

t-SNE algorithm implementation

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Implementation is in `src/neuralnetwork/TSNE.h` and `TSNE.cpp` in `dinrhiw2` repository.

We maximize KL-divergence (p_{ij} calculated from data).

$$D_{\text{KL}}(\mathbf{y}_1 \dots \mathbf{y}_N) = \sum_{i \neq j} p_{ij} \log\left(\frac{p_{ij}}{q_{ij}}\right), \quad q_{ij} = \frac{(1 + \|\mathbf{y}_i - \mathbf{y}_j\|^2)^{-1}}{\sum_k \sum_{l \neq k} (1 + \|\mathbf{y}_k - \mathbf{y}_l\|^2)^{-1}}$$

The p_{ij} values are calculated from data using formulas.

$$p_{i|j} = \frac{e^{-\|\mathbf{x}_i - \mathbf{x}_j\|^2 / 2\sigma_i^2}}{\sum_{k \neq i} e^{-\|\mathbf{x}_i - \mathbf{x}_k\|^2 / 2\sigma_i^2}}, \quad p_{i|i} = 0, \quad \sum_j p_{j|i} = 1$$

Symmetric probability values are computed from conditional probabilities using the formula

$$p_{ij} = \frac{p_{j|i} + p_{i|j}}{2N}, \quad \sum_{i,j} p_{ij} = 1$$

Gradient

We need to calculate gradient for each \mathbf{y}_i in D_{KL} .

$$\nabla_{\mathbf{y}_m} D_{\text{KL}} = \nabla_{\mathbf{y}_m} \sum_{i \neq j} -p_{ij} \log(q_{ij}) = -\sum_{i \neq j} \frac{p_{ij}}{q_{ij}} \nabla_{\mathbf{y}_m} q_{ij}$$

The general rule to derivate q_{ij} terms is:

$$\nabla_{\frac{f}{g}} = \nabla f g^{-1} = f' g^{-2} g - f g^{-2} g' = \frac{f' g - f g'}{g^2}$$

And when $m \neq i \neq j$ we need to derivate only the second part

$$\begin{aligned} & \nabla_{\mathbf{y}_m \neq i \neq j} \left(\frac{(1 + \|\mathbf{y}_i - \mathbf{y}_j\|^2)^{-1}}{\sum_k \sum_{l \neq k} (1 + \|\mathbf{y}_k - \mathbf{y}_l\|^2)^{-1}} \right) \\ &= -\frac{(1 + \|\mathbf{y}_i - \mathbf{y}_j\|^2)^{-1}}{(\sum_k \sum_{l \neq k} (1 + \|\mathbf{y}_k - \mathbf{y}_l\|^2)^{-1})^2} \nabla_{\mathbf{y}_m} \sum_k \sum_{l \neq k} (1 + \|\mathbf{y}_k - \mathbf{y}_l\|^2)^{-1} \end{aligned}$$

$$\begin{aligned} & \nabla_{\mathbf{y}_m \neq i \neq j} \sum_k \sum_{l \neq k} (1 + \|\mathbf{y}_k - \mathbf{y}_l\|^2)^{-1} \\ &= \nabla_{\mathbf{y}_m} \sum_{l \neq m} (1 + \|\mathbf{y}_m - \mathbf{y}_l\|^2)^{-1} + \nabla_{\mathbf{y}_m} \sum_{k \neq m} (1 + \|\mathbf{y}_k - \mathbf{y}_m\|^2)^{-1} \\ &= 2 \nabla_{\mathbf{y}_m} \sum_{l \neq m} (1 + \|\mathbf{y}_m - \mathbf{y}_l\|^2)^{-1} \\ &= 2 \sum_{l \neq m} \nabla_{\mathbf{y}_m} (1 + \|\mathbf{y}_m - \mathbf{y}_l\|^2)^{-1} \\ &= 4 \sum_{l \neq m} -(1 + \|\mathbf{y}_m - \mathbf{y}_l\|^2)^{-2} (\mathbf{y}_m - \mathbf{y}_l) \end{aligned}$$

And when $y = i$ we need to derivate the upper part too.

$$\begin{aligned} & \nabla_{\mathbf{y}_i} \frac{(1 + \|\mathbf{y}_i - \mathbf{y}_j\|^2)^{-1}}{\sum_k \sum_{l \neq k} (1 + \|\mathbf{y}_k - \mathbf{y}_l\|^2)^{-1}} = \frac{1}{\sum_k \sum_{l \neq k} (1 + \|\mathbf{y}_k - \mathbf{y}_l\|^2)^{-1}} \nabla_{\mathbf{y}_i} (1 + \|\mathbf{y}_i - \mathbf{y}_j\|^2)^{-1} - \frac{f g'}{g^2} \\ & \nabla_{\mathbf{y}_i} (1 + \|\mathbf{y}_i - \mathbf{y}_j\|^2)^{-1} = -2 (1 + \|\mathbf{y}_i - \mathbf{y}_j\|^2)^{-2} (\mathbf{y}_i - \mathbf{y}_j) \end{aligned}$$

With these derivatives we can then calculate derivative of D_{KL} for each \mathbf{y} . We just select step length for the gradient which causes increase in D_{KL} .

Optimization of computation

For large number of points the update rule is slow ($O(N^2)$ scaling). Extra speed can be achieved by combining large away data points to a single point which is then used to calculate the divergence and gradient. This can be done by using *Barnes-Hut approximation* which changes computational complexity to near linear $O(N \log(N))$.