

Stochastic Neighbor Embedding (SNE)

Pham Van Hong

11201638

Problem 1:

Definition: (SNE)

$$q_{j|i} = \frac{e^{-\|y_i - y_j\|^2}}{\sum_{l \neq i} e^{-\|y_i - y_l\|^2}} = \frac{E_{ij}}{E_{ik}} = \frac{E_{ij}}{Z_i}$$

And $E_{ij} = E_{ji}$. Conclusion, the loss function is defined as:

$$C = \sum_{k, l \neq k} p_{l|k} \log \frac{p_{l|k}}{q_{l|k}} = \sum_{k, l \neq k} p_{l|k} \log p_{l|k} - p_{l|k} \log q_{l|k}$$

$$C = \sum_{k, l \neq k} p_{l|k} \log p_{l|k} - p_{l|k} \log E_{lk} + p_{l|k} \log Z_k$$

We derive with respect to y_i :

$$\begin{aligned} \frac{\partial C}{\partial y_i} &= \sum_{k, l \neq k} -p_{l|k} \partial \log E_{kl} + \sum_{k, l \neq k} p_{l|k} \partial \log Z_k \\ \sum_{k, l \neq k} -p_{l|k} \partial \log E_{kl} &= \sum_{j \neq i} -p_{j|i} \partial \log E_{ij} - p_{i|j} \partial \log E_{ji} \end{aligned}$$

Since $E_{ij} = E_{ji} \left(-2(y_i - y_j) \right)$ we have

$$\begin{aligned} \sum_{j \neq i} -\frac{p_{j|i} E_{ij}}{E_{ij}} \left(-2(y_i - y_j) \right) - \frac{p_{i|j} E_{ji}}{E_{ji}} \left(2(y_j - y_i) \right) \\ = 2 \sum_{j \neq i} (p_{j|i} + p_{i|j}) (y_i - y_j) \end{aligned}$$

Since $\sum_{l \neq j} p_{l|j} = 1$ and Z_j does not depend on k , we can write

$$\begin{aligned}
\sum_{j,k \neq j} p_{k|j} \partial \log Z_j &= \sum_j \partial \log Z_j \\
&= \sum_j \frac{1}{Z_j} \sum_{k \neq j} \partial E_{jk} \\
&= \sum_j \frac{E_{ji}}{Z_j} (2(y_j - y_i)) + \sum_{j \neq i} \frac{E_{ij}}{Z_i} (-2(y_i - y_j)) \\
&= 2 \sum_{j \neq i} (-q_{j|i} - q_{i|j})(y_i - y_j) \\
C &= 2 \sum_{j \neq i} (p_{j|i} - q_{j|i} + p_{i|j} - q_{i|j})(y_i - y_j)
\end{aligned}$$

t-distributed SNE

Definition:

$$\begin{aligned}
q_{ji} &= q_{ij} = \frac{(1 + ||y_i - y_j||^2)^{-1}}{\sum_{k,l \neq k} (1 + ||y_k - y_l||^2)^{-1}} \\
&= \frac{E_{ij}^{-1}}{\sum_{k,l \neq k} E_{kl}^{-1}} \\
&= \frac{E_{ij}^{-1}}{Z}
\end{aligned}$$

We have $E_{ij} = E_{ji}$, the loss function is defined as

$$\begin{aligned}
C &= \sum_{k,l \neq k} p_{lk} \log \frac{p_{lk}}{q_{lk}} = \sum_{k,l \neq k} p_{lk} \log p_{lk} - p_{lk} \log q_{lk} \\
&= \sum_{k,l \neq k} p_{lk} \log p_{lk} - p_{lk} \log E_{kl}^{-1} + p_{lk} \log Z
\end{aligned}$$

We derive with respect to y_i

$$\frac{\partial C}{\partial y_i} = \sum_{k,l \neq k} -p_{lk} \partial \log E_{kl}^{-1} + \sum_{k,l \neq k} p_{lk} \partial \log Z$$

We start with the first term, noting that the derivative is non-zero when $\forall j, k = i$ or $l = i$, that $p_{ij} = p_{ji}$ and $E_{ij} = E_{ji}$

$$\sum_{k,l \neq k} -p_{lk} \partial \log E_{kl}^{-1} = -2 \sum_{j \neq i} p_{ij} \partial \log E_{ij}^{-1}$$

Since $\partial E_{ij}^{-1} = E_{ij}^{-2} (-2(y_i - y_j))$ we have:

$$-2 \sum_{j \neq i} \frac{p_{ji} E_{ij}^{-2}}{E_{ij}^{-1}} (-2(y_i - y_j)) = 4 \sum_{j \neq i} p_{ji} E_{ij}^{-1} (y_i - y_j)$$

$$\sum_{k,l \neq k} p_{lk} \partial \log Z = \frac{1}{Z} \sum_{k', l' \neq k'} \partial E_{kl}^{-1}$$

$$= 2 \sum_{k,l \neq k} p_{lk} \partial \log Z$$

$$= \frac{1}{Z} \sum_{k', l' \neq k'} \partial E_{kl}^{-1}$$

$$= 2 \sum_{j \neq i} \frac{E_{ji}^{-2}}{Z} (-2(y_j - y_i))$$

$$= -4 \sum_{j \neq i} q_{ij} E_{ji}^{-1} (y_i - y_j)$$

$$= \frac{\partial C}{\partial y_i} = 4 \sum_{j \neq i} (p_{ji} - q_{ji}) E_{ji}^{-1} (y_i - y_j)$$

$$= \frac{\partial C}{\partial y_i} = 4 \sum_{j \neq i} (p_{ji} - q_{ji}) \left(1 + \|y_i - y_j\|^2\right)^{-1} (y_i - y_j)$$