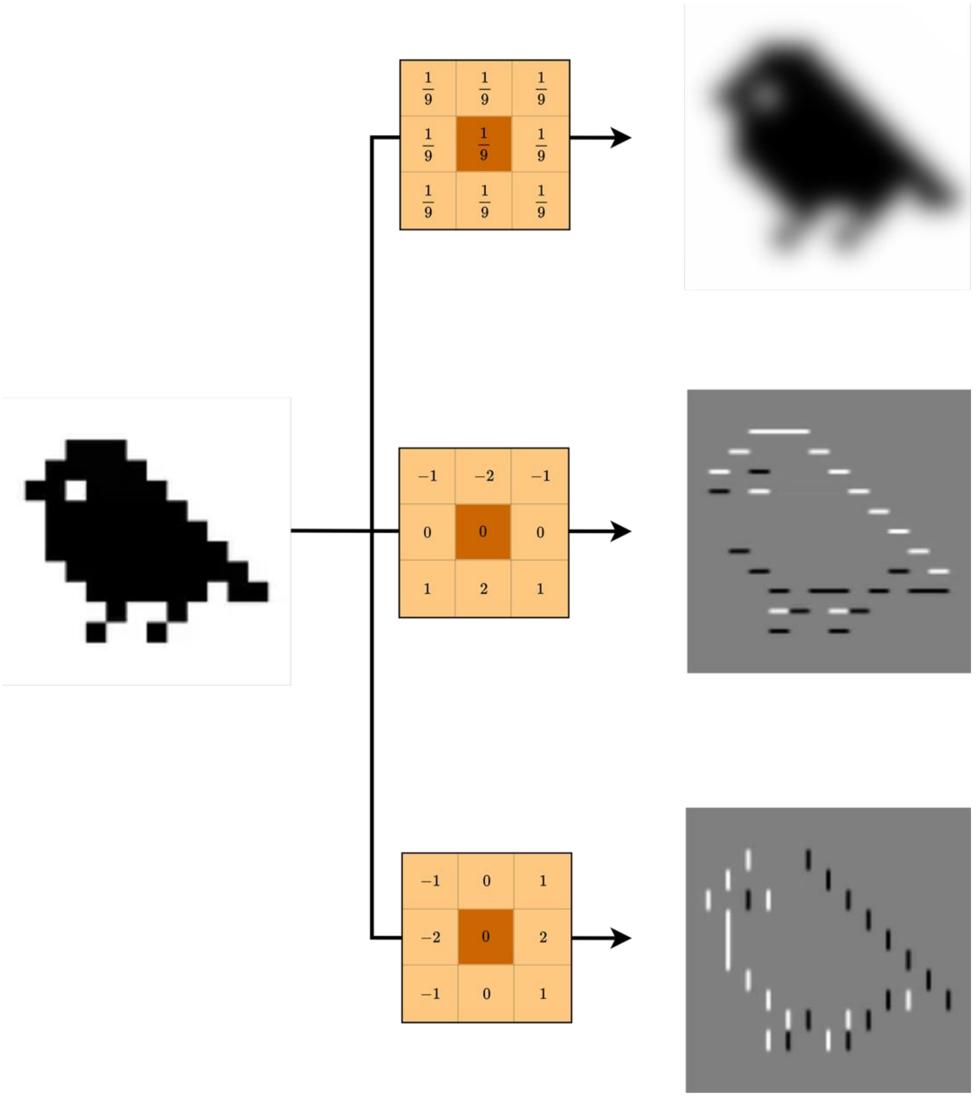
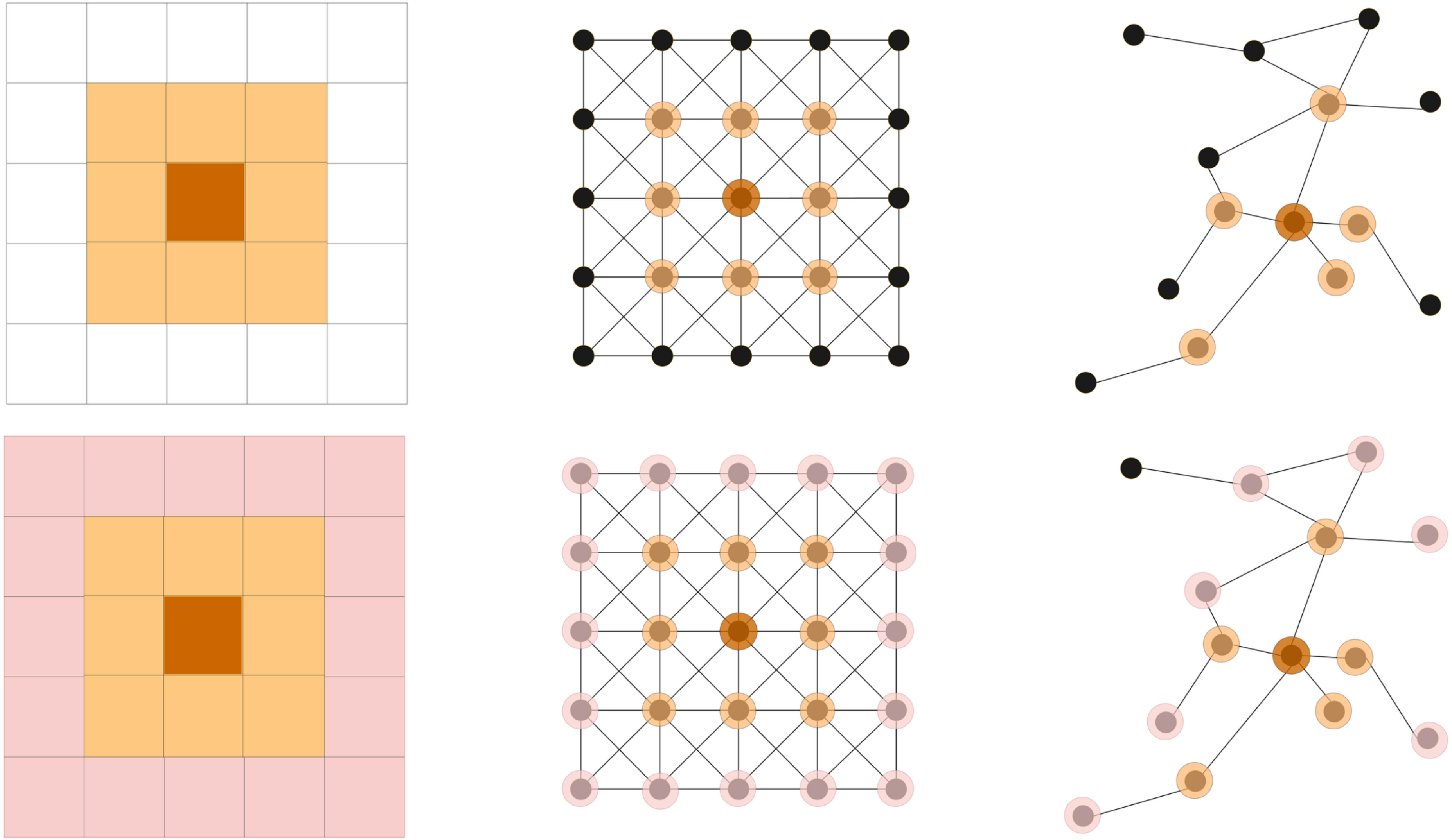


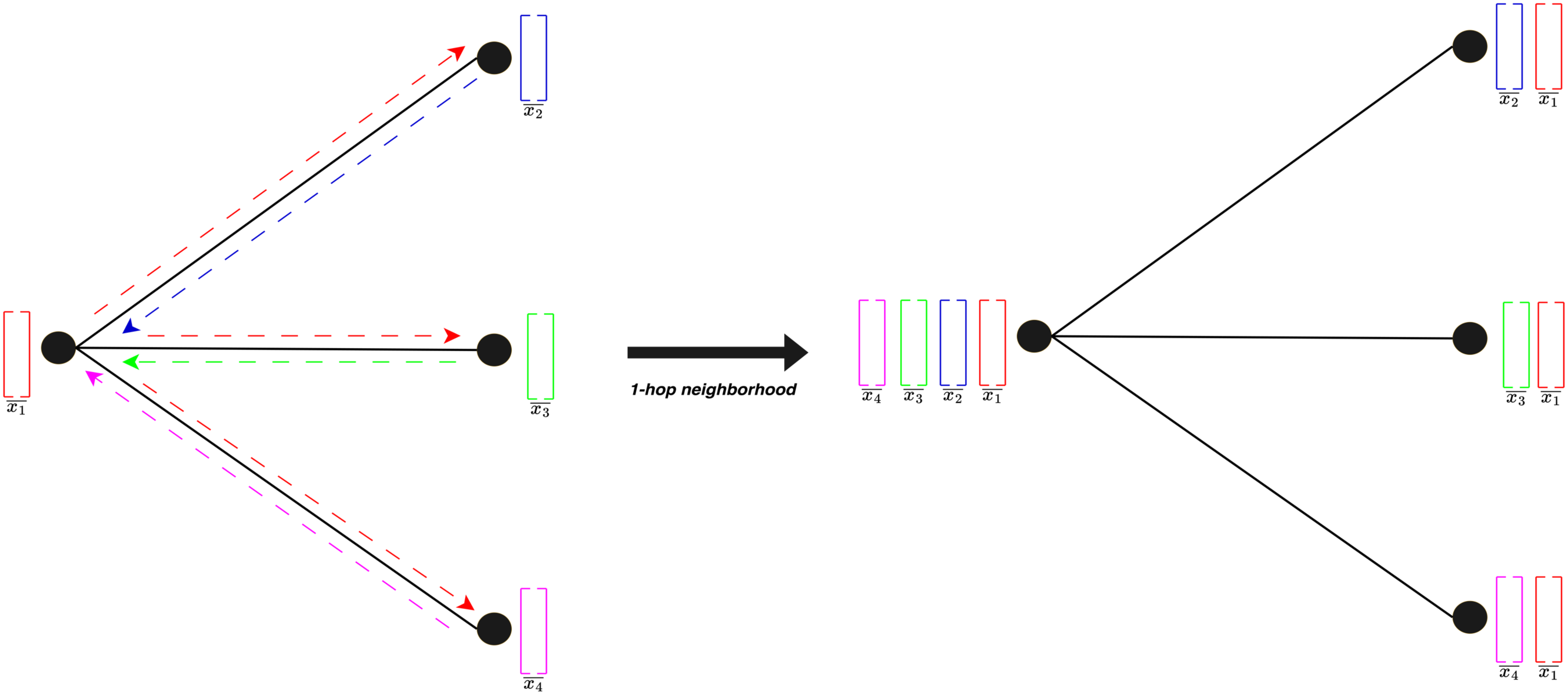
Image Convolution – Kernel Effect



Grids as Special Graphs



Message Passing on Graphs



Unnormalized Message Passing Step

$$H^{(l+1)} = \widetilde{A}H^{(l)} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \overrightarrow{x_1} \\ \overrightarrow{x_2} \\ \overrightarrow{x_3} \\ \overrightarrow{x_4} \end{bmatrix} = \begin{bmatrix} \overrightarrow{x_1} + \overrightarrow{x_2} + \overrightarrow{x_3} + \overrightarrow{x_4} \\ \overrightarrow{x_1} + \overrightarrow{x_2} \\ \overrightarrow{x_1} + \overrightarrow{x_3} \\ \overrightarrow{x_1} + \overrightarrow{x_4} \end{bmatrix}$$

(Where $\widetilde{A} = A + I$)

Degree Normalized Message Passing Step

$$H^{(l+1)} = \boxed{\widetilde{D}^{-\frac{1}{2}}\widetilde{A}\widetilde{D}^{-\frac{1}{2}}} H^{(l)} = \begin{bmatrix} \frac{1}{4}\vec{x}_1 + \frac{1}{\sqrt{8}}\vec{x}_2 + \frac{1}{\sqrt{8}}\vec{x}_3 + \frac{1}{\sqrt{8}}\vec{x}_4 \\ \frac{1}{\sqrt{8}}\vec{x}_1 + \frac{1}{2}\vec{x}_2 \\ \frac{1}{\sqrt{8}}\vec{x}_1 + \frac{1}{2}\vec{x}_3 \\ \frac{1}{\sqrt{8}}\vec{x}_1 + \frac{1}{2}\vec{x}_4 \end{bmatrix}$$

$$\boxed{\widetilde{a}_{ij} = \frac{\widetilde{a}_{ij}}{\sqrt{d_i d_j}}}$$

A layer in a Graph Convolutional Network

$$H^{(l+1)} = \boxed{\sigma}\left(\widetilde{D}^{-\frac{1}{2}}\widetilde{A}\widetilde{D}^{-\frac{1}{2}}H^{(l)}\boxed{W^{(l)}}\right)$$

Non-linear Activation Function

Linear Projection Matrix

$$W^{(l)} = \begin{bmatrix} \overrightarrow{w_1} \\ \overrightarrow{w_2} \\ \overrightarrow{w_3} \\ \overrightarrow{w_4} \end{bmatrix}$$

References

Daigavane, Ameya, Balaraman Ravindran, and Gaurav Aggarwal. 2021. "Understanding Convolutions on Graphs." *Distill* 6 (9): e32. https://doi.org/10.23915/distill.00032.

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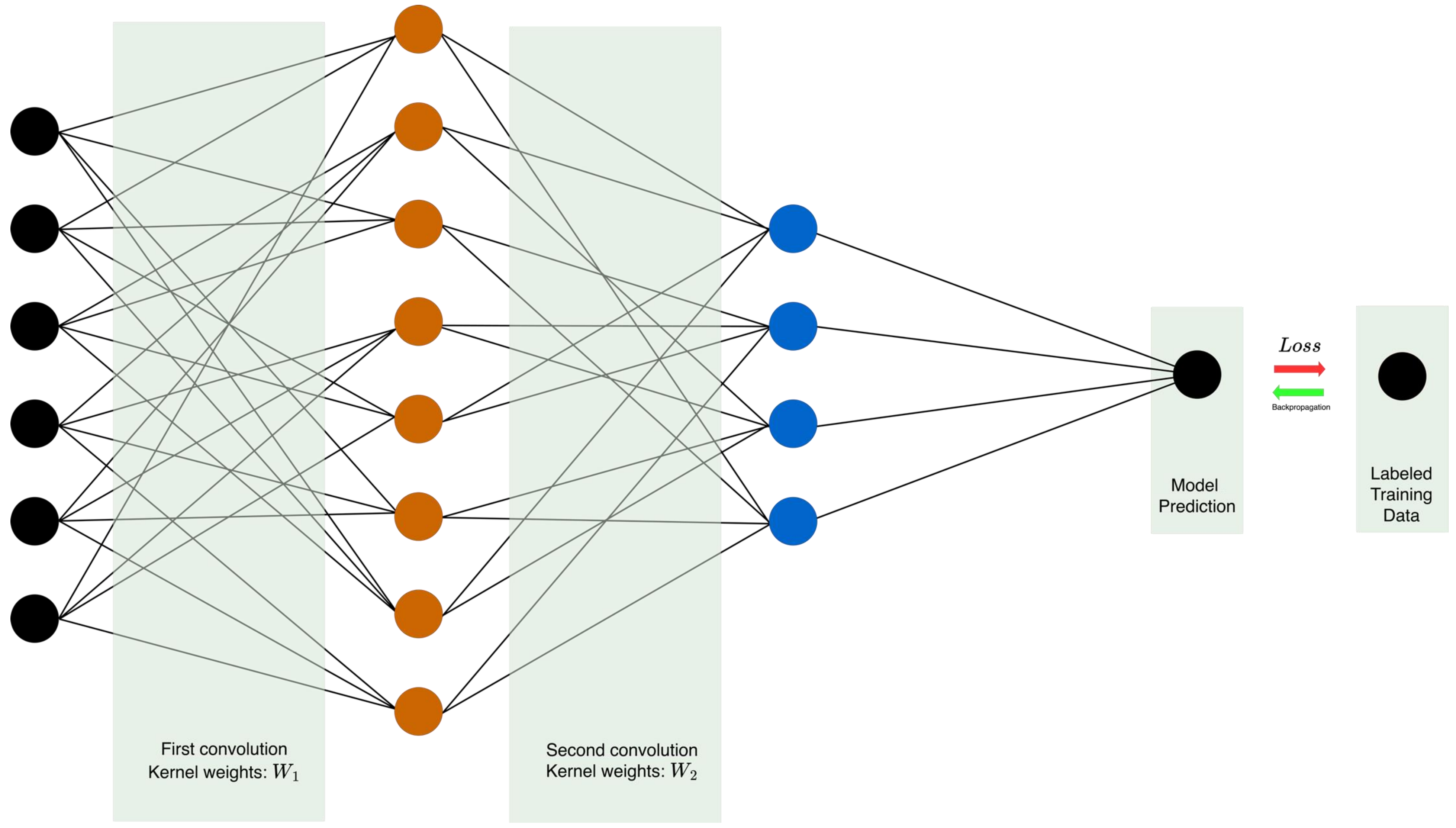
Jiang, Hao, Peng Cao, MingYi Xu, Jinzhu Yang, and Osmar Zaiane. 2020. "Hi-GCN: A Hierarchical Graph Convolution Network for Graph Embedding Learning of Brain Network and Brain Disorders Prediction." *Computers in Biology and Medicine* 127 (December):104096. https://doi.org/10.1016/j.compbiomed.2020.104096.

Kipf, Thomas N., and Max Welling. 2017. "Semi-Supervised Classification with Graph Convolutional Networks." arXiv. https://doi.org/10.48550/arXiv.1609.02907.

Sanchez-Lengeling, Benjamin, Emily Reif, Adam Pearce, and Alexander B. Wiltschko. 2021. "A Gentle Introduction to Graph Neural Networks." *Distill* 6 (9): e33. https://doi.org/10.23915/distill.00033.

Wilson, Robin J. 1972. *Introduction to Graph Theory*. New York, Academic Press. http://archive.org/details/introductiontogr00wils.

Extras: Convolutional Neural Network



Degree Normalized Adjacency

$$\widetilde{D} = \begin{bmatrix} 4 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix} \longrightarrow \widetilde{D}^{-\frac{1}{2}} = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} \end{bmatrix} \longrightarrow \widetilde{D}^{-\frac{1}{2}}\widetilde{A}\widetilde{D}^{-\frac{1}{2}} = \begin{bmatrix} \frac{1}{4} & \frac{1}{\sqrt{8}} & \frac{1}{\sqrt{8}} & \frac{1}{\sqrt{8}} \\ \frac{1}{\sqrt{8}} & \frac{1}{2} & 0 & 0 \\ \frac{1}{\sqrt{8}} & 0 & \frac{1}{2} & 0 \\ \frac{1}{\sqrt{8}} & 0 & 0 & \frac{1}{2} \end{bmatrix}$$

GCN Layer

$$H^{(l+1)} = \sigma\left(\widetilde{D}^{-\frac{1}{2}}\widetilde{A}\widetilde{D}^{-\frac{1}{2}}H^{(l)}W^{l}\right) = \begin{bmatrix} \frac{1}{4}\overrightarrow{x_1} + \frac{1}{\sqrt{8}}\overrightarrow{x_2} + \frac{1}{\sqrt{8}}\overrightarrow{x_3} + \frac{1}{\sqrt{8}}\overrightarrow{x_4} \\ \frac{1}{\sqrt{8}}\overrightarrow{x_1} + \frac{1}{2}\overrightarrow{x_2} \\ \frac{1}{\sqrt{8}}\overrightarrow{x_1} + \frac{1}{2}\overrightarrow{x_3} \\ \frac{1}{\sqrt{8}}\overrightarrow{x_1} + \frac{1}{2}\overrightarrow{x_4} \end{bmatrix} \begin{bmatrix} \overrightarrow{W_1} \\ \overrightarrow{W_2} \\ \overrightarrow{W_3} \\ \overrightarrow{W_4} \end{bmatrix}$$