

We have dataset,

$$X = \{x_1, x_2, x_3, \dots, x_n \in \mathbb{R}^d\}$$

SNE converts euclidean distances to similarities

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

$$q_{j|i} = \frac{\exp(-\|y_i - y_j\|^2)}{\sum_{k \neq i} \exp(-\|y_i - y_k\|^2)} = \frac{w_{ij}}{\sum_{k \neq i} w_{ik}} = \frac{w_{ij}}{z_i}$$

Kullback-Leiber Divergence (KL) compares two distributions

$$C = \sum_i KL(p_i \| q_i) = \sum_i \sum_j p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}$$

Cost function

$$\begin{aligned} L &= \sum_i \sum_j p_{j|i} \log \frac{p_{j|i}}{q_{j|i}} \\ &= \sum_i \sum_j p_{j|i} \log \frac{\exp(-\|y_i - y_j\|^2)}{\exp(-\|x_i - x_j\|^2 / 2\sigma_i^2)} \\ &= \sum_{i,j} p_{j|i} \log p_{j|i} - \log q_{j|i} \\ &= \sum_{i,j} p_{j|i} \log p_{j|i} - p_{j|i} \log w_{ij} + p_{j|i} \log z_i \end{aligned}$$

$$\frac{\partial L}{\partial y_i} = \sum_{i,j} -p_{j|i} \partial \log w_{ij} + \sum_{i,j} p_{j|i} \partial \log z_i$$

$$\approx \sum_{i,j} -p_{j|i} \partial \log w_{ij} = \sum_{j \neq i} -p_{j|i} \partial \log w_{ij} - p_{i|i} \partial \log w_{ji}$$

Because $\partial w_{ij} = w_{ij} (-2(y_i - y_j))$

$$\begin{aligned} \sum_{j \neq i} p_{j|i} \frac{w_{ij}}{w_{ij}} (-2(y_i - y_j)) &= p_{i|i} \frac{w_{ii}}{w_{ii}} (2(y_j - y_i)) \\ &= 2 \sum_{j \neq i} (p_{j|i} + p_{i|i}) (y_i - y_j) \end{aligned}$$

$$\sum_{j,i} p_{j|i} 2 \log z_i = \sum_i 2 \log z_i$$

$$\sum_j \frac{1}{z_j} \sum_{j,i} \partial w_{ji}$$

$$= \sum_{j \neq i} \frac{w_{ji}}{z_j} (2(y_j - y_i)) + \sum_{j \neq i} \frac{w_{ij}}{z_i} (-2(y_i - y_j))$$

$$= 2 \sum_{j \neq i} (1 - q_{j|i} - q_{i|j}) (y_i - y_j)$$

$$\Rightarrow \frac{\partial L}{\partial y_i} = 2 \sum_{j \neq i} (p_{j|i} - q_{j|i} + p_{i|j} - q_{i|j}) (y_i - y_j)$$

t-SNE

$$q_{ji} = q_{ij} = \frac{(1 + \|y_i - y_j\|^2)^{-1}}{\sum_{k,l} (1 + \|y_k - y_l\|^2)^{-1}} = \frac{w_{ij}^{-1}}{\sum_{k,l} w_{kl}^{-1}} = \frac{w_{ij}^{-1}}{2}$$

The loss function

$$L = \sum_{k,l} p_{kl} \log \frac{p_{kl}}{q_{kl}} = \sum_{k,l} p_{kl} \log p_{kl} - p_{kl} \log q_{kl}$$

$$= \sum_{k,l} p_{kl} \log p_{kl} - p_{kl} \log w_{kl}^{-1} + p_{kl} \log 2$$

$$\frac{\partial L}{\partial y_i} = \sum_{k,l} -p_{kl} 2 \log w_{kl}^{-1} + \sum_{k,l} p_{kl} 2 \log 2$$

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

because $\partial w_{ij}^{-1} = w_{ji}^{-2} (-2(y_i - y_j))$

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

$$\sum_{k,l} p_{kl} \partial \log Z = \frac{1}{2} \sum_{k,l} \partial w_{kl}^{-1}$$

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

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

In conclusion

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

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