INF2978 Algoritmos para Data Science

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1 Exercício 3.27

2 Exercício 3.30

1. Mostre que os elementos de XX^T são dados por

$$x_i x_j^T = -\frac{1}{2}\left(d_{ij}^2 - \frac{1}{n}\sum_{k=1}^{n} d_{ik}^2 - \frac{1}{n}\sum_{k=1}^{n} d_{kj}^2 + \frac{1}{n^2}\sum_{k=1}^{n}\sum_{l=1}^{n} d_{kl}^2\right) \tag{1}$$

Solução

Dado que $d_{ij}^2 = d_{ji}^2 = |x_i|^2 + |x_j|^2 - 2x_i x_j^T$ pela definição de D.

$$\begin{aligned}
\sum_{k=1}^{n} d_{kj}^2 &= \sum_{k=1}^{n} \left(|x_k|^2 + |x_j|^2 - 2x_k x_j^T\right) \\
&= \sum_{k=1}^{n} |x_k|^2 + \sum_{k=1}^{n} |x_j|^2 - 2\sum_{k=1}^{n} x_k x_j^T \\
&= \sum_{k=1}^{n} |x_k|^2 + n|x_j|^2 - 2x_j^T \sum_{k=1}^{n} x_k \\
&= \sum_{k=1}^{n} |x_k|^2 + n|x_j|^2
\end{aligned} \tag{2}$$

De modo análogo:

$$
\begin{aligned}
\sum_{k=1}^{n} d_{ik}^2 &= \sum_{k=1}^{n} \left(|x_i|^2 + |x_k|^2 - 2x_i x_k^T\right) \\
&= \sum_{k=1}^{n} |x_i|^2 + \sum_{k=1}^{n} |x_k|^2 - 2\sum_{k=1}^{n} x_i x_k^T \\
&= n|x_i|^2 + \sum_{k=1}^{n} |x_j|^2 - 2x_i \sum_{k=1}^{n} x_j^T \\
&= n|x_i|^2 + \sum_{k=1}^{n} |x_k|^2
\end{aligned} \tag{3}
$$

Além disso, tenho que:

$$
\begin{aligned}
\sum_{k=1}^{n}\sum_{l=1}^{n} d_{kl}^2 &= \sum_{k=1}^{n}\sum_{l=1}^{n} \left(|x_k|^2 + |x_l|^2 - 2x_k x_l^T\right) \\
&= \sum_{k=1}^{n}\sum_{l=1}^{n} |x_k|^2 + \sum_{k=1}^{n}\sum_{l=1}^{n} |x_l|^2 - 2\sum_{k=1}^{n}\sum_{l=1}^{n} x_k x_l^T \\
&= n\sum_{k=1}^{n} |x_k|^2 + n\sum_{l=1}^{n} |x_l|^2 - 2\sum_{k=1}^{n} x_k \sum_{l=1}^{n} x_j^T \\
&= 2n\sum_{k=1}^{n} |x_k|^2
\end{aligned} \tag{4}
$$

Combinando (2), (3) e (4), temos:

$$
\begin{aligned}
x_i x_j^T &= -\frac{1}{2}\left(d_{ij}^2 - \frac{1}{n}\sum_{k=1}^{n} d_{ik}^2 - \frac{1}{n}\sum_{k=1}^{n} d_{kj}^2 + \frac{1}{n^2}\sum_{k=1}^{n}\sum_{l=1}^{n} d_{kl}^2\right) \\
&= -\frac{1}{2}\left[|x_i|^2 + |x_j|^2 - 2x_i x_j^T - \frac{1}{n}\left(n|x_i|^2 + \sum_{k=1}^{n} |x_k^2|\right) - \frac{1}{n}\left(\sum_{k=1}^{n} |x_k|^2 + n|x_j|^2\right) + \frac{1}{n^2}\left(2n\sum_{k=1}^{n} |x_k^2|\right)\right] \\
&= -\frac{1}{2}\left[|x_i|^2 + |x_j|^2 - 2x_i x_j^T - |x_i|^2 - \frac{1}{n}\sum_{k=1}^{n} |x_k|^2 - \frac{1}{n}\sum_{k=1}^{n} |x_k|^2 - |x_j|^2 + \frac{2}{n}\sum_{k=1}^{n} |x_k|^2\right] \\
&= -\frac{1}{2}\left[-2x_i x_j^T - \frac{2}{n}\sum_{k=1}^{n} |x_k|^2 + \frac{2}{n}\sum_{k=1}^{n} |x_k|^2\right] \\
&= x_i x_j^T
\end{aligned}
$$

2. Descreva um algoritmo para determinar X cujas linhas são x_i.

   Seja $B = XX^T$, a partir do item anterior podemos concluir que $x_i x_j^T = x_j x_i^T$, logo B é uma matriz simétrica. Nós podemos aplicar o SVD em B de modo que $B = XX^T$, então teremos a matriz $X = UL^{\frac{1}{2}}$.