

tSNE

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1 Xây dựng bài toán t-SNE. Tính o hàm loss vì các parameter (y) trong bài toán t-SNE

SNE converts euclidean distances to similarities, that can be interpreted as probabilities

$$p_{j|i} = \frac{\exp(-\|x_i - x_j\|^2 / 2\sigma_i^2)}{\sum_{k \neq i} \exp(-\|x_i - x_k\|^2 / 2\sigma_i^2)}$$
$$q_{j|i} = \frac{\exp(-\|y_i - y_j\|^2)}{\sum_{k \neq i} \exp(-\|y_i - y_k\|^2)}$$
$$p_{i|j} = 0, q_{i|j} = 0$$

t-SNE minimizes the Kullback-Leibler divergence between the joint probabilities p_{ij} in the high-dimensional space and the joint probabilities q_{ij} in the low-dimensional space. The values of p_{ij} are defined to be the symmetrized conditional probabilities, whereas the values of q_{ij} are obtained by means of a Student-t distribution with one degree of freedom:

$$p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}$$
$$q_{ij} = \frac{(1 + \|y_i - y_j\|^2)^{-1}}{\sum_{k \neq l} (1 + \|y_k - y_l\|^2)^{-1}}$$

The Kullback-Leibler divergence between the two joint probability distributions P and Q is given by:

$$C = \sum_i KL(P_i || Q_i) = \sum_i \sum_j p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}$$
$$= \sum_i \sum_j p_{ij} \log p_{ij} - p_{ij} \log q_{ij}$$

In order to make the derivation less cluttered, we define two auxiliary variables d_{ij} and Z as follows:

$$d_{ij} = \|y_i - y_j\|$$

$$Z = \sum_{k \neq l} = (1 + d_{kl}^2)^{-1}$$

If y_i changes, the only pairwise distance that change are d_{ij} and d_{ji} for $\forall j$. Therefore, the gradient of the cost function C with respect to y_i is given by

$$\begin{aligned} \frac{\delta C}{\delta y_i} &= \sum_j \left(\frac{\delta C}{\delta d_{ij}} + \frac{\delta C}{\delta d_{ji}} \right) (y_i - y_j) \\ &= 2 \sum_j \frac{\delta C}{\delta d_{ij}} (y_i - y_j) \end{aligned} \quad (1)$$

The gradient $\frac{\delta C}{\delta d_{ij}}$ The gradient $\frac{\delta C}{\delta d_{ij}}$ is computed from the definition of the Kullback-Leibler divergence:

$$\begin{aligned} \frac{\delta C}{\delta d_{ij}} &= - \sum_{k \neq l} p_{kl} \frac{\delta(\log q_{kl})}{\delta d_{ij}} \\ &= - \sum_{k \neq l} p_{kl} \frac{\delta(\log q_{kl} Z - \log Z)}{\delta d_{ij}} \\ &= - \sum_{k \neq l} p_{kl} \left(\frac{1}{q_{kl} Z} \frac{\delta((1 + d_{kl}^2)^{-1})}{\delta d_{ij}} - \frac{1}{Z} \frac{\delta Z}{\delta d_{ij}} \right) \end{aligned}$$

The gradient $\frac{\delta((1 + d_{kl}^2)^{-1})}{\delta d_{ij}}$ is only nonzero when $k = i$ and $l = j$. So:

$$\frac{\delta C}{\delta d_{ij}} = 2 \frac{p_{ij}}{p_{ij} Z} (1 + d_{ij}^2)^{-1} - 2 \sum_{k \neq l} p_{kl} \frac{(1 + d_{ij}^2)^{-2}}{Z}$$

Note that $\sum_{k \neq l} p_{kl} = 1$, we have:

$$\begin{aligned} \frac{\delta C}{\delta d_{ij}} &= 2p_{ij}(1 + d_{ij}^2)^{-1} - 2q_{ij}(1 + d_{ij}^2)^{-1} \\ &= 2(p_{ij} - q_{ij})(1 + d_{ij}^2)^{-1} \end{aligned}$$

Substitute it into (1), the gradient:

$$\frac{\delta C}{\delta y_i} = 4 \sum_j (p_{ij} - q_{ij})(1 + \|y_i - y_j\|^2)^{-1} (y_i - y_j)$$