Semi-supervised classification with graph convolutional networks by Kipf and Welling

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Node representations $H^{(l)}$ are embedded recursively following

$$H^{(l+1)} = \sigma\left(W^{(l)} H^{(l)} \hat{A}\right), \tag{1}$$

where

1. column i of $H^{(l)}$ is the l-th embedding $h_i^{(l)}$ of node i
2. $H^{(0)} = X$ where X are graph feature vectors
3. $W^{(l)}$ is a matrix of adjustable weights
4. σ is a nonlinear function such as ReLU or tanh
5. $\hat{A}$ is a symmetrically normalised Laplacian with entries

$$\hat{A}_{ij} = \frac{A_{ij} + I_{ij}}{\sqrt{(k_i + 1)(k_j + 1)}}.$$

$$
\begin{aligned}
H^{(0)} &= X && \text{(2a)}\\
M^{(0)} &= H^{(0)}\hat{A} && \text{(2b)}\\
H^{(1)} &= \mathsf{ReLU}\left(W^{(0)}M^{(0)}\right) && \text{(2c)}\\
M^{(1)} &= H^{(1)}\hat{A} && \text{(2d)}\\
H^{(2)} &= \mathsf{softmax}\left(W^{(1)}M^{(1)}\right) && \text{(2e)}
\end{aligned}
$$

Figure 1: Zachary karate club coloured using Louvain method in *Gephi*.

$$
\begin{aligned}
\mathrm{H}^{(0)} &= \mathrm{X} && \text{(3a)}\\
\mathrm{M}^{(0)} &= \mathrm{H}^{(0)}\hat{\mathrm{A}} && \text{(3b)}\\
\mathrm{H}^{(1)} &= \tanh\left(W^{(0)}\mathrm{M}^{(0)}\right) && \text{(3c)}\\
\mathrm{M}^{(1)} &= \mathrm{H}^{(1)}\hat{\mathrm{A}} && \text{(3d)}\\
\mathrm{H}^{(2)} &= \tanh\left(W^{(1)}\mathrm{M}^{(1)}\right) && \text{(3e)}\\
\mathrm{M}^{(2)} &= \mathrm{H}^{(2)}\hat{\mathrm{A}} && \text{(3f)}\\
\mathrm{H}^{(3)} &= \tanh\left(W^{(2)}\mathrm{M}^{(2)}\right) && \text{(3g)}\\
\mathrm{M}^{(3)} &= \mathrm{H}^{(3)}\hat{\mathrm{A}} && \text{(3h)}\\
Z = \mathrm{H}^{(4)} &= \mathrm{softmax}\left(W^{(4)}\mathrm{M}^{(4)}\right) && \text{(3i)}
\end{aligned}
$$

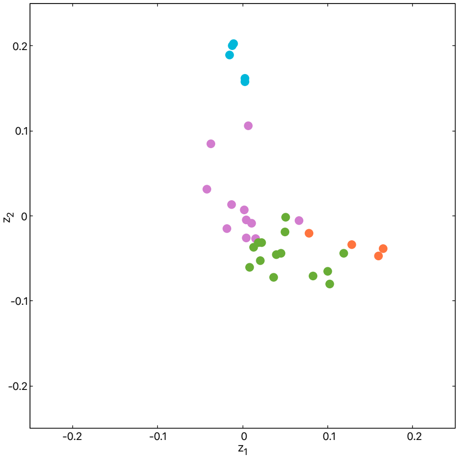


Figure 2: Unsupervised embedding of Zachary karate club.

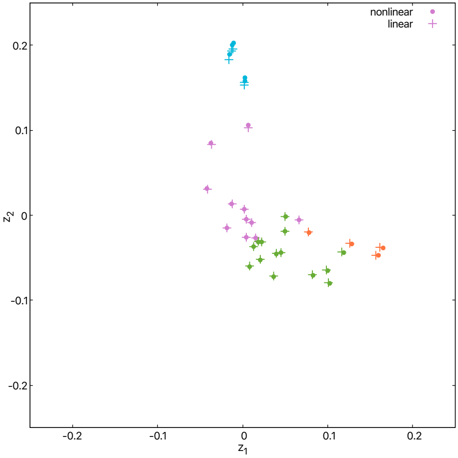


Figure 3: Comparing $\sigma(\tilde{H}^{(l)}) = \tanh(\tilde{H}^{(l)})$ and $\mathrm{id}(\tilde{H}^{(l)})$.

We add a softmax layer and apply the cross-entropy loss

$$\mathcal{L} = -\sum_{l \in \mathcal{Y}_L} \sum_{f} Y_{fl} \ln Z_{fl} \tag{4}$$

where

1. $\mathcal{Y}_L$ contains indices of nodes that are labelled
2. $f \in \{0, 1, 2, 3\}$ indexes the node classes in Zachary
3. $Y_{fl} \in \{0, 1\}$ indicates class membership of node l
4. $Z_{fl} = H_{fl}^{(4)} = \text{softmax}(h_{fl}^{(4)})$ is normalised output data.

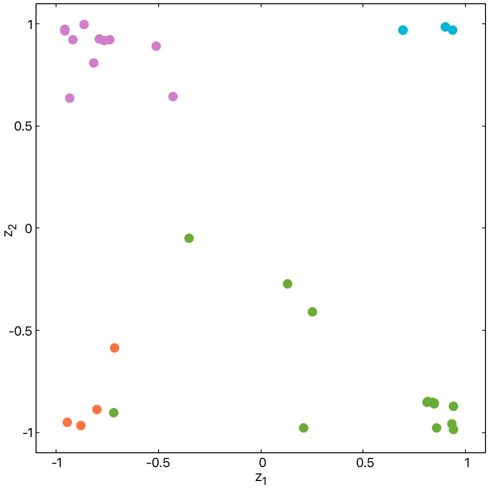
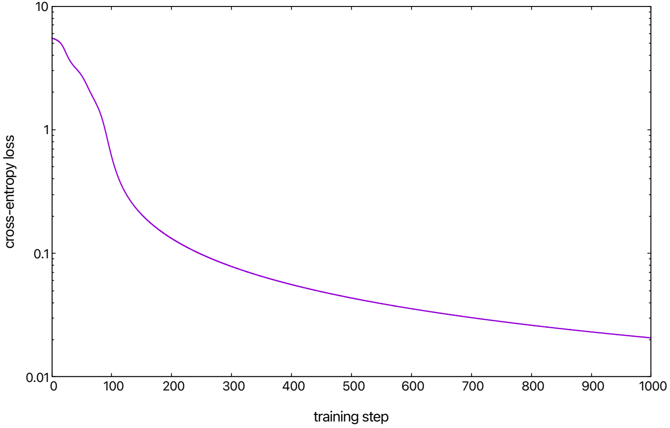


Figure 4: Semi-supervised embedding of Zachary in two dimensions


10
1
0.1
0.01
0
100
200
300
400
500
600
700
800
900
1000
training step
cross-entropy loss

Change in $\mathcal{L}$ due to a change in w_{ji} is

$$\frac{\partial \mathcal{L}}{\partial w_{ji}} = \sum_{\alpha} \frac{\partial \mathcal{L}}{\partial h_j^\alpha} \frac{\partial h_j^\alpha}{\partial w_{ji}} = \sum_{\alpha} \delta_j^\alpha m_i^\alpha, \tag{5}$$

where α runs over node indices $\{1, \ldots, |\mathcal{V}|\}$. Then,

$$\begin{aligned} \delta_j^\alpha \equiv \frac{\partial \mathcal{L}}{\partial h_j^\alpha} &= \sum_k \frac{\partial \mathcal{L}}{\partial h_k^\alpha} \frac{\partial h_k^\alpha}{\partial h_j^\alpha} + \sum_\beta \sum_k \frac{\partial \mathcal{L}}{\partial h_k^\beta} \frac{\partial h_k^\beta}{\partial h_j^\alpha} \\ &= \sum_k \delta_k^\alpha \frac{\partial h_k^\alpha}{\partial h_j^\alpha} + \sum_\beta \sum_k \delta_k^\beta \frac{\partial h_k^\beta}{\partial h_j^\alpha} \end{aligned} \tag{6}$$

where k runs over all cells from j, and $\beta \in \text{neighbours}(\alpha)$, with

$$\frac{\partial h_k^\alpha}{\partial h_j^\alpha} = w_{kj} \frac{\sigma'(h_j^\alpha)}{k_\alpha + 1} \quad \text{and} \quad \frac{\partial h_k^\beta}{\partial h_j^\alpha} = w_{kj} \frac{\sigma'(h_j^\alpha)}{\sqrt{(k_\alpha + 1)(k_\beta + 1)}}. \tag{7}$$

Compare backpropagation $\nabla\mathcal{L}^{(\mathsf{b})}$ to numerical differentiation $\nabla\mathcal{L}^{(\mathsf{b})}$,

$$\frac{\partial\mathcal{L}^{(\mathsf{d})}}{\partial w_{ji}} = \frac{\mathcal{L}(w_{ji}+\epsilon)-\mathcal{L}(w_{ji}-\epsilon)}{2\epsilon} + \mathcal{O}(\epsilon^2). \tag{8}$$

Both forward and backward passes involve $\mathcal{O}(|\mathcal{E}|)$ operations.

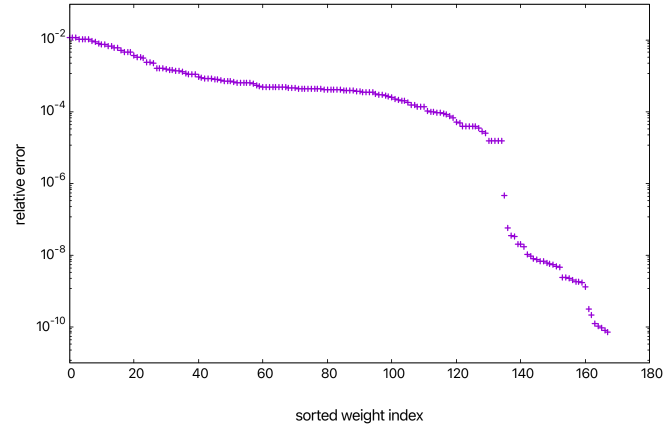


Figure 5: Sorted relative error in the gradients $\left|\nabla\mathcal{L}_i^{(b)} - \nabla\mathcal{L}_i^{(n)}\right| / \left|\nabla\mathcal{L}_i^{(b)}\right|$