Step-By-Step Derivation of SNE and t-SNE gradients

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January 6, 2020

Please contact me if you find errors or have doubts. There is always room for improvement and learning.

Stochastic Neighbor Embedding (SNE)

If you have stumbled upon this document, you probably already know the formulation of the problem, therefore I will avoid writing things that can be easily found in the article.

Define

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

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

$$\begin{aligned} C &= \sum_{k, l \neq k} p_{l|k} \log \frac{p_{l|k}}{q_{l|k}} = \sum_{k, l \neq k} p_{l|k} \log p_{l|k} - p_{l|k} \log q_{l|k} \\ &= \sum_{k, l \neq k} p_{l|k} \log p_{l|k} - p_{l|k} \log E_{kl} + p_{l|k} \log Z_k \end{aligned} \tag{2}$$

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

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

We start with the first term, noting that the derivative is non-zero when $\forall j \neq i$, $k = i$ or $l = i$

$$\sum_{k,l\neq k} -p_{l|k}\partial \log E_{kl} = \sum_{j\neq i} -p_{j|i}\partial \log E_{ij} - p_{i|j}\partial \log E_{ji} \tag{3}$$

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

$$\begin{aligned}\sum_{j\neq i} -p_{j|i}\frac{\cancel{E_{ij}}}{\cancel{E_{ij}}}(-2(y_i - y_j)) - p_{i|j}\frac{\cancel{E_{ji}}}{\cancel{E_{ji}}}(2(y_j - y_i))\\ = 2\sum_{j\neq i}(p_{j|i} + p_{i|j})(y_i - y_j))\end{aligned} \tag{4}$$

We conclude with the second term. Since $\sum_{l\neq j} p_{l|j} = 1$ and Z_j does not depend on k, we can write (changing variable from l to j to make it more similar to the already computed terms)

$$\sum_{j,k\neq j} p_{k|j}\partial \log Z_j = \sum_j \partial \log Z_j$$

The derivative is non-zero when $k = i$ or $j = i$ (also, in the latter case we can move Z_i inside the summation because constant)

$$\begin{aligned}&= \sum_j \frac{1}{Z_j}\sum_{k\neq j}\partial E_{jk}\\ &= \sum_{j\neq i}\frac{E_{ji}}{Z_j}(2(y_j - y_i)) + \sum_{j\neq i}\frac{E_{ij}}{Z_i}(-2(y_i - y_j))\\ &= 2\sum_{j\neq i}(-q_{j|i} - qi|j)(y_i - y_j)\end{aligned} \tag{5}$$

Combining eq. (4) and (5) we arrive at the final result

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

t-distributed Stochastic Neighbor Embedding (t-SNE)

Define

$$q_{ji} = q_{ij} = \frac{(1 + \|y_i - y_j\|^2)^{-1}}{\sum_{k,l\neq k}(1 + \|y_k - y_l\|^2)^{-1}} = \frac{E_{ij}^{-1}}{\sum_{k,l\neq k} E_{kl}^{-1}} = \frac{E_{ij}^{-1}}{Z} \tag{7}$$

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

$$C = \sum_{k,l \neq k} p_{lk} \log \frac{p_{lk}}{q_{lk}} = \sum_{k,l \neq k} p_{lk} \log p_{lk} - p_{lk} \log q_{lk}$$
$$= \sum_{k,l \neq k} p_{lk} \log p_{lk} - p_{lk} \log E_{kl}^{-1} + p_{lk} \log Z \tag{8}$$

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

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

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

$$\sum_{k,l \neq k} -p_{lk} \partial \log E_{kl}^{-1} = -2 \sum_{j \neq i} p_{ji} \partial \log E_{ij}^{-1} \tag{9}$$

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

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

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

$$\sum_{k,l \neq k} p_{lk} \partial \log Z = \frac{1}{Z} \sum_{k',l' \neq k'} \partial E_{kl}^{-1}$$
$$= 2 \sum_{j \neq i} \frac{E_{ji}^{-2}}{Z} (-2(yj - yi))$$
$$= -4 \sum_{j \neq i} q_{ij} E_{ji}^{-1} (yi - yj) \tag{11}$$

Combining eq. (10) and (11) we arrive at the final result

$$\frac{\partial C}{\partial y_i} = 4 \sum_{j \neq i} (p_{ji} - q_{ji}) E_{ji}^{-1} (y_i - y_j)$$
$$\frac{\partial C}{\partial y_i} = 4 \sum_{j \neq i} (p_{ji} - q_{ji})(1 + \|y_i - y_j\|^2)^{-1} (y_i - y_j) \quad \square \tag{12}$$