My solutions to

Deep Learning: Foundations and Concepts

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13 Graph Neural Networks

13.1

The adjacency matrices corresponding to (b) and (c) in Figure 13.2 are

$$A := \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \end{pmatrix} \text{ and } \tilde{A} := \begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

respectively. With (13.1) it follows that

$$\begin{aligned} PAP^\top &= \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix} \\ &= \begin{pmatrix} 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix} \\ &= \tilde{A} \end{aligned}$$

13.2

Consider node m of a given simple graph with N nodes, and denote by N_m the number of edges connected to that node. It follows immediately from the definition of adjacency matrix A that $N_m = \sum_{n=1}^{N} A_{mn}$. It then holds that

$$\begin{aligned}
(AA)_{m,m} &= \sum_{n=1}^{N} A_{m,n} A_{n,m} \\
&= \sum_{n=1}^{N} A_{m,n}^2 \qquad \text{by symmetry of } A \\
&= \sum_{n=1}^{N} A_{m,n} \qquad A_{m,n} \in \{0,1\} \text{ f.a. } n \\
&= N_m
\end{aligned}$$

13.4

For every $m \in \{1, \dots, N\}$ it holds that

$$\begin{aligned}
(PX)_{m,:} &= \sum_{k=1}^{N} P_{m,k} X_{k,:} \\
&= \sum_{k=1}^{N} \left(u_{\pi(m)}^{\top}\right)_k X_{k,:} \qquad (13.3) \\
&= \sum_{k=1}^{N} \delta_{\pi(m),k} X_{k,:} \qquad \text{by def. of } u \\
&= X_{\pi(m),:}
\end{aligned}$$

13.5

For every $m \in \{1, \dots, N\}$, $n \in \{1, \dots, N\}$ it holds that

$$\begin{aligned}
\left(PAP^{\top}\right)_{m,n} &= \sum_{k=1}^{N} (PA)_{m,k} \left(P^{\top}\right)_{k,n} \\
&= \sum_{k=1}^{N} A_{\pi(m),k} \left(P^{\top}\right)_{k,n} \qquad \text{analogous to exercise 13.4} \\
&= \sum_{k=1}^{N} A_{\pi(m),k} P_{n,k} \qquad \text{by def. of transpose}
\end{aligned}$$

$$
\begin{aligned}
&= \sum_{k=1}^{N} A_{\pi(m),k} \left(u_{\pi(n)}^{\top}\right)_k && (13.3)\\
&= \sum_{k=1}^{N} A_{\pi(m),k} \delta_{\pi(n),k} && \text{by def. of } u\\
&= A_{\pi(m),\pi(n)}
\end{aligned}
$$