Question 1

Word2Vec creates the node-embeddings based on the the context of each node which in this case is the neighbouring nodes in the generated random walks. In a connected component, which is complete, the generated random walks will tend to have the same context as they are all connected. Therefore the embeddings of the nodes in a connected component will be approximately closer together in the embedding space. However two different connected components since they do not share an edge/node and hence context, their embeddings would not be the same. Therefore two different connected components will have 2 different clusters of embeddings in the embedding space when DeepWalk algorithm is applied i.e. random walks + word2vec.

Question 2

The cyclic subgraphs (v_1, v_2, v_3) and (v_5, v_6, v_4) are structurally symmetrical. One notices that the embeddings of (v_1, v_2, v_3) are respectively the negatives of the embeddings of (v_5, v_6, v_4) in both X_1 and X_2.

X_1 differs from X_2 by the second-dimension of the embeddings. Specifically, the second column of X_1 is the negative of the second column of X_2. From the above reasoning, we can assume that the for the second time, the DeepWalk algorithm generated random walks which were symmetrical to those of the first time. Neither of X_1 or X_2 give more information than the other.

Question 3

A message passing layer aggregates the information of a node's neighbours. By stacking n message passing layers a node will have information about the n following neighbouring nodes. Therefore it is better for the model to have more than one message passing layer as it allows to get a more complete understanding of the graph. However n should not exceed the diameter of the input graph (the greatest distance between any pairs of nodes) as that would be useless, since we are trying to aggregate information from nodes which are at a greater distance than the longest possible distance, which is impossible.

Question 4

We have:

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad \hat{\mathbf{A}} = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \cdot \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{2} & \frac{1}{\sqrt{6}} & 0 & 0 \\ \frac{1}{\sqrt{6}} & \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{\sqrt{6}} \\ 0 & 0 & \frac{1}{\sqrt{6}} & \frac{1}{2} \end{pmatrix}$$

$$
\begin{aligned}
\mathbf{Z}^0 &= ReLU(\hat{\mathbf{A}}\,\mathbf{X}\,\mathbf{W}^0) \\
&= ReLU\left(\begin{pmatrix} \frac{1}{2}+\frac{1}{\sqrt{6}} \\ \frac{2}{3}+\frac{1}{\sqrt{6}} \\ \frac{2}{3}+\frac{1}{\sqrt{6}} \\ \frac{1}{2}+\frac{1}{\sqrt{6}} \end{pmatrix} \cdot \begin{pmatrix} 0.5 & -0.2 \end{pmatrix}\right) = ReLU\left(\begin{pmatrix} \frac{1}{2}\left(\frac{1}{2}+\frac{1}{\sqrt{6}}\right) & \frac{1}{5}\left(-\frac{1}{2}-\frac{1}{\sqrt{6}}\right) \\ \frac{1}{2}\left(\frac{2}{3}+\frac{1}{\sqrt{6}}\right) & \frac{1}{5}\left(-\frac{2}{3}-\frac{1}{\sqrt{6}}\right) \\ \frac{1}{2}\left(\frac{2}{3}+\frac{1}{\sqrt{6}}\right) & \frac{1}{5}\left(-\frac{2}{3}-\frac{1}{\sqrt{6}}\right) \\ \frac{1}{2}\left(\frac{1}{2}+\frac{1}{\sqrt{6}}\right) & \frac{1}{5}\left(-\frac{1}{2}-\frac{1}{\sqrt{6}}\right) \end{pmatrix}\right) \\
&\simeq ReLU\left(\begin{pmatrix} 0.454124 & -0.18165 \\ 0.537457 & -0.214983 \\ 0.537457 & -0.214983 \\ 0.454124 & -0.18165 \end{pmatrix}\right) = \begin{pmatrix} 0.454124 & 0 \\ 0.537457 & 0 \\ 0.537457 & 0 \\ 0.454124 & 0 \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{Z}^1 &= ReLU(\hat{\mathbf{A}}\,\mathbf{Z}^0\,\mathbf{W}^1) \\
&= ReLU\left(\begin{pmatrix} 0.446478 & -0.178591 \\ 0.5437 & -0.21748 \\ 0.5437 & -0.21748 \\ 0.446478 & -0.178591 \end{pmatrix} \cdot \begin{pmatrix} 0.3 & -0.4 & 0.8 & 0.5 \\ -1.1 & 0.6 & -0.1 & 0.7 \end{pmatrix}\right) \\
&= ReLU\left(\begin{pmatrix} 0.330394 & -0.285746 & 0.375042 & 0.0982252 \\ 0.402338 & -0.347968 & 0.456708 & 0.119614 \\ 0.402338 & -0.347968 & 0.456708 & 0.119614 \\ 0.330394 & -0.285746 & 0.375042 & 0.0982252 \end{pmatrix}\right) \\
&\simeq \begin{pmatrix} 0.33 & 0 & 0.38 & 0.10 \\ 0.40 & 0 & 0.46 & 0.12 \\ 0.40 & 0 & 0.46 & 0.12 \\ 0.33 & 0 & 0.38 & 0.10 \end{pmatrix}
\end{aligned}
$$

We observe that there are two pairs of nodes which have the exact representation, namely nodes (1,4) and nodes (2,3). That makes sense since nodes (1,4) (resp. (2,3)) have the same degree of 1 (resp. 2) i.e they have the same structural properties and hence will have the same embeddings.