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

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

Equation (9) of main text transforms X as

$$H^{(0)} = X \tag{2a}$$

$$M^{(0)} = H^{(0)}\hat{A} \tag{2b}$$

$$H^{(1)} = \mathsf{ReLU}\left(W^{(0)}M^{(0)}\right) \tag{2c}$$

$$M^{(1)} = H^{(1)}\hat{A} \tag{2d}$$

$$H^{(2)} = \mathsf{softmax}\left(W^{(1)}M^{(1)}\right) \tag{2e}$$

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

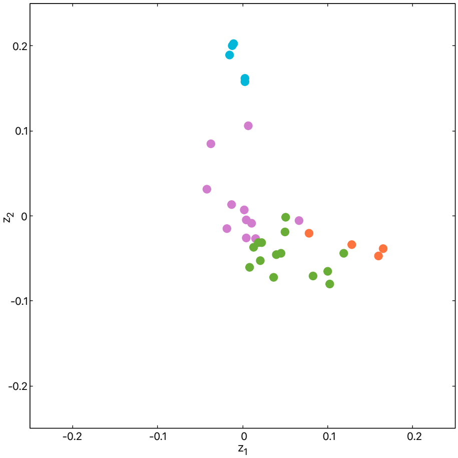


Figure 2: Unsupervised embedding of Zachary karate club.

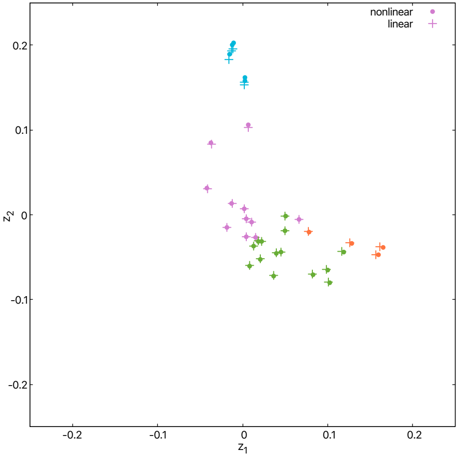


Figure 3: Comparing $\sigma(\tilde{H}^{(l)}) = \tanh(\tilde{H}^{(l)})$ and $\mathrm{id}(\tilde{H}^{(l)})$.

Semi-supervised embedding

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

$$\mathcal{L} = -\sum_{l \in \mathcal{Y}_L} \sum_{f} Y_{fl} \ln Z_{fl} \tag{3}$$

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. $Z_{fl} = H_{fl}^{(4)} = \mathrm{softmax}(h_{fl}^{(4)})$ is output data.

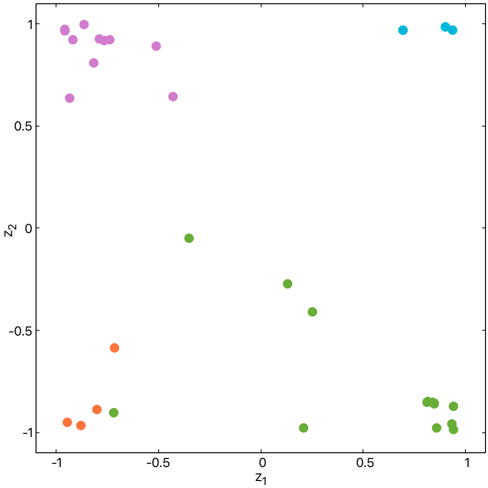
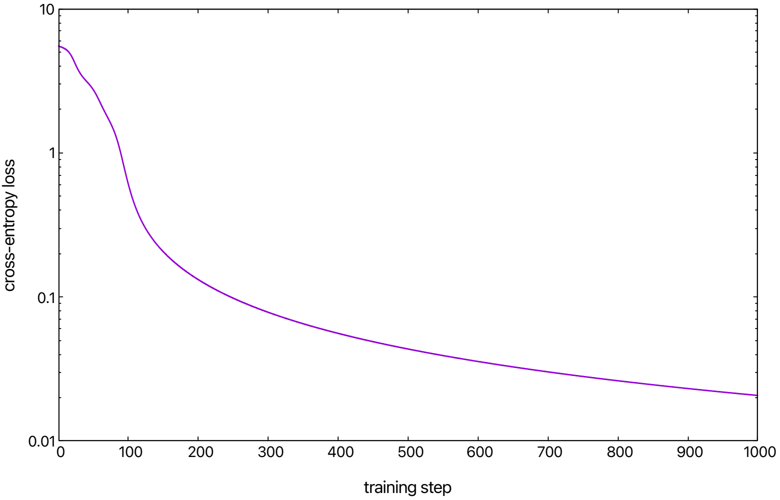


Figure 4: Semi-supervised embedding of Zachary in two dimensions


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