

## HOMEWORK 2: T-NSE

1. Biến đổi công thức toán SNE, t-SNE, có tính đạo hàm loss với các parameter.

- t-SNE is an alternative dimensionality reduction algorithm
- t-SNE tries to perserve local structure
  - Low dimensional neighborhood should be the same as original neighborhood

a) Find low dimensional points such that their neighborhood distribution is similar.

The probability that point  $x_i$  chooses  $x_j$  as it neighbor:

$$p_{j|i} = \frac{e^{-\frac{\|x^{(i)} - x^{(j)}\|^2}{2\sigma_i^2}}}{\sum_{k \neq i} e^{-\frac{\|x^{(i)} - x^{(k)}\|^2}{2\sigma_i^2}}}$$

With  $p_{j|i} = 0$

$$p_{j|i} = \frac{e^{-\|y_i - y_j\|^2}}{\sum_{k \neq i} e^{-\|y_i - y_k\|^2}}$$

So we now need to minimize the KL divergence values. Hence our cost function is based on this

$$C = \sum_i KL(P_i || Q_1)$$

Final distribution over pairs is symmetrized:

$$p_{ij} = \frac{1}{2N} (p_{i|j} + p_{j|i})$$

- The parameter  $\sigma_i$  sets the size of the neighborhood
  - Very low  $\sigma_i$  - all the probability is in the nearest neighbor
  - Very high  $\sigma_i$  - Uniform weights
- Here we set  $\sigma_i$  differently for each data point
- For each distribution  $P_{j|i}$  ( depends on  $\sigma_i$ ) we define the perplexity

$$perp(P_{j|i}) = 2^{H(P_{j|i})}$$

Where  $H(P) = -\sum_i P_i \log(P_i)$  is the entropy

b) Tính đạo hàm loss với các parameter.

❖ SNE (Stochastic Neighbor Embedding).

- Given  $x^{(1)}, x^{(2)}, x^{(3)}, \dots, x^{(N)} \in \mathbb{R}^D$  we define the distribution  $P_{ij}$
- We will have good embedding  $y^{(1)}, y^{(2)}, y^{(3)}, \dots, y^{(N)} \in \mathbb{R}^d$  for some  $d < D$  and we can define distribution  $Q$  similarly the same (notice no  $\sigma_i$  and not symmetric):

$$Q_{ij} = \frac{e^{-\|y^{(i)} - y^{(j)}\|^2}}{\sum_k \sum_{l \neq k} e^{-\|y^{(i)} - y^{(k)}\|^2}}$$

- Optimize  $Q$  to be close to  $P$  by use Minimize KL- divergence:  $L(Q) = KL(P||Q)$

$$\begin{aligned} KL(P||Q) &= \sum_{ij} P_{ij} \log\left(\frac{P_{ij}}{Q_{ij}}\right) \\ &= - \sum_{ij} P_{ij} \log(Q_{ij}) + const \end{aligned}$$

$$\Rightarrow \frac{\partial L}{\partial y^{(i)}} = \sum_j (P_{ij} - Q_{ij})(y^{(i)} - y^{(j)})$$

❖ t-SNE (t-distribution Stochastic Neighbor Embedding).

- Probability goes to zero much slower than a Gaussian
- We have redefine  $Q_{ij}$ :

$$Q_{ij} = \frac{(1 + \|y_i - y_j\|^2)^{-1}}{\sum_k \sum_{l \neq k} (1 + \|y_k - y_l\|^2)^{-1}}$$

- We need minimize  $KL(P||Q)$ :

$$\begin{aligned} KL(P||Q) &= \sum_{ij} P_{ij} \log\left(\frac{P_{ij}}{Q_{ij}}\right) \\ &= \sum_{ij} P_{ij} \log(Q_{ij}) + const \end{aligned}$$

$$\Rightarrow \frac{\partial L}{\partial y^{(i)}} = \sum_j (P_{ij} - Q_{ij})(y^{(i)} - y^{(j)}) (1 + \|y^{(i)} - y^{(j)}\|^2)^{-1}$$

2. So sánh t-SNE and PCA

PCA	t-SNE
<ul style="list-style-type: none"> <li>- PCA is a linear dimensionality reduction technique for very high dimensional data</li> <li>- PCA tries to find a global structure (+ Low dimensional subspace + Can lead to local inconsistencies -&gt; Far away point can become nearest neighbors</li> </ul>	<ul style="list-style-type: none"> <li>- It is an alternative (non-linear) dimensionality reduction algorithm</li> <li>- It tries to perserve local structure (Low dimensional neighborhood should be the same as original neighborhood)</li> </ul>