

Dimensionality Reduction techniques solve optimization problems.

Three approaches for Dimensionality Reduction:

- Distance preservation
- Topology preservation
- Information preservation

t-SNE converts Euclidean distance to similarity, which can be interpreted as probability. t-SNE is distance-based but tends to reserve topology.

1. SNE

$$\text{Problem: } X = \{x_1, x_2, \dots, x_n \in R^h\} \rightarrow Y = \{y_1, y_2, \dots, y_n \in R^i\}$$

$$\min_Y C(X, Y)$$

We have $p_{j|i}$ as the probability of x_j lies near x_i and $q_{j|i}$ as the probability of y_j lies near y_i

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

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

$\Rightarrow p_{j|i}$ and $q_{j|i}$ should be the same

Kullback-Leiber Divergence measures the faithfulness with which $q_{j|i}$ models $p_{j|i}$.

$P_i = \{p_{1|i}, p_{2|i}, \dots, p_{n|i}\}$ and $Q_i = \{q_{1|i}, q_{2|i}, \dots, q_{n|i}\}$ are the distributions on the neighbour of data i .

$$D_{KL}(P_i || Q_i) = \sum P(x_i) \log \left(\frac{P(x_i)}{Q(x_i)} \right)$$

Loss function is defined as

$$C = \sum_i \sum_j KL(P_{j|i} || Q_{j|i}) = \sum_i \sum_j p_{j|i} \log \left(\frac{p_{j|i}}{q_{j|i}} \right)$$

- KL divergence is asymmetric
- KL divergence is always positive

\Rightarrow Minimize loss function to find $\{y_1, y_2, \dots, y_n\}$

$$C = \sum_i \sum_j p_{j|i} \log \left(\frac{p_{j|i}}{q_{j|i}} \right)$$

$$= \sum_i \sum_j p_{j|i} \log(p_{j|i}) - \sum_i \sum_j p_{j|i} \log(q_{j|i})$$

$$\begin{aligned} \frac{\partial C}{\partial y_i} &= \frac{\partial \sum_i \sum_j p_{j|i} \log(q_{j|i})}{\partial y_i} \\ &= \frac{\partial \left(\sum_j p_{j|i} \log(q_{j|i}) + \sum_i p_{i|j} \log(q_{i|j}) \right)}{\partial y_i} \end{aligned} \quad (1)$$

$$\begin{aligned} \frac{\partial \sum_i p_{i|j} \log(q_{i|j})}{\partial y_i} &= \frac{\partial \sum_i p_{i|j} \log(q_{i|j})}{\partial y_i} = \frac{\partial \sum_i p_{i|j} \left((-\|y_j - y_i\|^2) - \sum_{k \neq i} (-\|y_k - y_j\|^2) \right)}{\partial y_i} \\ &= 2 \sum_j p_{j|i} (y_i - y_j) \end{aligned} \quad (2)$$

$$\frac{\partial \sum_i p_{j|i} \log(q_{j|i})}{\partial y_i} = \frac{\partial \sum_j p_{j|i} \left((-\|y_j - y_i\|^2) - \sum_{k \neq j} (-\|y_k - y_j\|^2) \right)}{\partial y_i} \quad (3)$$

$$= 2 \sum_j p_{j|i} \left((y_i - y_j) - \sum_{k \neq j} (y_k - y_j) \right) \quad (4)$$

From (1), (2), (4)

$$\begin{aligned} \frac{\partial C}{\partial y_i} &= \frac{\partial \sum_j p_{i|j} \log(q_{i|j})}{\partial y_i} + \frac{\partial \sum_i p_{i|j} \log(q_{i|j})}{\partial y_i} \\ &= 2 \sum_j p_{j|i} (y_i - y_j) + 2 \sum_i p_{i|j} \left((y_i - y_j) - \sum_{k \neq j} (y_k - y_i) \right) \\ &= 2 \sum_j (y_i - y_j) \left(p_{j|i} + p_{i|j} - \sum_{k \neq j} (y_k - y_j) \right) \\ &= 2 \sum_j (y_i - y_j) (p_{j|i} + p_{i|j} - q_{i|j} - q_{j|i}) \end{aligned}$$