Homework Dimensionality Reduction

Friday, 5 February 2021 11:00

Problem 1: The similarity in the low dimensional space is defined as:

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

The objective is to obtain a low-dimensional projection capturing the similarity structure of the high-dimensional data. This is achieved via optimizing the Kullback-Leibler divergence

$$C = \mathrm{KL}(P||Q) = \sum_i \sum_{j \neq i} p_{ij} \log \frac{p_{ij}}{q_{ij}}$$

Please derive the gradient $\frac{\partial C}{\partial y_s}$ for t-SNE for the coordinate y_s in the low dimensional space. Please note that this gradient can be used to update y_s with first-order methods.

p_{ij} high dimensional pairs

q_{ij} low dimensiondl pairs

$x_i \to y_i$

Arguably, the most difficult part is to keep track of y_s in various sums. To simplify this we denote the intermediate distance term $d_{ij} = 1 + \|y_i - y_j\|^2$.

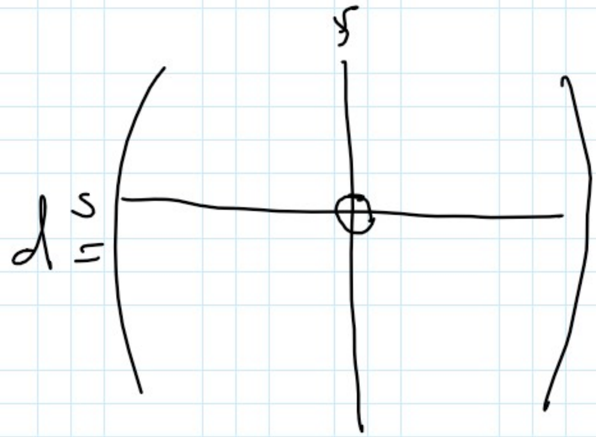
Next, we use the chain rule on C, so that we can take the derivative with respect to the individual "interactions" d_{ij} instead of the coordinate y_s.

$$\frac{\partial C}{\partial y_s} = \frac{\partial C(d(y))}{\partial y_s}$$

$$= \sum_i \sum_j \frac{\partial C}{\partial d_{ij}} \frac{\partial d_{ij}}{\partial y_s}$$

$\frac{\partial d_{ij}}{\partial y_s}$ is only non-zero if either $i = s$ or $j = s$. Furthermore, $d_{ij} = d_{ji}$.

d_{ii}



$$= 2 \sum_j \frac{\partial C}{\partial d_{sj}} \frac{\partial d_{sj}}{\partial y_s}$$

$s = j$

At this point we can already compute $\frac{\partial d_{sj}}{\partial y_s}$.

$$= 4 \sum_j (y_s - y_j) \frac{\partial C}{\partial d_{sj}}$$

Now we are left with computing the gradient of C with respect to some d_{nm}.

$$\frac{\partial C}{\partial d_{nm}} = \frac{\partial}{\partial d_{nm}} \left[\sum_i \sum_{j \neq i} p_{ij} \log \frac{p_{ij}}{q_{ij}} \right]$$

$$= \frac{\partial}{\partial d_{nm}} \left[\sum_i \sum_{j \neq i} \text{[redacted]} - p_{ij} \log q_{ij} \right]$$

Linearity of differentiation and p is constant with respect to d.

$$= - \sum_i \sum_{j \neq i} p_{ij} \frac{\partial \log q_{ij}}{\partial d_{nm}}$$

Expand the definition of q_{ij}.

$$= - \sum_i \sum_{j \neq i} p_{ij} \frac{\partial}{\partial d_{nm}} \left[\log \frac{d_{ij}^{-1}}{\sum_k \sum_{k \neq l} d_{kl}^{-1}} \right]$$

$$= - \sum_i \sum_{j \neq i} p_{ij} \frac{\partial}{\partial d_{nm}} \left[- \log d_{ij} - \log \sum_k \sum_{k \neq l} d_{kl}^{-1} \right]$$

$$= \sum_i \sum_{j \neq i} p_{ij} \frac{\partial \log d_{ij}}{\partial d_{nm}} + \sum_i \sum_{j \neq i} p_{ij} \frac{\partial}{\partial d_{nm}} \log \sum_k \sum_{k \neq l} d_{kl}^{-1}$$

$\frac{\partial \log d_{ij}}{\partial d_{nm}}$ is only non-zero for $i = n$ and $j = m$.

$$= p_{nm} d_{nm}^{-1} + \sum_i \sum_{j \neq i} p_{ij} \frac{1}{\sum_k \sum_{k \neq l} d_{kl}^{-1}} \frac{\partial}{\partial d_{nm}} \sum_k \sum_{k \neq l} d_{kl}^{-1}$$

The same is true for $\frac{\partial d_{kl}^{-1}}{\partial d_{nm}}$.

$$= p_{nm} d_{nm}^{-1} + \sum_i \sum_{j \neq i} p_{ij} \frac{1}{\sum_k \sum_{k \neq l} d_{kl}^{-1}} \frac{\partial d_{nm}^{-1}}{\partial d_{nm}}$$

$$= p_{nm} d_{nm}^{-1} - \frac{1}{\sum_k \sum_{k \neq l} d_{kl}^{-1}} d_{nm}^{-2} \sum_i \sum_{j \neq i} p_{ij}$$

$\sum_i \sum_{j \neq i} p_{ij} = 1$ and we can also find the definition of q_{nm} in there.

$$= p_{nm} d_{nm}^{-1} - \frac{d_{nm}^{-1}}{\sum_k \sum_{k \neq l} d_{kl}^{-1}} d_{nm}^{-1}$$

$$= (p_{nm} - q_{nm})\, d_{nm}^{-1}$$

Finally, we plug this result into $\frac{\partial C}{\partial y_s}$ and resolve the definition of d_{sj}.

$$\frac{\partial C}{\partial y_s} = 4 \sum_j (y_s - y_j) \frac{\partial C}{\partial d_{sj}}$$

$$= 4 \sum_j (y_s - y_j)(p_{sj} - q_{sj})\, d_{sj}^{-1}$$

$$= 4 \sum_j (y_s - y_j)(p_{sj} - q_{sj})\left(1 + \|y_s - y_j\|^2\right)^{-1}$$

Problem 2: We train a linear autoencoder to D-dimensional data. The autoencoder has a single K-dimensional hidden layer, there are no biases, and all activation functions are identity ($\sigma(x) = x$).

- Why is it usually impossible to get zero reconstruction error in this setting if $K < D$?
- Under which conditions is this possible?

We have $f(x) = \boldsymbol{X}\boldsymbol{W}_1\boldsymbol{W}_2$ where $\boldsymbol{X}$ is the data matrix and the dimensions of the weight matrices are $D \times K$ for $\boldsymbol{W}_1$ and $K \times D$ for $\boldsymbol{W}_2$.

The final multiplication $\boldsymbol{W}_2$ brings points from K-dimensions up into D-dimensions but the points will still all be in a K-dimensional linear subspace. Unless the data happen to lie exactly in a K-dimensional linear subspace, they can't be exactly fitted.