

we derive with respect to y_i . To make the derivation less cluttered, I will omit the ∂y_i term at the denominator

$$\frac{\partial \mathcal{L}}{\partial y_i} = \sum_{k, l \neq k} -P_{kl} \partial \log E_{kl}^{-1} + \sum_{k, l \neq k} P_{kl} \partial \log Z$$

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

$$\sum_{k, l \neq k} -P_{kl} \partial \log E_{kl}^{-1} = -2 \sum_{j \neq i} P_{ji} \partial \log E_{ij}^{-1} \quad (9)$$

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

$$-2 \sum_{j \neq i} P_{ji} \frac{E_{ij}^{-2}}{E_{ij}^{-1}} (-2(y_i - y_j)) = 4 \sum_{j \neq i} P_{ji} E_{ij}^{-1} (y_i - y_j) \quad (10)$$

we conclude with the second term. Using the fact that

$\sum_{k, l \neq k} P_{kl} = 1$ and that Z does not depend on k or l

$$\begin{aligned} \sum_{k, l \neq k} P_{kl} \partial \log Z &= \frac{1}{Z} \sum_{k', l' \neq k'} \partial E_{kl}^{-1} \\ &= 2 \sum_{j \neq i} \frac{E_{ji}^{-2}}{Z} (-2(y_j - y_i)) \\ &= -4 \sum_{j \neq i} q_{ij} E_{ji}^{-1} (y_i - y_j) \quad (11) \end{aligned}$$

Combining (10) and (11)

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

$$\frac{\partial \mathcal{L}}{\partial y_i} = 4 \sum_{j \neq i} (P_{ji} - q_{ji}) (1 + \|y_i - y_j\|^2)^{-1} (y_i - y_j)$$

we conclude with second term, since $\sum_{l \neq j} P_{lj} = 1$ and Z_j does not depend on h , we can write

$$\sum_{j, h \neq j} P_{hj} \partial \log Z_j = \sum_j \partial \log Z_j$$

The derivative is non-zero when $h = i$ or $j = i$

$$\begin{aligned} &= \sum_j \frac{1}{Z_j} \sum_{h \neq j} \partial E_{jh} \\ &= \sum_{j \neq i} \frac{E_{ji}}{Z_j} (2(y_j - y_i)) + \sum_{j \neq i} \frac{E_{ij}}{Z_j} (-2(y_i - y_j)) \\ &= 2 \sum_{j \neq i} (-q_{j|i} - q_{i|j}) (y_i - y_j) \quad (5) \end{aligned}$$

Combining (4) and (5) we have

$$\frac{\partial C}{\partial y_i} = 2 \sum_{j \neq i} (P_{j|i} - q_{j|i} + P_{i|j} - q_{i|j}) (y_i - y_j) \quad (6)$$

t-SNE

Define

$$q_{ji} = q_{ij} = \frac{(1 + \|y_i - y_j\|^2)^{-1}}{\sum_{h, l \neq h} (1 + \|y_h - y_l\|^2)^{-1}} = \frac{E_{ij}^{-1}}{\sum_{h, l \neq h} E_{hl}^{-1}} = \frac{E_{ij}^{-1}}{Z} \quad (7)$$

Notice that $E_{ij} = E_{ji}$. The loss function:

$$\begin{aligned} C &= \sum_{h, l \neq h} P_{lh} \log \frac{P_{lh}}{q_{lh}} = \sum_{h, l \neq h} P_{lh} \log P_{lh} - P_{lh} \log q_{lh} \\ &= \sum_{h, l \neq h} P_{lh} \log P_{lh} - P_{lh} \log E_{hl}^{-1} + P_{lh} \log Z \quad (8) \end{aligned}$$

Question 1: SNE
Define

①

$$q_{j|i} = \frac{e^{-\|y_i - y_j\|^2}}{\sum_{k \neq i} e^{-\|y_i - y_k\|^2}} = \frac{E_{ij}}{\sum_{k \neq i} E_{ik}} = \frac{E_{ij}}{Z_i} \quad (1)$$

Notice that: $E_{ij} = E_{ji}$. The loss function is defined as

$$\begin{aligned} C &= \sum_{k, l \neq k} P_{kl} \log \frac{P_{kl}}{q_{kl}} = \sum_{k, l \neq k} P_{kl} \log P_{kl} - P_{kl} \log q_{kl} \\ &= \sum_{k, l \neq k} P_{kl} \log P_{kl} - P_{kl} \log E_{kl} + P_{kl} \log Z_k \quad (2) \end{aligned}$$

We derive with respect to y_i . To make the derivation less cluttered, I will omit the ∂y_i term at the denominator.

$$\frac{\partial C}{\partial y_i} = \sum_{k, l \neq k} -P_{kl} \partial \log E_{kl} + \sum_{k, l \neq k} P_{kl} \partial \log Z_k$$

we start with the first item, ~~note~~ note that the derivative is non-zero when $\forall j \neq i, k=i$ or $l=i$

$$\sum_{k, l \neq k} -P_{kl} \partial \log E_{kl} = \sum -P_{ji} \partial \log E_{ij} - P_{ij} \partial \log E_{ji} \quad (3)$$

since $\partial E_{ij} = E_{ij}(-2(y_i - y_j))$ we have

$$\begin{aligned} &\sum_{j \neq i} -P_{ji} \frac{E_{ij}}{E_{ij}} (-2(y_i - y_j)) - P_{ij} \frac{E_{ji}}{E_{ji}} (2(y_j - y_i)) \\ &= 2 \sum_{j \neq i} (P_{ji} + P_{ij})(y_i - y_j) \quad (4) \end{aligned}$$