Stochastic Neighbor Embedding with Gaussian and Student-t Distributions: Tutorial and Survey

Benyamin Ghojogh
Department of Electrical and Computer Engineering, Machine Learning Laboratory, University of Waterloo, Waterloo, ON, Canada

Ali Ghodsi
Department of Statistics and Actuarial Science & David R. Cheriton School of Computer Science, Data Analytics Laboratory, University of Waterloo, Waterloo, ON, Canada

Fakhri Karray
Department of Electrical and Computer Engineering, Centre for Pattern Analysis and Machine Intelligence, University of Waterloo, Waterloo, ON, Canada

Mark Crowley
Department of Electrical and Computer Engineering, Machine Learning Laboratory, University of Waterloo, Waterloo, ON, Canada

Abstract
Stochastic Neighbor Embedding (SNE) is a manifold learning and dimensionality reduction method with a probabilistic approach. In SNE, every point is considered to be the neighbor of all other points with some probability and this probability is tried to be preserved in the embedding space. SNE considers Gaussian distribution for the probability in both the input and embedding spaces. However, t-SNE uses the Student-t and Gaussian distributions in these spaces, respectively. In this tutorial and survey paper, we explain SNE, symmetric SNE, t-SNE (or Cauchy-SNE), and t-SNE with general degrees of freedom. We also cover the out-of-sample extension and acceleration for these methods.

1. Introduction
Stochastic Neighbor Embedding (SNE) (Hinton & Roweis, 2003) is a manifold learning and dimensionality reduction method which can be used for feature extraction (Ghojogh et al., 2019). It has a probabilistic approach. It fits the data in the embedding space locally hoping to preserve the global structure of data (Saul & Roweis, 2003). 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. It is noteworthy that there exist some other similar probabilistic dimensionality reduction methods which make use of Gaussian distribution for neighborhood. Some examples are Neighborhood Component Analysis (NCA) (Goldberger et al., 2005), deep NCA (Liu et al., 2020), and Proxy-NCA (Movshovitz-Attias et al., 2017).

SNE uses the Gaussian distribution for neighbors in both the input and embedding spaces. The Student-t distributed SNE, or so-called t-SNE (van der Maaten & Hinton, 2008), considers the Student-t and Gaussian distributions in these 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 (Kobak & Berens, 2019). In this paper, we explain SNE, symmetric SNE, t-SNE (or Cauchy-SNE), t-SNE with general degrees of freedom, their out-of-sample extensions, and their accelerations. We also show the results of simulations for visualization of embeddings.

The goal of SNE is to embed the high-dimensional data
\{x_i\}_{i=1}^n \text{ into the lower dimensional data } \{y_i\}_{i=1}^n \text{ where } n \text{ is the number of data points. We denote the dimensionality of high- and low-dimensional spaces by } d \text{ and } p, \text{ respectively, i.e. } x_i \in \mathbb{R}^d \text{ and } y_i \in \mathbb{R}^p. \text{ We usually have } p \ll d. \text{ For data visualization, we have } p \in \{2, 3\}. \text{ The remainder of this paper is organized as follows. In Sections 2 and 3, we explain SNE and symmetric SNE, respectively. Section 4 introduces the crowding problem and the t-SNE or Cauchy-SNE method. The out-of-sample embedding and acceleration of these methods are introduced in Sections 6 and 7, respectively. Recent improvements of t-SNE are briefly mentioned in Section 8. Finally, Section 9 concludes the paper.}

2. Stochastic Neighbor Embedding (SNE)

In SNE (Hinton & Roweis, 2003), we consider a Gaussian probability around every point \(x_i\), where the point \(x_i\) is on the mean and the distribution is for probability of accepting any other point as the neighbor of \(x_i\); the farther points are neighbors with less probability. Hence, the variance is distance, denoted by \(d \in \mathbb{R}\), and the Gaussian probability is:

\[
 f(d) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{d^2}{2\sigma^2}\right),
\]

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 \(x_i \in \mathbb{R}^d\) takes \(x_j \in \mathbb{R}^d\) as its neighbor is:

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

where:

\[
 \mathbb{R} \ni d_{ij}^2 := \frac{||x_i - x_j||^2}{2\sigma_i^2}.
\]

Note that this trick is also used for \(q_{ij}\) in SNE and also for \(p_{ij}\) and \(q_{ij}\) in t-SNE (and its variants) as we will see later. It is noteworthy that the mentioned trick is also used in other methods such as Continuous Bag-of-Word (CBOW) model of Word2Vec (Mikolov et al., 2013a; Rong, 2014), Euclidean Embedding (Globerson et al., 2007), and Parametric Embedding (Iwata et al., 2005). In this trick, the summation in the denominator can get very time-consuming especially when the dataset (or corpus for Word2Vec) is large. This plus the slow pace of gradient descent (Boyd & Vandenberghe, 2004) are the reasons that SNE, t-SNE, and Word2Vec are very slow and even infeasible for large datasets. The Word2Vec tackled the problem of the slow pace by introducing Negative Sampling Skip-Gram model (Mikolov et al., 2013b; Goldberg & Levy, 2014) which uses logistic function similar to the approach of logistic regression (Kleinbaum et al., 2002). In logistic function, we deal with inner product (similarity) of data points rather than distance of data points and there is no summation in the denominator. The Negative Sampling Skip-Gram model also uses Newton’s method, which is much faster than gradient descent (Boyd & Vandenberghe, 2004), similar to logistic regression.

The \(\sigma_i^2\) is the variance which we consider for the Gaussian distribution used for the \(x_i\). It can be set to a fixed number or determined by a binary search to make the entropy of distribution some specific value (Hinton & Roweis, 2003). 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 \(y_i \in \mathbb{R}^p\) to take \(y_j \in \mathbb{R}^p\) as its neighbor:

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

where:

\[
 \mathbb{R} \ni z_{ij}^2 := ||y_i - y_j||^2.
\]

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.

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 (Kullback, 1997) over the \(n\) points:

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

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 (Im et al., 2018).

**Proposition 1.** The gradient of \(c_1\) with respect to \(y_i\) is:

\[
 \mathbb{R}^p \ni \frac{\partial c_1}{\partial y_i} = 2 \sum_{j=1}^{n} (p_{ij} - q_{ij} + p_{ji} - q_{ji})(y_i - y_j),
\]

where \(p_{ij}\) and \(q_{ij}\) are the Eqs. (2) and (4), and \(p_{ii} = q_{ii} = 0\).
Proof. Proof is inspired by (van der Maaten & Hinton, 2008). Let:

\[ R \ni r_{ij} := z^2_{ij} = ||y_i - y_j||^2. \tag{8} \]

By changing \( y_i \), we only have change impact in \( z_{ij} \) and \( z_{ji} \) (or \( r_{ij} \) and \( r_{ji} \) for all \( j \)’s. According to chain rule, we have:

\[ R^p \ni \frac{\partial c_1}{\partial y_i} = \sum_j \left( \frac{\partial c_1}{\partial r_{ij}} \frac{\partial r_{ij}}{\partial y_i} + \frac{\partial c_1}{\partial r_{ji}} \frac{\partial r_{ji}}{\partial y_i} \right). \]

According to Eq. (8), we have:

\[ r_{ij} = ||y_i - y_j||^2 \implies \frac{\partial r_{ij}}{\partial y_i} = 2(y_i - y_j), \]

\[ r_{ji} = ||y_j - y_i||^2 \implies \frac{\partial r_{ji}}{\partial y_i} = 2(y_i - y_j). \]

Therefore:

\[ \therefore \frac{\partial c_1}{\partial y_i} = 2 \sum_j \left( \frac{\partial c_1}{\partial r_{ij}} + \frac{\partial c_1}{\partial r_{ji}} \right)(y_i - y_j). \tag{9} \]

The cost function can be re-written as:

\[ c_1 = \sum_k \sum_{i \neq k} p_{kl} \log \left( \frac{p_{kl}}{q_{kl}} \right) = \sum_{k \neq l} p_{kl} \log \left( \frac{p_{kl}}{q_{kl}} \right) \]

\[ = \sum_{k \neq l} (p_{kl} \log(p_{kl}) - p_{kl} \log(q_{kl})), \]

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

\[ R \ni \frac{\partial c_1}{\partial r_{ij}} = -\sum_{k \neq l} p_{kl} \frac{\partial \log(q_{kl})}{\partial r_{ij}}. \]

According to Eq. (4), the \( q_{kl} \) is:

\[ q_{kl} := \frac{\exp(-z^2_{kl})}{\sum_{k \neq f} \exp(-z^2_{kf})} = \frac{\exp(-r_{kl})}{\sum_{k \neq f} \exp(-r_{kf})}. \]

We take the denominator of \( q_{kl} \) as:

\[ \beta := \sum_{k \neq f} \exp(-z^2_{kf}) = \sum_{k \neq f} \exp(-r_{kf}). \tag{10} \]

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

\[ \therefore \frac{\partial c_1}{\partial r_{ij}} = -\sum_{k \neq l} p_{kl} \frac{\partial \left( \log(q_{kl} \beta) - \log(\beta) \right)}{\partial r_{ij}} \]

\[ = -\sum_{k \neq l} p_{kl} \left[ \frac{\partial (\log(q_{kl} \beta))}{\partial r_{ij}} - \frac{\partial (\log(\beta))}{\partial r_{ij}} \right] \]

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

The \( q_{kl} \) is:

\[ q_{kl} \beta = \frac{\exp(-r_{kl})}{\sum_{f \neq k} \exp(-r_{kf})} \times \sum_{k \neq f} \exp(-r_{kf}) = \exp(-r_{kl}). \]

Therefore, we have:

\[ \therefore \frac{\partial c_1}{\partial r_{ij}} = -\sum_{k \neq l} p_{kl} \left[ \frac{1}{q_{kl} \beta} \frac{\partial (\exp(-r_{kl}))}{\partial r_{ij}} - \frac{1}{\beta} \frac{\partial (\exp(-r_{kl}))}{\partial r_{ij}} \right]. \]

The \( \frac{\partial (\exp(-r_{kl}))}{\partial r_{ij}}/\partial r_{ij} \) is non-zero for only \( k = i \) and \( l = j \); therefore:

\[ \frac{\partial (\exp(-r_{kl}))}{\partial r_{ij}} = -\exp(-r_{ij}), \]

\[ \frac{\partial \beta}{\partial r_{ij}} = \frac{\partial \sum_{k \neq f} \exp(-r_{kf})}{\partial r_{ij}} = \frac{\partial \exp(-r_{ij})}{\partial r_{ij}} = -\exp(-r_{ij}). \]

Therefore:

\[ \therefore \frac{\partial c_1}{\partial r_{ij}} = -\left( p_{ij} \left[ \frac{-1}{q_{ij} \beta} \exp(-r_{ij}) + 0 + \cdots + 0 \right] \right) \]

\[ -\sum_{k \neq l} p_{kl} \left[ \frac{1}{\beta} \exp(-r_{ij}) \right]. \]

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

\[ \frac{\partial c_1}{\partial r_{ij}} = -p_{ij} \left[ \frac{-1}{q_{ij} \beta} \exp(-r_{ij}) \right] - \left[ \frac{1}{\beta} \exp(-r_{ij}) \right] \]

\[ = \exp(-r_{ij}) \left[ p_{ij} - q_{ij} \right] = p_{ij} - q_{ij}. \tag{11} \]

Similarly, we have:

\[ \frac{\partial c_1}{\partial r_{ji}} = p_{ji} - q_{ji}. \tag{12} \]

Substituting the obtained derivatives in Eq. (9) gives us:

\[ \frac{\partial c_1}{\partial y_i} = 2 \sum_j (p_{ij} - q_{ij} + p_{ji} - q_{ji})(y_i - y_j), \]

which is the gradient mentioned in the proposition. Q.E.D.

The update of the embedded point \( y_i \) is done by gradient descent. Every iteration is:

\[ \Delta y_i^{(t)} := -\eta \frac{\partial c_1}{\partial y_i} + \alpha(t) \Delta y_i^{(t-1)}, \]

\[ y_i^{(t)} := y_i^{(t-1)} + \Delta y_i^{(t)}, \tag{13} \]
where momentum is used for better convergence (Qian, 1999). The $\alpha(t)$ is the momentum. It can be smaller for initial iterations and larger for further iterations. For example, we can have (van der Maaten & Hinton, 2008):

$$\alpha(t) := \begin{cases} 0.5 & t < 250, \\ 0.8 & t \geq 250. \end{cases}$$ (14)

In the original paper of SNE (Hinton & Roweis, 2003), the momentum term is not mentioned but it is suggested in (van der Maaten & Hinton, 2008).

The $\eta$ is the learning rate which can be a small positive constant (e.g., $\eta = 0.1$) or can be updated adaptively according to (Jacobs, 1988).

Moreover, in both (Hinton & Roweis, 2003) and (van der Maaten & Hinton, 2008), 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.

3. Symmetric Stochastic Neighbor Embedding

In symmetric SNE (van der Maaten & Hinton, 2008), we consider a Gaussian probability around every point $x_i$. The probability that the point $x_i \in \mathbb{R}^d$ takes $x_j \in \mathbb{R}^d$ as its neighbor is:

$$\mathbb{R} \ni p_{ij} := \frac{\exp(-d_{ij}^2)}{\sum_{k \neq i} \exp(-d_{ik}^2)},$$ (15)

where:

$$\mathbb{R} \ni d_{ij}^2 := \frac{||x_i - x_j||^2}{2\sigma_i^2}.$$(16)

Note that the denominator of Eq. (15) for all points is fixed and thus it is symmetric for $i$ and $j$. Compare this with Eq. (2) which is not symmetric.

The $\sigma_i^2$ is the variance which we consider for the Gaussian distribution used for the $x_i$. It can be set to a fixed number or determined by a binary search to make the entropy of distribution some specific value (Hinton & Roweis, 2003).

The Eq. (15) has a problem with outliers. If the point $x_i$ 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 $p_{ij}$, 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. (15) and rather we use:

$$\mathbb{R} \ni p_{ij} := \frac{p_{ji} + p_{ij}}{2n},$$ (17)

where:

$$\mathbb{R} \ni p_{ji} := \frac{\exp(-d_{ji}^2)}{\sum_{k \neq i} \exp(-d_{ki}^2)}.$$(18)

is the probability that $x_i \in \mathbb{R}^d$ takes $x_j \in \mathbb{R}^d$ as its neighbor.

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

$$\mathbb{R} \ni q_{ij} := \frac{\exp(-z_{ij}^2)}{\sum_{k \neq i} \exp(-z_{ki}^2)},$$ (19)

where:

$$\mathbb{R} \ni z_{ij}^2 := ||y_i - y_j||^2.$$(20)

Note that the Eq. (19) does not have the problem of outliers as in Eq. (15) because even for an outlier, the embedded points are initialized close together and not far.

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 (Kullback, 1997) over the $n$ points:

$$\mathbb{R}^p \ni c_2 := \sum_{i=1}^{n} KL(P_i||Q_i) = \sum_{i=1}^{n} \sum_{j=1, j \neq i}^{n} p_{ij} \log \left( \frac{p_{ij}}{q_{ij}} \right),$$ (21)

where $p_{ij}$ and $q_{ij}$ are the Eqs. (17) and (19).

**Proposition 2.** The gradient of $c_2$ with respect to $y_i$ is:

$$\mathbb{R}^p \ni \frac{\partial c_2}{\partial y_i} = 4 \sum_{j=1}^{n} (p_{ij} - q_{ij}) (y_i - y_j),$$ (22)

where $p_{ij}$ and $q_{ij}$ are the Eqs. (17) and (19), and $p_{ii} = q_{ii} = 0$.

**Proof.** Proof is inspired by (van der Maaten & Hinton, 2008).

Similar to Eq. (9), we have:

$$\frac{\partial c_2}{\partial y_i} = 2 \sum_{j} \left( \frac{\partial c_2}{\partial r_{ij}} + \frac{\partial c_2}{\partial r_{ji}} \right) (y_i - y_j),$$ (23)

Similar to the derivation of Eqs. (11) and (12), we can derive:

$$\frac{\partial c_2}{\partial r_{ij}} = p_{ij} - q_{ij},$$ (24)

and

$$\frac{\partial c_2}{\partial r_{ji}} = p_{ji} - q_{ji},$$

respectively. In the symmetric SNE, we have:

$$\frac{\partial c_2}{\partial r_{ji}} = p_{ji} - q_{ji} \rightarrow p_{ji} - q_{ji},$$ (25)
where \( \langle a \rangle \) is because in symmetric SNE, the \( p_{ij} \) and \( q_{ij} \) are symmetric for \( i \) and \( j \) according to Eqs. (17) and (19).

Substituting Eqs. (24) and (25) in Eq. (23) gives us:

\[
\frac{\partial c_2}{\partial y_i} = 4 \sum_j (p_{ij} - q_{ij})(y_i - y_j),
\]

which is the gradient mentioned in the proposition. Q.E.D.

The update of the embedded point \( y_i \) is done by gradient descent whose every iteration is as Eq. (13) where \( c_1 \) is replaced by \( c_2 \). Note that the momentum term can be omitted in the symmetric SNE. Like in SNE, in symmetric 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.

4. t-distributed Stochastic Neighbor Embedding (t-SNE)

4.1. The Crowding Problem

In SNE (Hinton & Roweis, 2003), 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. 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.

The main idea of t-SNE (van der Maaten & Hinton, 2008) is addressing the crowding problem which exists in SNE (Hinton & Roweis, 2003). In the example of fitting people in a room, t-SNE enlarges the room to solve the crowding problem. Therefore, in the formulation of t-SNE, we use Student-t distribution (Gosset (Student), 1908) 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:

\[
q_{ij} = \frac{(1 + z_{ij}^2)^{-1}}{\sum_{k \neq i}(1 + z_{ki}^2)^{-1}},
\]

which is based on the standard Cauchy distribution:

\[
f(z) = \frac{1}{\pi(1 + z^2)},
\]

where \( \pi \) is canceled from the numerator and the normalizing denominator in \( q_{ij} \) (see the explanations of this trick in Section 2).

If the Student-t distribution (Gosset (Student), 1908) with the general degrees of freedom \( \delta \) is used, we would have:

\[
f(z) = \frac{\Gamma((\delta+1)/2)\Gamma(1 + \frac{z^2}{\delta})}{\Gamma(\delta)\sqrt{\delta\pi}}(1 + \frac{z^2}{\delta})^{-\frac{\delta+1}{2}},
\]

where \( \Gamma \) is the gamma function. Cancelling out the scaling factors from the numerator and denominator, we would have (van der Maaten, 2009):

\[
q_{ij} = \frac{(1 + z_{ij}^2/\delta)^{-(\delta+1)/2}}{\sum_{k \neq i}(1 + z_{ki}^2/\delta)^{-(\delta+1)/2}}.
\]

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 (van der Maaten, 2009), which we explain in Section 5.

4.2. t-SNE Formulation

In t-SNE (van der Maaten & Hinton, 2008), we consider a Gaussian probability around every point \( x_i \) in the input space because the crowding problem does not exist in the high dimensional data. The probability that the point \( x_i \in \mathbb{R}^d \) takes \( x_j \in \mathbb{R}^d \) as its neighbor is:

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

where:

\[
d_{ij}^2 := \frac{||x_i - x_j||^2}{2\sigma_i^2}.
\]

Note that Eq. (29) is not symmetric for \( i \) and \( j \) because of the denominator. We take the symmetric \( p_{ij} \) as the scaled average of \( p_{ij} \) and \( p_{ji} \):

\[
\mathbb{R} \ni p_{ij} := \frac{p_{ij} + p_{ji}}{2n}.
\]

In the low-dimensional embedding space, we consider a Student’s \( t \)-distribution with one degree of freedom (Cauchy distribution) for the point \( y_i \in \mathbb{R}^p \) to take \( y_j \in \mathbb{R}^p \) as its neighbor:

\[
\mathbb{R} \ni q_{ij} := \frac{(1 + z_{ij}^2)^{-1}}{\sum_{k \neq i}(1 + z_{ki}^2)^{-1}},
\]
where:

\[ \mathbb{R} \ni z_{ij}^2 := \|y_i - y_j\|^2_2. \]  

(33)

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 (Kullback, 1997) over the n points:

\[ \mathbb{R} \ni c_3 := \sum_{i=1}^{n} KL(P_i||Q_i) = \sum_{i=1}^{n} \sum_{j=1,j\neq i}^{n} p_{ij} \log\left(\frac{p_{ij}}{q_{ij}}\right), \]

(34)

where \( p_{ij} \) and \( q_{ij} \) are the Eqs. (31) and (32).

**Proposition 3.** The gradient of \( c_3 \) with respect to \( y_i \) is:

\[ \frac{\partial c_3}{\partial y_i} = 4 \sum_{j=1}^{n} (p_{ij} - q_{ij})(1 + ||y_i - y_j||_2^2)^{-1}(y_i - y_j), \]

where \( p_{ij} \) and \( q_{ij} \) are the Eqs. (31) and (32), and \( p_{ii} = q_{ii} = 0 \).

**Proof.** Proof is according to (van der Maaten & Hinton, 2008). Let:

\[ \mathbb{R} \ni r_{ij} := z_{ij}^2 = ||y_i - y_j||_2^2. \]  

(36)

By changing \( y_i \), we only have change impact in \( z_{ij} \) and \( z_{ji} \) for all \( j \)'s. According to chain rule, we have:

\[ \mathbb{R}^P \ni \frac{\partial c_3}{\partial y_i} = \sum_{j} \left( \frac{\partial c_3}{\partial r_{ij}} \frac{\partial r_{ij}}{\partial y_i} + \frac{\partial c_3}{\partial r_{ji}} \frac{\partial r_{ji}}{\partial y_i} \right). \]

According to Eq. (36), we have:

\[ r_{ij} = ||y_i - y_j||_2^2 \implies \frac{\partial r_{ij}}{\partial y_i} = 2(y_i - y_j), \]

\[ r_{ji} = ||y_i - y_j||_2^2 \implies \frac{\partial r_{ji}}{\partial y_i} = 2(y_i - y_j). \]

Therefore:

\[ \therefore \frac{\partial c_3}{\partial y_i} = 2 \sum_{j} \left( \frac{\partial c_3}{\partial r_{ij}} + \frac{\partial c_3}{\partial r_{ji}} \right)(y_i - y_j). \]  

(37)

The cost function can be re-written as:

\[ c_3 = \sum_{k \neq l} p_{kl} \log\left(\frac{p_{kl}}{q_{kl}}\right) = \sum_{k \neq l} p_{kl} \log\left(\frac{p_{kl}}{q_{kl}}\right) \]

\[ = \sum_{k \neq l} \left( p_{kl} \log(p_{kl}) - p_{kl} \log(q_{kl}) \right), \]

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. (32), the \( q_{kl} \) is:

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

(38)

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

\[ \therefore \frac{\partial c_3}{\partial r_{ij}} = - \sum_{k \neq l} p_{kl} \left[ \frac{1}{q_{kl}\beta} \frac{\partial (q_{kl})}{\partial r_{ij}} - \frac{1}{\beta} \frac{\partial \beta}{\partial r_{ij}} \right]. \]

The \( q_{kl} \) is:

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

\[ = (1 + r_{kl})^{-1}. \]

Therefore, we have:

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

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

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

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

\[ = -(1 + r_{ij})^{-2}. \]

Therefore:

\[ \therefore \frac{\partial c_3}{\partial r_{ij}} = - \left( p_{ij} \left[ \frac{1}{q_{ij}\beta} (1 + r_{ij})^{-2} \right] + 0 \cdots + 0 \right) \]

\[ - \sum_{k \neq l} p_{kl} \left[ \frac{1}{\beta} (1 + r_{ij})^{-2} \right]. \]
We have $\sum_{k\neq l} p_{kl} = 1$ because summation of all possible probabilities is one. Thus:

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

$$= (1 + r_{ij})^{-1} \frac{1}{\beta} \left[ rac{p_{ij}}{q_{ij}} - 1 \right]$$

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

Similarly, we have:

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

where $(a)$ is because in t-SNE, the $p_{ij}$, $q_{ij}$, and $r_{ij}$ are symmetric for $i$ and $j$ according to Eqs. (31), (32), and (36).

Substituting the obtained derivatives in Eq. (37) gives us:

$$\frac{\partial c_3}{\partial y_i} = 4 \sum_j (p_{ij} - q_{ij}) (1 + r_{ij})^{-1} (y_i - y_j),$$

which is the gradient mentioned in the proposition. Q.E.D.

Note that in (van der Maaten & Hinton, 2008), the proof uses $z_{ij}$ rather than $r_{ij} = z_{ij}^2$ in Eq. (36) and the rest of the proof. In our opinion, it is better to use $z_{ij}^2$ rather than $z_{ij}$ for the proof. □

The update of the embedded point $y_i$ is done by gradient descent whose every iteration is as Eq. (13) where $c_1$ is replaced by $c_3$. For t-SNE, there is no need to add jitter to the solution of initial iterations (van der Maaten & Hinton, 2008) because it is more robust than SNE. The $\alpha(t)$ is the momentum which can be updated according to Eq. (14). The $\eta$ is the learning rate which can be a small positive constant (e.g., $\eta = 0.1$) or can be updated according to (Jacobs, 1988) (in van der Maaten & Hinton, 2008), the initial $\eta$ is 100.

Note that in (van der Maaten & Hinton, 2008), the update of $y_i(t)$ is $\Delta y_i(t) := +\eta \frac{\partial c_3}{\partial y_i} + \alpha(t) \Delta y_i(t-1)$ which we think is a typo in that paper because the positive direction of gradient is used in gradient ascent for maximizing and not minimizing the objective function. We also checked the implementation of t-SNE in Python scikit-learn library and it was gradient descent and not gradient ascent.

4.3. Early Exaggeration

In t-SNE, it is better to multiply all $p_{ij}$’s by a constant (e.g., 4) in the initial iterations:

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

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.

5. General Degrees of Freedom in t-SNE

We can have general degrees of freedom for Student-t distribution in t-SNE (van der Maaten, 2009). As we saw in Eqs. (27) and (28), we can have any degrees of freedom for $q_{ij}$ (note that $\alpha$ is a positive integer). We repeat Eq. (28) here for more convenience:

$$q_{ij} = \frac{(1 + z_{ij}^2/\delta)^{-(\delta+1)/2}}{\sum_k (1 + z_{ij}^2/\delta)^{-(\delta+1)/2}}.$$

If $\delta \to \infty$, the Student-t distribution formulated in Eq. (27) tends to Gaussian distribution used in SNE (Hinton & Roweis, 2003). SNE and t-SNE use degrees $\delta \to \infty$ and $\delta = 1$ in Eq. (40), respectively. Note that the kernel $q_{ij}$ in the low-dimensional space has no need to be a probability distribution necessarily, but it is enough for it to be a decaying function. It has been shown in (Kobak et al., 2019) the degree $\delta < 1$ works properly well for embedding.

There are three ways to determine $\delta$ (van der Maaten, 2009):

1. We can set $\delta$ to be fixed. For example, $\delta = 1$ is used in the original t-SNE (van der Maaten & Hinton, 2008) which uses the Cauchy distribution in Eq. (32).
2. The problem of the first approach is not considering the relation of the crowding problem with the dimensionality of the embedded space. Recall the crowding problem discussed in Section 4.1. On the one hand, as Eq. (27) shows, the degree of freedom is in the power so the tail thickness of Student-t distribution decreases exponentially with $\delta$. On the other hand, the volume of a hyper-sphere grows exponentially with the dimension; for example, in two and three dimensions, the volume is $\pi r^2$ and $(4/3)\pi r^3$, respectively, where $r$ is the radius. The crowding volume in the embedded space to store the embedded data points is $\propto \pi r^h$ and grows exponentially with $h$. Therefore, the relation of $\delta$ and $h$ (dimensionality of embedded space) is linear, i.e., $h \propto \delta$. In order to be consistent with the original t-SNE (van der Maaten & Hinton, 2008), we take $\delta = h - 1$ which gives $\delta = 1$ for $h = 2$ (van der Maaten, 2009).
3. The problem of the second approach is that $\delta$ might not “only” depend on $h$. In this approach, we find the

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1The link is: https://github.com/scikit-learn/scikit-learn/blob/7b136e9/sklearn/manifold/t_sne.py
best α which minimizes the cost c3, i.e., Eq. (34), (van der Maaten, 2009) where p_{ij} is obtained using Eqs. (29) and (31) and q_{ij} is Eq. (28). We use gradient descent (Boyd & Vandenberghe, 2004) for optimization of both δ and \{\mathbf{y}_i\}_{i=1}^n, where the gradients are as mentioned and proved before. The parametric t-SNE (van der Maaten, 2009) has used restricted Boltzmann machine (Hinton & Salakhutdinov, 2006; Hinton, 2012; Ghoghoj et al., 2021b) to learn the optimal δ and \{\mathbf{y}_i\}_{i=1}^n by a neural network. One can use an alternating optimization approach (Jain & Kar, 2017) to solve for both δ and \{\mathbf{y}_i\}_{i=1}^n simultaneously. In this approach, \{\mathbf{y}_i\}_{i=1}^n are updated with gradient descent using Eq. (47); then, the degree δ is updated with gradient descent using Eq. (46), and this procedure is repeated until convergence.

Note that the degree δ is an integer greater than or equal to one. However, the gradient in Eq. (46) is a float number. For updating the degree using gradient descent in the alternating optimization approach, one can update the degree using the sign of gradient, i.e.:

\[ \delta := \delta - \text{sign}(\frac{\partial c_3}{\partial \delta}), \]  

because the direction of updating is opposite to the gradient direction.

For convenience, we list \( p_{ij} \), \( q_{ij} \), and \( c_3 \) here again:

\[ R \ni p_{ji} := \frac{\exp(-d_{ij}^2)}{\sum_{k \neq i} \exp(-d_{ik}^2)}, \]  
\[ R \ni p_{ij} := \frac{p_{ij} + p_{ji}}{2n}, \]  
\[ R \ni q_{ij} := \frac{(1 + \frac{z_{ij}^2}{\delta})^{-(\delta+1)/2}}{\sum_{k \neq l} (1 + \frac{z_{kl}^2}{\delta})^{-(\delta+1)/2}}, \]  
\[ R \ni c_3 := \sum_i KL(P_i || Q_i) = \sum_i \sum_{j \neq i} p_{ij} \log(\frac{p_{ij}}{q_{ij}}). \]  

**Proposition 4.** The gradient of \( c_3 \) with respect to δ is:

\[ \frac{\partial c_3}{\partial \delta} = \sum_{i \neq j} \left( \frac{1 + \delta}{2 \delta^2 (1 + \frac{z_{ij}^2}{\delta})} + \frac{1}{2} \log(1 + \frac{z_{ij}^2}{\delta}) \right) (p_{ij} - q_{ij}), \]  

where \( p_{ij} \) and \( q_{ij} \) are the Eqs. (43) and (44), respectively, and \( z_{ij}^2 := ||y_i - y_j||_2^2. \)

No matter which of the three ways of determining δ is used, we need to optimize the cost function \( c_3 \) (Eq. (45)) using gradient descent.

**Proposition 5.** The gradient of \( c_3 \) with respect to \( y_i \) is:

\[ \frac{\partial c_3}{\partial y_i} = \frac{2\delta + 2}{\delta} \times \sum_j (p_{ij} - q_{ij})(1 + \frac{||y_i - y_j||_2^2}{\delta})^{-1} (y_i - y_j), \]  

where \( p_{ij} \) and \( q_{ij} \) are the Eqs. (43) and (44), respectively.

**Proof.** Let:

\[ R \ni r_{ij} := z_{ij}^2 = ||y_i - y_j||_2^2. \]  

By changing \( y_i \), we only have change impact in \( z_{ij} \) and \( z_{ji} \) for all \( j \)’s. Considering Eq. (48) and according to chain rule, we have:

\[ R^p \ni \frac{\partial c_3}{\partial r_{ij}} = \sum_j \left( \frac{\partial c_3}{\partial r_{ij}} \frac{\partial r_{ij}}{\partial y_i} \right) + \left( \frac{\partial c_3}{\partial r_{ji}} \frac{\partial r_{ji}}{\partial y_i} \right). \]

According to Eq. (48), we have:

\[ r_{ij} = ||y_i - y_j||_2^2 \Rightarrow \frac{\partial r_{ij}}{\partial y_i} = 2(y_i - y_j), \]
\[ r_{ji} = ||y_j - y_i||_2^2 = ||y_i - y_j||_2^2 \Rightarrow \frac{\partial r_{ji}}{\partial y_i} = 2(y_i - y_j). \]

Therefore:

\[ \Rightarrow \frac{\partial c_3}{\partial y_i} = 2 \sum_j \left( \frac{\partial c_3}{\partial r_{ij}} \frac{\partial r_{ij}}{\partial y_i} + \frac{\partial c_3}{\partial r_{ji}} \frac{\partial r_{ji}}{\partial y_i} \right)(y_i - y_j). \]

The cost function can be re-written as:

\[ c_3 = \sum_k \sum_{i \neq k} p_{kl} \log(\frac{p_{kl}}{q_{kl}}) = \sum_k \sum_{k \neq l} p_{kl} \log(\frac{p_{kl}}{q_{kl}}), \]

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

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

According to Eq. (44), the \( q_{kl} \) is:

\[ q_{kl} = \frac{(1 + r_{kl}/\delta)^{-(\delta+1)/2}}{\sum_{m \neq k} (1 + r_{mf}/\delta)^{-(\delta+1)/2}}, \]

We take the denominator of \( q_{kl} \) as:

\[ \beta := \sum_{m \neq f} (1 + r_{mf}/\delta)^{-(\delta+1)/2}. \]
We have \( \log(q_{kl}) = \log(q_{kl}) + \log\beta - \log\beta = \log(q_{kl}/\beta) - \log\beta. \) Therefore:

\[
\frac{\partial c_3}{\partial r_{ij}} = - \sum_{k \neq l} p_{kl} \left( \frac{\log(q_{kl}/\beta) - \log\beta}{r_{ij}} \right)
\]

\[
= - \sum_{k \neq l} p_{kl} \left[ \frac{\partial \left( \log(q_{kl}/\beta) \right)}{\partial r_{ij}} - \frac{\partial \log\beta}{\partial r_{ij}} \right]
\]

\[
= - \sum_{k \neq l} p_{kl} \left[ \frac{1}{q_{kl}/\beta} \frac{\partial q_{kl}}{\partial r_{ij}} - \frac{1}{\beta} \frac{\partial c_3}{\partial r_{ij}} \right].
\]

The \( q_{kl}/\beta \) is:

\[
q_{kl}/\beta = \frac{(1 + r_{kl}/\delta)^{-(\delta+1)/2}}{m \neq f} \frac{(1 + r_{mf}/\delta)^{-(\delta+1)/2}}{m \neq f}
\]

The \( \frac{\partial ((1 + r_{kl}/\delta)^{-(\delta+1)/2})}{\partial r_{ij}} \) is non-zero for only \( k = i \) and \( l = j \); therefore:

\[
\frac{\partial (q_{kl}/\beta)}{\partial r_{ij}} = \frac{\partial ((1 + r_{kl}/\delta)^{-(\delta+1)/2})}{\partial r_{ij}}
\]

\[
= - \frac{\delta + 1}{2\delta} \frac{1}{(1 + r_{ij}/\delta)} \cdot \frac{-\frac{\delta}{\delta + 1}}{\beta}
\]

\[
\frac{\partial c_3}{\partial r_{ij}} = 2 \sum_{j} \frac{\delta + 1}{\delta} (1 + \frac{r_{ij}}{\delta})^{-\frac{\delta}{\delta + 1}} (p_{ij} - q_{ij})(y_i - y_j),
\]

which is the gradient mentioned in the proposition. Q.E.D.

Note that in (van der Maaten, 2009), the gradient is mentioned to:

\[
\frac{\partial c_3}{\partial y_i} = 2 \sum_{j} \frac{\delta + 1}{\delta} (1 + \frac{r_{ij}}{\delta})^{-\frac{\delta}{\delta + 1}} (p_{ij} - q_{ij})(y_i - y_j),
\]

which we think is wrong. We conjecture that, in the paper (van der Maaten, 2009), there might have been a small mistake in derivation of Eq. (51) where possibly \((1 + \frac{r_{ij}}{\delta})^{-1/\beta}\) has been taken rather than \((1 + \frac{r_{ij}}{\delta})^{-\frac{\delta}{\delta + 1}}\) to be \(q_{ij}\) because of the habit of the original t-SNE (van der Maaten & Hinton, 2008).

Comparing Eqs. (35) and (47) shows that the original t-SNE (van der Maaten & Hinton, 2008) is a special case with \(\delta = 1\).

### 6. Out-of-sample Embedding

Recall that we have \(n\) high-dimensional data points \(\{x_i\}_{i=1}^{n}\) and we want to embed them into the lower dimensional data \(\{y_i\}_{i=1}^{n}\) where \(x_i \in \mathbb{R}^d\) and \(y_i \in \mathbb{R}^p\). Assume we have \(n_t\) out-of-sample data points \(\{x_i^{(t)}\}_{t=1}^{n_t}\) and we want to embed them into the lower dimensional data \(\{y_i^{(t)}\}_{t=1}^{n_t}\) where \(x_i^{(t)} \in \mathbb{R}^d\) and \(y_i^{(t)} \in \mathbb{R}^p\). There are several different methods for out-of-sample extension of SNE and t-SNE methods. One approach, which we do not cover in this manuscript, is based on optimization (Bunte et al., 2012). Another method is based on kernel mapping (Gisbrecht et al., 2012; 2015) which we explain in the following.

We define a map which maps any data point as \(x \mapsto y(x)\), where:

\[
\mathbb{R}^p \ni y(x) := \sum_{j=1}^{n} \alpha_j \frac{k(x, x_j)}{\sum_{\ell=1}^{n} k(x, x_{\ell})},
\]

and \(\alpha_j \in \mathbb{R}^p\), and \(x_j\) and \(x_{\ell}\) denote the \(j\)-th and \(\ell\)-th training data points, respectively. The \(k(x, x_j)\) is a kernel such
as the Gaussian kernel:

$$k(x, x_j) = \exp\left(-\frac{||x - x_j||^2_2}{2\sigma_j^2}\right),$$  \hspace{1cm} (54)

where \(\sigma_j\) is calculated as \((\text{Gisbrecht et al., 2015})::

$$\sigma_j := \gamma \cdot \min_i(||x_j - x_i||_2),$$  \hspace{1cm} (55)

where \(\gamma\) is a small positive number.

Assume we have already embedded the training data points using SNE or t-SNE; therefore, the set \(\{y_i\}_{i=1}^n\) is available. If we map the training data points, we want to minimize the following least-squares cost function in order to get \(y_i\) close to \(y_i\) for the \(i\)-th training point:

$$\min_{\alpha_j} \sum_{i=1}^n ||y_i - y(x_i)||_2^2,$$  \hspace{1cm} (56)

where the summation is over the training data points. We can write this cost function in matrix form as:

$$\min_A ||Y - KA||_F^2,$$  \hspace{1cm} (57)

where \(\mathbb{R}^{n \times p} \ni Y := [y_1, \ldots, y_n]^\top\) and \(\mathbb{R}^{n \times p} \ni A := [\alpha_1, \ldots, \alpha_n]^\top\). The \(K \in \mathbb{R}^{n \times n}\) is the kernel matrix whose \((i, j)\)-th element is:

$$K(i, j) := \frac{k(x_i, x_j)}{\sum_{\ell=1}^n k(x_i, x_\ell)},$$  \hspace{1cm} (58)

The Eq. (57) is always non-negative; thus, its smallest value is zero. Therefore, the solution to this equation is:

$$Y - KA = 0 \implies Y = KA$$

\((\alpha)\) \implies A = K^+ Y,$$  \hspace{1cm} (59)

where \(K^+\) is the pseudo-inverse of \(K\):

$$K^+ = (K^\top K)^{-1} K^\top,$$  \hspace{1cm} (60)

and \((\alpha)\) is because \(K^+ K = I\).

Finally, the mapping of Eq. (53) for the \(n_t\) out-of-sample data points is:

$$Y^{(t)} = K^{(t)} A,$$  \hspace{1cm} (61)

where \(\mathbb{R}^{n_t \times p} \ni Y^{(t)} := [y_1^{(t)}, \ldots, y_{n_t}^{(t)}]^\top\) and the \((i, j)\)-th element of the out-of-sample kernel matrix \(K^{(t)} \in \mathbb{R}^{n_t \times n}\) is:

$$K^{(t)}(i, j) := \frac{k(x_i^{(t)}, x_j)}{\sum_{\ell=1}^n k(x_i^{(t)}, x_\ell)},$$  \hspace{1cm} (62)

where \(x_i^{(t)}\) is the \(i\)-th out-of-sample data point, and \(x_j\) and \(x_\ell\) are the \(j\)-th and \(\ell\)-th training data points, respectively.

In Eq. (59), if \(Y\) is the embedding of training data using SNE/t-SNE, then the out-of-sample embedding of SNE/t-SNE are obtained. As mentioned in (Gisbrecht et al., 2015), this method can also be used for out-of-sample extension in Isomap (Tenenbaum et al., 2000; Ghojogh et al., 2020), Locally Linear Embedding (LLE) (Roweis & Saul, 2000), and Maximum Variance Embedding (MVU) (Weinberger & Saul, 2006). The only difference is in obtaining the embedded training points \(Y\) using different non-parametric dimensionality reduction methods (Gisbrecht et al., 2012, 2015).

### 7. Accelerating SNE and t-SNE

The SNE and t-SNE methods are very slow because of numerical iterative optimization. Different methods have been proposed for accelerating these methods (Linderman et al., 2017). Some of these methods are the tree-based algorithms (van der Maaten, 2014; Robinson & Pierce-Hoffman, 2020). This type of t-SNE is also referred to as Barnes-Hut t-SNE (Van Der Maaten, 2013; van der Maaten, 2014). We do not cover the tree-based algorithms (van der Maaten, 2014) in this paper for the sake of brevity. Some other methods exist for accelerating SNE and t-SNE which are based on landmarks. In these methods, we randomly sample from the dataset in order to have a subset of data. The sampled data points are called landmarks. In the following, we mention three methods for accelerating t-SNE and/or SNE which use landmarks. In the following, we review the methods based on landmarks.

#### 7.1. Acceleration Using Out-of-sample Embedding

One way to speed up SNE and t-SNE is the kernel mapping (Gisbrecht et al., 2015) introduced in Section 6. We consider the landmarks as the training data points and train SNE or t-SNE with them. Thereafter, we treat the non-landmark data points as out-of-sample points. We use kernel SNE or kernel t-SNE (or Fisher kernel t-SNE for supervised cases) in order to embed the out-of-sample data points.

Another method is to again consider the landmarks as training points and embed the training points using SNE or t-SNE. Then, the non-landmarks, which are out-of-sample points, are embedded using optimization (Bunte et al., 2012) as was mentioned in Section 6.

#### 7.2. Acceleration Using Random Walk

Another way of accelerating t-SNE is random walk (van der Maaten & Hinton, 2008). First, a \(k\)-Nearest Neighbor (kNN) graph is constructed using all points including landmarks and non-landmarks. This method has an acceptable robustness to the choice of \(k\); for example, \(k = 20\) can be used (van der Maaten & Hinton, 2008). Also, note that calculation of kNN is time-consuming for
large dataset; however, it is not a big deal as it is done only once. Then, multiple random walks are performed in this $k$NN graph (Spitzer, 2013). For every random walk, we start from a random landmark and randomly select the edges and go further randomly until we reach another landmark and then we terminate for that random walk. After performing all the random walks, the fraction of random walks which pass through the point $x_i$ (either landmark or non-landmark) and then reach the point $x_j$ (either landmark or non-landmark) is a good approximation for $p_{ij}$. In t-SNE, we use this approximation in place of Eq. (29), which is then used in Eq. (31). The rest of t-SNE is similar to the original t-SNE. Therefore, for $p_{ij}$ in Eq. (35), we use the approximation rather than Eq. (31) and this makes the t-SNE much faster.

8. Recent Improvements of t-SNE

Here, we just list some of the recent improvements of t-SNE and do not explain them in detail for brevity. Recall that the variance $\sigma_i^2$ is determined for every point $x_i$ using binary search. This cancels the local density information for points in the lower density regions will have a smaller $\sigma_i^2$. Dense t-SNE (Narayan et al., 2021) resolves this problem by a density radius to include the density information. LargeVis (Tang et al., 2016) and UMAP (McInnes et al., 2018; Ghojogh et al., 2021c) are closely related methods to t-SNE. Parametric t-SNE (van der Maaten, 2009) and parametric kernel t-SNE (Gisbrecht et al., 2015) implement t-SNE formulation in a neural network structure. The optimization of t-SNE can be seen as optimizing attractive and repulsive forces between points. Some discussions on the attractive and repulsive forces in t-SNE can be found in (Linderman et al., 2017; Sainburg et al., 2020). Many algorithms such as t-SNE, which are based on these forces, can be unified as a family of neighborhood embedding methods (Böhm et al., 2020; Böhm, 2020). Finally, note that a combination of variational autoencoder (Kingma & Welling, 2014; Ghojogh et al., 2021a) and SNE exists (Graving & Couzin, 2020).

9. Conclusion

This paper was a tutorial and survey paper on SNE and its variants. These methods have a probabilistic approach where the probabilities of neighborhood in the input space are tried to be preserved in the embedding space. We explained SNE, symmetric SNE, t-SNE (or Cauchy-SNE), and t-SNE with general degrees of freedom. We also covered out-of-sample extension and their acceleration methods. Finally, some simulations were provided for visualization of embeddings. Some newer variants of SNE and t-SNE were not covered in this manuscript and we refer the reader to those papers for more information. An example is Fisher kernel t-SNE (Gisbrecht et al., 2015) for supervised embedding using t-SNE. This method uses $T$-point approximation of Riemannian distance (Peltonen et al., 2004) in the formulation of probability. There is also some other technique for heavy-tailed SNE such as (Yang et al., 2009).

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