ML 813: Topics on Dimensionality Reduction and Manifold Learning

SNE and t-SNE

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Spring 2025

Introduction

Introduction (1)

Stochastic Neighbor Embedding (SNE) (2003) [1] is a manifold learning and **dimensionality reduction** method which can be used for feature extraction [2].

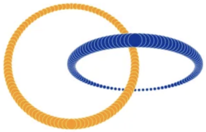
- It has a **probabilistic** approach. It fits the data in the embedding space **locally hoping to preserve the global structure** of data [3].
- The idea of SNE is to **consider every point as neighbors of other points with some probability where the closer points are neighbors with higher probability**. Therefore, rather than considering k nearest neighbors in a binary manner (whether being neighbors or not), it considers **neighbors in a stochastic way** (for how probable it is to be neighbors).
- It tries to **preserve the probability of neighborhoods** in the low-dimensional embedding space.
- There exist some other similar probabilistic dimensionality reduction methods which make use of Gaussian distribution for neighborhood. Some examples are **Neighborhood Component Analysis (NCA)** [4], deep NCA [5], and **Proxy-NCA** [6].

Introduction (2)

SNE uses the **Gaussian distribution** for neighbors in both the input and embedding spaces. The **Student-t distributed SNE**, or so-called **t-SNE** [7], considers the **Student-t and Gaussian distributions** in the input and embedding spaces, respectively. The reason of using Student-t distribution in t-SNE is because of its heavier tails so it can include more information from the high-dimensional data.

- t-SNE is one of the state-of-the-art methods for **data visualization**; for example, it has been used for **DNA and single-cell** data visualization [8].
- The goal of SNE is to embed the high-dimensional data $\{\boldsymbol{x}_i\}_{i=1}^n$ into the lower dimensional data $\{\boldsymbol{y}_i\}_{i=1}^n$ where n is the number of data points. We denote the dimensionality of high- and low-dimensional spaces by d and p, respectively, i.e. $\boldsymbol{x}_i \in \mathbb{R}^d$ and $\boldsymbol{y}_i \in \mathbb{R}^p$. We usually have $p \ll d$. For **data visualization**, we have $p \in \{2, 3\}$.

Example of SNE Embedding



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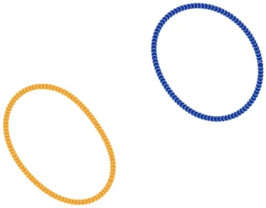

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Stochastic Neighbor Embedding (SNE)

Stochastic Neighbor Embedding (SNE)

- In **SNE** (2003) [1], we consider a **Gaussian probability** around every point $\boldsymbol{x}_i$ where the distribution is for probability of accepting any other point as the neighbor of $\boldsymbol{x}_i$; the farther points are neighbors with less probability. Hence, the variable is distance, denoted by $d \in \mathbb{R}$, and the Gaussian probability is:

$$f(d) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{d^2}{2\sigma^2}), \tag{1}$$

  where the mean of distribution is assumed to be zero.

- The fixed multiplier $\frac{1}{\sqrt{2\pi\sigma^2}}$ can be **dropped**; however, $\exp(-d^2/2\sigma^2)$ does not add (integrate) to one and thus it is not a probability density function. In order to tackle this problem, we can do a trick and divide $\exp(-d^2/2\sigma^2)$ by the summation of all possible values of $\exp(-d^2/2\sigma^2)$ to have a **softmax** function. Therefore, the probability that the point $\boldsymbol{x}_i \in \mathbb{R}^d$ takes $\boldsymbol{x}_j \in \mathbb{R}^d$ as its neighbor is:

$$\mathbb{R} \ni p_{ij} := \frac{\exp(-d_{ij}^2)}{\sum_{k \neq i} \exp(-d_{ik}^2)}, \tag{2}$$

  where:

$$\mathbb{R} \ni d_{ij}^2 := \frac{||\boldsymbol{x}_i - \boldsymbol{x}_j||_2^2}{2\sigma_i^2}. \tag{3}$$

Stochastic Neighbor Embedding (SNE)

- The σ_i^2 is the **variance** which we consider for the Gaussian distribution used for the $\boldsymbol{x}_i$. It can be set to a **fixed number** or determined by a **binary search** to make the entropy of distribution some specific value [1]. Note that according to the distribution of data in the input space, the best value for the variance of Gaussian distributions can be found.
- In the low-dimensional embedding space, we again consider a **Gaussian probability** distribution for the point $\boldsymbol{y}_i \in \mathbb{R}^p$ to take $\boldsymbol{y}_j \in \mathbb{R}^p$ as its neighbor:

$$\mathbb{R} \ni q_{ij} := \frac{\exp(-z_{ij}^2)}{\sum_{k \neq i} \exp(-z_{ik}^2)}, \tag{4}$$

where:

$$\mathbb{R} \ni z_{ij}^2 := ||\boldsymbol{y}_i - \boldsymbol{y}_j||_2^2. \tag{5}$$

- It is noteworthy that the variance of distribution is not used (or is set to $\sigma_i^2 = 0.5$ to cancel 2 in the denominator) because the variance of distribution in the embedding space is the choice of algorithm.

Stochastic Neighbor Embedding (SNE)

- We want the probability distributions in both the input and embedded spaces to be as similar as possible; therefore, the cost function to be minimized can be summation of the **Kullback-Leibler (KL) divergences** [9] over the n points:

$$\mathbb{R} \ni c_1 := \sum_{i=1}^{n} \text{KL}(P_i || Q_i) = \sum_{i=1}^{n} \sum_{j=1, j \neq i}^{n} p_{ij} \log(\frac{p_{ij}}{q_{ij}}), \tag{6}$$

  where p_{ij} and q_{ij} are the Eqs. (2) and (4).
- Note that divergences other than the KL divergence can be used for the SNE optimization; e.g., see [10].
- The gradient of c_1 with respect to $\boldsymbol{y}_i$ is:

$$\mathbb{R}^p \ni \frac{\partial c_1}{\partial \boldsymbol{y}_i} = 2 \sum_{j=1}^{n} (p_{ij} - q_{ij} + p_{ji} - q_{ji})(\boldsymbol{y}_i - \boldsymbol{y}_j), \tag{7}$$

  where p_{ij} and q_{ij} are the Eqs. (2) and (4), and $p_{ii} = q_{ii} = 0$.
- For proof of this, refer to our tutorial "Stochastic neighbor embedding with Gaussian and student-t distributions: Tutorial and survey" [11] or our textbook.

Stochastic Neighbor Embedding (SNE)

- The update of the embedded point $\boldsymbol{y}_i$ is done by **gradient descent**. Every iteration is:

$$\begin{aligned} \Delta \boldsymbol{y}_i^{(t)} &:= -\eta \frac{\partial c_1}{\partial \boldsymbol{y}_i} + \alpha(t)\, \Delta \boldsymbol{y}_i^{(t-1)}, \\ \boldsymbol{y}_i^{(t)} &:= \boldsymbol{y}_i^{(t-1)} + \Delta \boldsymbol{y}_i^{(t)}, \end{aligned} \tag{8}$$

  where **momentum** is used for better convergence [12].
- The $\alpha(t)$ is the **momentum**. It can be smaller for initial iterations and larger for further iterations. For example, we can have [7]:

$$\alpha(t) := \begin{cases} 0.5 & t < 250, \\ 0.8 & t \geq 250. \end{cases} \tag{9}$$

  In the original paper of SNE [1], the momentum term is not mentioned but it is suggested in [7].
- The η is the **learning rate** which can be a small positive constant (e.g., $\eta = 0.1$) or can be updated adaptively according to [13].
- Moreover, in both [1] and [7], it is mentioned that in SNE we should add some **Gaussian noise (random jitter)** to the solution of the **first iterations** before going to the next iterations. It helps **avoiding the local optimum** solutions.

Symmetric Stochastic Neighbor Embedding

Symmetric Stochastic Neighbor Embedding

- In **symmetric SNE** (2008) [7], we consider a Gaussian probability around every point $\boldsymbol{x}_i$. The probability that the point $\boldsymbol{x}_i \in \mathbb{R}^d$ takes $\boldsymbol{x}_j \in \mathbb{R}^d$ as its neighbor is:

$$\mathbb{R} \ni p_{ij} := \frac{\exp(-d_{ij}^2)}{\sum_{k \neq l} \exp(-d_{kl}^2)}, \tag{10}$$

  where:

$$\mathbb{R} \ni d_{ij}^2 := \frac{||\boldsymbol{x}_i - \boldsymbol{x}_j||_2^2}{2\sigma_i^2}. \tag{11}$$

- Note that the **denominator** of Eq. (10) for all points is fixed and thus it is symmetric for i and j. Compare this with Eq. (2):

$$\mathbb{R} \ni p_{ij} := \frac{\exp(-d_{ij}^2)}{\sum_{k \neq i} \exp(-d_{ik}^2)},$$

  which is not symmetric.

Symmetric Stochastic Neighbor Embedding

- The Eq. (10):

$$\mathbb{R} \ni p_{ij} := \frac{\exp(-d_{ij}^2)}{\sum_{k \neq l} \exp(-d_{kl}^2)},$$

has a **problem with outliers**. If the point $\boldsymbol{x}_i$ is an outlier, its p_{ij} will be **extremely small** because the denominator is fixed for every point and numerator will be small for the outlier.

- However, If we use Eq. (2) for p_{ij}:

$$\mathbb{R} \ni p_{ij} := \frac{\exp(-d_{ij}^2)}{\sum_{k \neq i} \exp(-d_{ik}^2)},$$

the denominator for all the points is not the same and therefore, **the denominator for an outlier will also be small waving out the problem of small numerator**.

- For this mentioned problem, we do not use Eq. (10) and rather we use:

$$\mathbb{R} \ni p_{ij} := \frac{p_{i|j} + p_{j|i}}{2n}, \tag{12}$$

where:

$$\mathbb{R} \ni p_{j|i} := \frac{\exp(-d_{ij}^2)}{\sum_{k \neq i} \exp(-d_{ik}^2)}, \tag{13}$$

is the probability that $\boldsymbol{x}_i \in \mathbb{R}^d$ takes $\boldsymbol{x}_j \in \mathbb{R}^d$ as its neighbor.

Symmetric Stochastic Neighbor Embedding

- In the low-dimensional embedding space, we consider a Gaussian probability distribution for the point $\boldsymbol{y}_i \in \mathbb{R}^p$ to take $\boldsymbol{y}_j \in \mathbb{R}^p$ as its neighbor and we make it **symmetric** (**fixed denominator for all points**):

$$\mathbb{R} \ni q_{ij} := \frac{\exp(-z_{ij}^2)}{\sum_{k \neq l} \exp(-z_{kl}^2)}, \tag{14}$$

  where:

$$\mathbb{R} \ni z_{ij}^2 := ||\boldsymbol{y}_i - \boldsymbol{y}_j||_2^2. \tag{15}$$

- Note that the Eq. (14) does **not have the problem of outliers** as in Eq. (10) because even for an **outlier**, the **embedded points are initialized close together and not far**.

Symmetric Stochastic Neighbor Embedding

- We want the probability distributions in both the input and embedded spaces to be as similar as possible; therefore, the cost function to be minimized can be summation of the **Kullback-Leibler (KL) divergences** [9] over the n points:

$$\mathbb{R} \ni c_2 := \sum_{i=1}^{n} \text{KL}(P_i || Q_i) = \sum_{i=1}^{n} \sum_{j=1, j \neq i}^{n} p_{ij} \log(\frac{p_{ij}}{q_{ij}}), \quad (16)$$

  where p_{ij} and q_{ij} are the Eqs. (12) and (14).

- The gradient of c_2 with respect to $\boldsymbol{y}_i$ is:

$$\mathbb{R}^p \ni \frac{\partial c_2}{\partial \boldsymbol{y}_i} = 4 \sum_{j=1}^{n} (p_{ij} - q_{ij})(\boldsymbol{y}_i - \boldsymbol{y}_j), \quad (17)$$

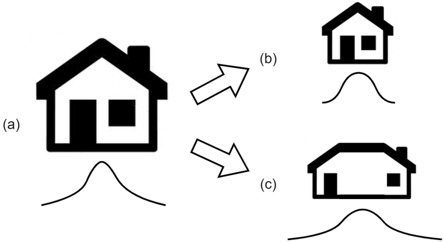
  where p_{ij} and q_{ij} are the Eqs. (12) and (14), and $p_{ii} = q_{ii} = 0$.

- For proof of this, refer to our tutorial "Stochastic neighbor embedding with Gaussian and student-t distributions: Tutorial and survey" [11] or our textbook.

t-distributed Stochastic Neighbor Embedding (t-SNE)

The Crowding Problem

- In SNE [1], we are considering **Gaussian** distribution for both input and embedded spaces.
- That is okay for the **input space** because it already has a high dimensionality.
- However, when we **embed the high-dimensional data into a low-dimensional space**, it is very hard to fit the **information** of all the points in the same neighborhood area.
- For better clarification, suppose the dimensionality is like the size of a room, as depicted in this figure. In high dimensionality, we have a large hall including a huge crowd of people. Now, we want to fit all the people into a small room; of course, we cannot! This problem is referred to as the **crowding problem**.



t-distributed Stochastic Neighbor Embedding (t-SNE)

- The main idea of **t-SNE** (2008) [7] is addressing the **crowding problem** which exists in SNE [1].
- In the example of fitting people in a room, t-SNE **enlarges** the room to solve the crowding problem (see the figure).
- Therefore, in the formulation of t-SNE, we use **Student-t distribution [14] rather than Gaussian distribution** for the **low-dimensional embedded space**.
- This is because the Student-t distribution has **heavier tails** than Gaussian distribution, which is like a larger room, and can fit the information of high dimensional data in the low dimensional embedding space.
- As we will see later, the q_{ij} in t-SNE is:

$$q_{ij} = \frac{(1 + z_{ij}^2)^{-1}}{\sum_{k \neq l} (1 + z_{kl}^2)^{-1}},$$

which is based on the **standard Cauchy distribution**:

$$f(z) = \frac{1}{\pi(1 + z^2)}, \tag{18}$$

where π is canceled from the numerator and the normalizing denominator in q_{ij} (similar to the technique of **softmax**).

t-distributed Stochastic Neighbor Embedding (t-SNE)

- If the **Student-t distribution** [14] with the **general degrees of freedom** δ is used, we would have:

$$f(z) = \frac{\Gamma(\frac{\delta+1}{2})}{\sqrt{\delta \times \pi}\ \ \Gamma(\frac{\delta}{2})}(1 + \frac{z^2}{\delta})^{-\frac{\delta+1}{2}}, \tag{19}$$

  where Γ is the gamma function.

- Cancelling out the scaling factors from the numerator and denominator, we would have [15]:

$$q_{ij} = \frac{(1 + z_{ij}^2/\delta)^{-(\delta+1)/2}}{\sum_{k \neq l}(1 + z_{kl}^2/\delta)^{-(\delta+1)/2}}. \tag{20}$$

- However, as the **first degree of freedom has the heaviest tails** amongst different degrees of freedom, it is the most suitable for the crowding problem; hence, we use the **first degree of freedom** which is the **Cauchy distribution**. Note that the t-SNE algorithm, which uses the Cauchy distribution, may also be called the **Cauchy-SNE**.
- Later, **t-SNE with general degrees of freedom** was proposed [15].

t-distributed Stochastic Neighbor Embedding (t-SNE)

- In t-SNE [7], we consider a **Gaussian** probability around every point $\boldsymbol{x}_i$ in the input space because the **crowding problem does not exist in the high dimensional data**. The probability that the point $\boldsymbol{x}_i \in \mathbb{R}^d$ takes $\boldsymbol{x}_j \in \mathbb{R}^d$ as its neighbor is:

$$\mathbb{R} \ni p_{j|i} := \frac{\exp(-d_{ij}^2)}{\sum_{k \neq i} \exp(-d_{ik}^2)}, \tag{21}$$

where:

$$\mathbb{R} \ni d_{ij}^2 := \frac{||\boldsymbol{x}_i - \boldsymbol{x}_j||_2^2}{2\sigma_i^2}. \tag{22}$$

- Note that Eq. (21) is not symmetric for i and j because of the denominator. We take the **symmetric** p_{ij} as the scaled average of $p_{i|j}$ and $p_{j|i}$:

$$\mathbb{R} \ni p_{ij} := \frac{p_{i|j} + p_{j|i}}{2n}. \tag{23}$$

- In the low-dimensional **embedding space**, we consider a **Student's *t*-distribution with one degree of freedom (Cauchy distribution)** for the point $\boldsymbol{y}_i \in \mathbb{R}^p$ to take $\boldsymbol{y}_j \in \mathbb{R}^p$ as its neighbor:

$$\mathbb{R} \ni q_{ij} := \frac{(1 + z_{ij}^2)^{-1}}{\sum_{k \neq l}(1 + z_{kl}^2)^{-1}}, \tag{24}$$

where:

$$\mathbb{R} \ni z_{ij}^2 := ||\boldsymbol{y}_i - \boldsymbol{y}_j||_2^2. \tag{25}$$

t-distributed Stochastic Neighbor Embedding (t-SNE)

- We want the probability distributions in both the input and embedded spaces to be as similar as possible; therefore, the cost function to be minimized can be summation of the **Kullback-Leibler (KL) divergences** [9] over the n points:

$$\mathbb{R} \ni c_3 := \sum_{i=1}^{n} \text{KL}(P_i || Q_i) = \sum_{i=1}^{n} \sum_{j=1, j \neq i}^{n} p_{ij} \log(\frac{p_{ij}}{q_{ij}}), \tag{26}$$

  where p_{ij} and q_{ij} are the Eqs. (23) and (24).

- The gradient of c_3 with respect to $\boldsymbol{y}_i$ is:

$$\frac{\partial c_3}{\partial \boldsymbol{y}_i} = 4 \sum_{j=1}^{n} (p_{ij} - q_{ij})(1 + ||\boldsymbol{y}_i - \boldsymbol{y}_j||_2^2)^{-1} (\boldsymbol{y}_i - \boldsymbol{y}_j), \tag{27}$$

  where p_{ij} and q_{ij} are the Eqs. (23) and (24), and $p_{ii} = q_{ii} = 0$.

t-distributed Stochastic Neighbor Embedding (t-SNE)

- Proof: Proof is according to [7]. Let:

$$\mathbb{R} \ni r_{ij} := z_{ij}^2 = ||\boldsymbol{y}_i - \boldsymbol{y}_j||_2^2. \tag{28}$$

- By changing $\boldsymbol{y}_i$, we only have change impact in z_{ij} and z_{ji} for all j's. According to chain rule, we have:

$$\mathbb{R}^p \ni \frac{\partial c_3}{\partial \boldsymbol{y}_i} = \sum_j \big(\frac{\partial c_3}{\partial r_{ij}} \frac{\partial r_{ij}}{\partial \boldsymbol{y}_i} + \frac{\partial c_3}{\partial r_{ji}} \frac{\partial r_{ji}}{\partial \boldsymbol{y}_i}\big).$$

- According to Eq. (28), we have:

$$r_{ij} = ||\boldsymbol{y}_i - \boldsymbol{y}_j||_2^2 \implies \frac{\partial r_{ij}}{\partial \boldsymbol{y}_i} = 2(\boldsymbol{y}_i - \boldsymbol{y}_j),$$
$$r_{ji} = ||\boldsymbol{y}_j - \boldsymbol{y}_i||_2^2 = ||\boldsymbol{y}_i - \boldsymbol{y}_j||_2^2 \implies \frac{\partial r_{ji}}{\partial \boldsymbol{y}_i} = 2(\boldsymbol{y}_i - \boldsymbol{y}_j).$$

- Therefore:

$$\therefore \quad \frac{\partial c_3}{\partial \boldsymbol{y}_i} = 2 \sum_j \big(\frac{\partial c_3}{\partial r_{ij}} + \frac{\partial c_3}{\partial r_{ji}}\big)(\boldsymbol{y}_i - \boldsymbol{y}_j). \tag{29}$$

t-distributed Stochastic Neighbor Embedding (t-SNE)

- The cost function can be re-written as:

$$c_3 = \sum_{k} \sum_{l \neq k} p_{kl} \log(\frac{p_{kl}}{q_{kl}}) = \sum_{k \neq l} p_{kl} \log(\frac{p_{kl}}{q_{kl}})$$
$$= \sum_{k \neq l} \big(p_{kl} \log(p_{kl}) - p_{kl} \log(q_{kl})\big),$$

  whose first term is a constant with respect to q_{kl} and thus to r_{kl}.
- We have:

$$\mathbb{R} \ni \frac{\partial c_3}{\partial r_{ij}} = -\sum_{k \neq l} p_{kl} \frac{\partial(\log(q_{kl}))}{\partial r_{ij}}.$$

- According to Eq. (24):

$$\mathbb{R} \ni q_{ij} := \frac{(1 + z_{ij}^2)^{-1}}{\sum_{k \neq l}(1 + z_{kl}^2)^{-1}},$$

  the q_{kl} is:

$$q_{kl} := \frac{(1 + z_{kl}^2)^{-1}}{\sum_{m \neq f}(1 + z_{mf}^2)^{-1}}, = \frac{(1 + r_{kl})^{-1}}{\sum_{m \neq f}(1 + r_{mf})^{-1}}.$$

- We take the denominator of q_{kl} as:

$$\beta := \sum_{m \neq f}(1 + z_{mf}^2)^{-1} = \sum_{m \neq f}(1 + r_{mf})^{-1}. \tag{30}$$

t-distributed Stochastic Neighbor Embedding (t-SNE)

- We had:

$$\mathbb{R} \ni \frac{\partial c_3}{\partial r_{ij}} = -\sum_{k \neq l} p_{kl} \frac{\partial(\log(q_{kl}))}{\partial r_{ij}}, \quad q_{kl} := \frac{(1+z_{kl}^2)^{-1}}{\sum_{m \neq f}(1+z_{mf}^2)^{-1}}, = \frac{(1+r_{kl})^{-1}}{\sum_{m \neq f}(1+r_{mf})^{-1}},$$

$$\beta := \sum_{m \neq f}(1+z_{mf}^2)^{-1} = \sum_{m \neq f}(1+r_{mf})^{-1}.$$

- We have $\log(q_{kl}) = \log(q_{kl}) + \log\beta - \log\beta = \log(q_{kl}\beta) - \log\beta$. Therefore:

$$\therefore \quad \frac{\partial c_3}{\partial r_{ij}} = -\sum_{k \neq l} p_{kl} \frac{\partial\big(\log(q_{kl}\beta) - \log\beta\big)}{\partial r_{ij}} = -\sum_{k \neq l} p_{kl} \Big[\frac{\partial\big(\log(q_{kl}\beta)\big)}{\partial r_{ij}} - \frac{\partial\big(\log\beta\big)}{\partial r_{ij}}\Big]$$

$$= -\sum_{k \neq l} p_{kl} \Big[\frac{1}{q_{kl}\beta} \frac{\partial\big(q_{kl}\beta\big)}{\partial r_{ij}} - \frac{1}{\beta}\frac{\partial\beta}{\partial r_{ij}}\Big].$$

- The $q_{kl}\beta$ is:

$$q_{kl}\beta = \frac{(1+r_{kl})^{-1}}{\sum_{m \neq f}(1+r_{mf})^{-1}} \times \sum_{m \neq f}(1+r_{mf})^{-1} = (1+r_{kl})^{-1}.$$

- Therefore, we have:

$$\therefore \quad \frac{\partial c_3}{\partial r_{ij}} = -\sum_{k \neq l} p_{kl} \Big[\frac{1}{q_{kl}\beta} \frac{\partial\big((1+r_{kl})^{-1}\big)}{\partial r_{ij}} - \frac{1}{\beta}\frac{\partial\beta}{\partial r_{ij}}\Big].$$

t-distributed Stochastic Neighbor Embedding (t-SNE)

- We found:

$$\frac{\partial c_3}{\partial r_{ij}} = -\sum_{k \neq l} p_{kl} \Big[\frac{1}{q_{kl}\beta} \frac{\partial\big((1+r_{kl})^{-1}\big)}{\partial r_{ij}} - \frac{1}{\beta} \frac{\partial \beta}{\partial r_{ij}} \Big].$$

- The $\partial\big((1+r_{kl})^{-1}\big)/\partial r_{ij}$ is non-zero for only $k = i$ and $l = j$; therefore:

$$\frac{\partial\big((1+r_{ij})^{-1}\big)}{\partial r_{ij}} = -(1+r_{ij})^{-2},$$

$$\frac{\partial \beta}{\partial r_{ij}} = \frac{\partial \sum_{m \neq f} (1+r_{mf})^{-1}}{\partial r_{ij}} = \frac{\partial (1+r_{ij})^{-1}}{\partial r_{ij}} = -(1+r_{ij})^{-2}.$$

- Therefore:

$$\therefore \quad \frac{\partial c_3}{\partial r_{ij}} = -\Big(p_{ij} \Big[\frac{-1}{q_{ij}\beta} (1+r_{ij})^{-2} \Big] + 0 + \dots + 0 \Big) - \sum_{k \neq l} p_{kl} \Big[\frac{1}{\beta} (1+r_{ij})^{-2} \Big].$$

- We have $\sum_{k \neq l} p_{kl} = 1$ because summation of all possible probabilities is one. Thus:

$$\frac{\partial c_3}{\partial r_{ij}} = -p_{ij} \Big[\frac{-1}{q_{ij}\beta} (1+r_{ij})^{-2} \Big] - \Big[\frac{1}{\beta} (1+r_{ij})^{-2} \Big] = (1+r_{ij})^{-1} \underbrace{\frac{(1+r_{ij})^{-1}}{\beta}}_{=q_{ij}} \Big[\frac{p_{ij}}{q_{ij}} - 1 \Big]$$

$$= (1+r_{ij})^{-1}(p_{ij} - q_{ij}).$$

t-distributed Stochastic Neighbor Embedding (t-SNE)

- We found:

$$\frac{\partial c_3}{\partial r_{ij}} = (1 + r_{ij})^{-1}(p_{ij} - q_{ij}).$$

- Similarly, we have:

$$\frac{\partial c_3}{\partial r_{ji}} = (1 + r_{ji})^{-1}(p_{ji} - q_{ji}) \overset{(a)}{=} (1 + r_{ij})^{-1}(p_{ij} - q_{ij}),$$

  where (a) is because in t-SNE, the p_{ij}, q_{ij}, and r_{ij} are symmetric for i and j according to Eqs. (23), (24), and (28).

- Substituting the obtained derivatives in Eq. (29):

$$\therefore \quad \frac{\partial c_3}{\partial \boldsymbol{y}_i} = 2 \sum_j \Big(\frac{\partial c_3}{\partial r_{ij}} + \frac{\partial c_3}{\partial r_{ji}}\Big)(\boldsymbol{y}_i - \boldsymbol{y}_j),$$

  gives us:

$$\frac{\partial c_3}{\partial \boldsymbol{y}_i} = 4 \sum_j (p_{ij} - q_{ij})(1 + r_{ij})^{-1}(\boldsymbol{y}_i - \boldsymbol{y}_j),$$

  which is the gradient mentioned before. Q.E.D.

t-distributed Stochastic Neighbor Embedding (t-SNE)

- The update of the embedded point $\boldsymbol{y}_i$ is done by gradient descent whose every iteration is as Eq. (8) where c_1 is replaced by c_3:

$$\Delta \boldsymbol{y}_i^{(t)} := -\eta \frac{\partial c_1}{\partial \boldsymbol{y}_i} + \alpha(t)\, \Delta \boldsymbol{y}_i^{(t-1)},$$
$$\boldsymbol{y}_i^{(t)} := \boldsymbol{y}_i^{(t-1)} + \Delta \boldsymbol{y}_i^{(t)}.$$

- For t-SNE, there is **no need to add jitter** to the solution of initial iterations [7] because it is **more robust than SNE**.
- In t-SNE, it is better to **multiply all p_{ij}'s by a constant (e.g., 4)** in the **initial iterations**:

$$p_{ij} := p_{ij} \times 4, \tag{31}$$

  which is called **early exaggeration**. This heuristic helps the optimization **focus on the large p_{ij}'s (close neighbors) more in the early iterations**.
- This is because **large p_{ij}'s are affected more by multiplying by 4 than the small p_{ij}'s.**
- **After the neighbours are embedded close to one another**, we are free not to do this multiplication any more and let far-away points be embedded using the probabilities without multiplication. Note that the early exaggeration is **optional** and not mandatory.

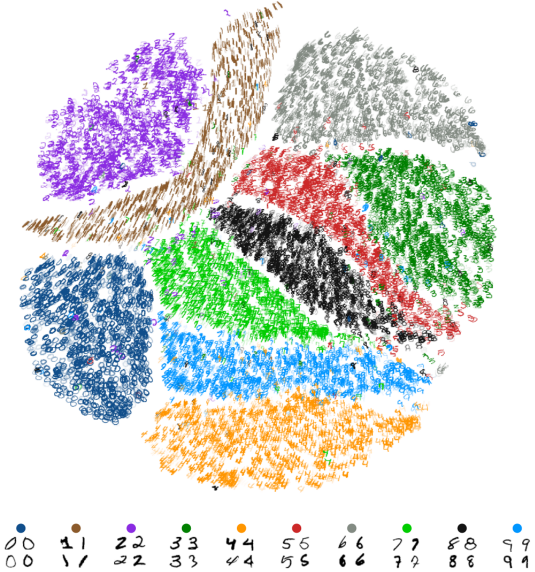
t-distributed Stochastic Neighbor Embedding (t-SNE)

- We can have **general degrees of freedom** for **Student-t distribution** in t-SNE [15].
- As we saw in Eqs. (19) and (20), we can have any degrees of freedom for q_{ij} (note that α is a positive integer). We repeat Eq. (20) here for more convenience:

$$q_{ij} = \frac{(1 + z_{ij}^2/\delta)^{-(\delta+1)/2}}{\sum_{k \neq l}(1 + z_{kl}^2/\delta)^{-(\delta+1)/2}}. \tag{32}$$

- If $\delta \rightarrow \infty$, the Student-t distribution formulated in Eq. (19) tends to Gaussian distribution used in SNE [1].
- SNE and t-SNE use degrees $\delta \rightarrow \infty$ and $\delta = 1$ in Eq. (32), respectively.

Example of t-SNE Embedding (Digit Dataset)



Credit of image: [16]

Acknowledgment

- Some slides are based on our tutorial paper: "Stochastic neighbor embedding with Gaussian and student-t distributions: Tutorial and survey" [11]
- For more information on SNE and t-SNE, refer to our tutorial paper [11].
- Some slides of this slide deck are inspired by teachings of Prof. Ali Ghodsi at University of Waterloo, Department of Statistics.
- The code of SNE and t-SNE in my GitHub: `https://github.com/bghojogh/SNE-tSNE`
- t-SNE in sklearn: `https://scikit-learn.org/stable/modules/generated/sklearn.manifold.TSNE.html`

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