# High Dimension Visualization: t-SNE

Stands for **t-distributed Stochastic Neighborhood Embedding** which was presented by **Laurens van der Maaten** and **Geoffrey Hinton** in 2008.

## Limitations of PCA

The limitations of PCA are that it does not preserve the neighborhood when points are projected from a higher dimension to a lower dimension.

## The idea of tSNE

- If one wants to project data from a higher dimension to a lower dimension, t-SNE will try to preserve the distances of the points that are close to each other.

- t-SNE tries to create an embedding that preserves the neighborhood using some probabilistic methods.

- Hence, the core idea behind t-SNE is;
    - When we go from $d$-dimensions to $d'$-dimensions where $d<d'$, the core idea behind t-SNE is to preserve the pairwise distance in a neighborhood as best as possible.
- However, there is a problem that t-SNE faces while preserving neighborhood information. It is known as **The Crowding Problem**.

## Crowding Problem

- Suppose we have 2D data and we want to project it in 1D data using any neighborhood embedding method.

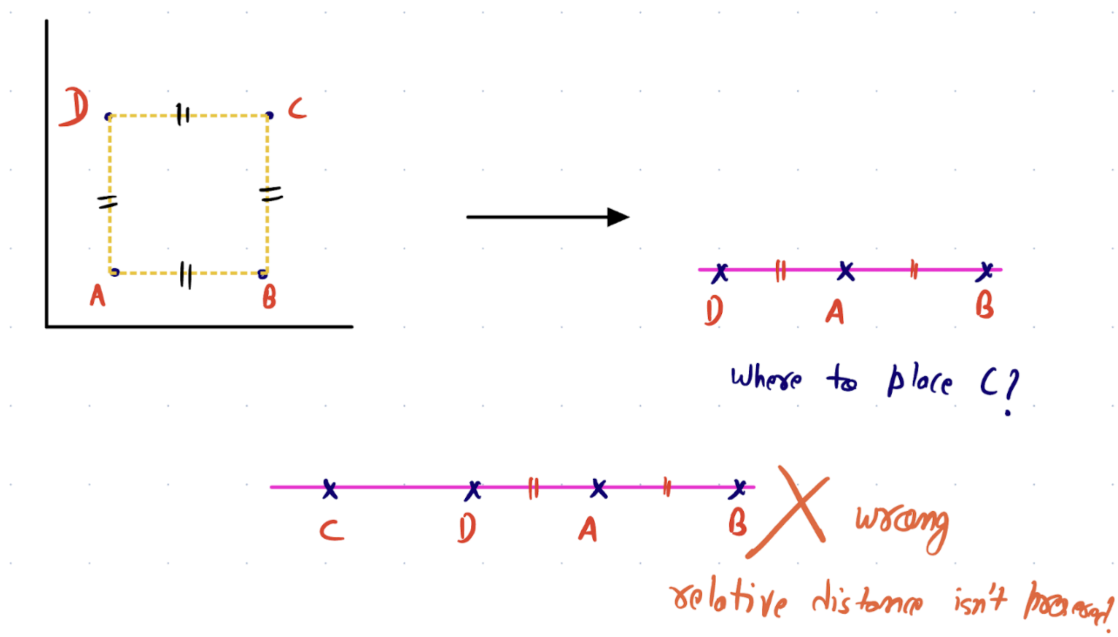
- We have four data points in the shape of a square, where $a$ is at the origin, $b$ is on the X-axis, and $d$ is on the Y-axis as shown in the diagram given below.

- Now, consider a case, when we choose the neighborhood of the point $a$ that contains all the other points.

Let's try to project this data into 1D such that the pairwise distance is preserved

- We place point $a$ on a 1D axis, point $b$ on the right of point $a$, and point $d$ on the left of point $a$. Here, the distance of both the points $d$ and $b$ to point $a$ is the same.

- Now, if you try to project point $c$, it will be exactly projected at the coordinates of point $a$. Because, as $a$ is equidistant from point $b$ and $d$, so is the point $c$.




- This was just a simple case we saw for better understanding.

- In real-life data, there will be hundreds, probably thousands of points that will not be able to preserve pairwise distance when projected from a higher dimension to a lower dimension

## Math for t-SNE

- Our objective is to project data points $xi \in R^d$ to $y_i$ using t-SNE, where $y_i \in R^2$
- In t-SNE, we compute the pairwise similarities as probabilities.
- We compute $P_{ij}$ for $d$-dimensions and $Q_{ij}$ for $d'$-dimensions where $d > d'$

- $P_{ij}$ is the probability that the points $x_i$ and $x_j$ are neighbors in $d$-dimensional space.
- The pairwise similarities in the low-dimensional map $Q_{ij}$ are given by:

$$= \frac{\exp\left(-\|y_i - y_j\|^2\right)}{\sum_{k\neq l}\exp\left(-\|y_k - y_l\|^2\right)},$$

- The pairwise similarities in the high-dimensional space $P_{ij}$ are:

$$= \frac{\exp\left(-\|x_i - x_j\|^2/2\sigma^2\right)}{\sum_{k\neq l}\exp\left(-\|x_k - x_l\|^2/2\sigma^2\right)}.$$

- As you can see in the equation above, the numerator term in $P_{ij}$ is nothing but a sort of normal distribution with a variance of σ.
  - The term $|x_i - x_j|^2$ computes the Euclidean distance between $x_i$ and $x_j$.
  - As $x_i$ and $x_j$ move farther and farther away, we give the lower probability that $x_i$ and $x_j$ our neighbors
- Now, as we are computing probabilities, probabilities across all points should be equal to 1
- So, the denominator terms is just a normalization factor to make sure that the sum of all the probabilities is equal to 1

$$\sum_i \sum_j P_{ij} = 1$$

- This technique is known as SNE.

- Now, in $d'$-dimensions space, every $x_i$ and $x_j$ would have corresponding $y_i$ and $y_j$.
- So, again we define $Q_{ij}$ with the same formulation as $P_{ij}$
- Hence, if $x_i$ and $x_j$ are similar, then $P_{ij}$ would be higher and we want our $y_i$ and $y_j$ such a representation such that $Q_{ij}$ is also high.
- Because of the crowding problem, we can never perfectly preserve the distance.
- So, in t-SNE, we try to preserve the probabilities when going from high dimension to low dimension space
- We compare probabilities $P_{ij}$ and $Q_{ij}$ with something known as KL-Divergence.

## KL-Divergence

- It measures the dissimilarity between the distributions.
- So, the KL-Divergence between two distributions $P$ and $Q$ can be written as:

$$KL - div(P_{ij}, Q_{ij}) = \sum_i \sum_j [P_{ij} \ . \ log(\frac{P_{ij}}{Q_{ij}})]$$

- KL divergence is also known as **relative entropy.**

## Interpreting KL-Divergence

- If $P_{ij}$ and $Q_{ij}$ are the same, then KL-divergence will be equal to 0.
- If $P_{ij}$ is very small and, $P_{ij}$ and $Q_{ij}$ are the same, then KL-divergence will have a small value.
    - Think of $P_{ij}$ working as a weightage, because if $P_{ij}$ is small we don't really care as points $xi$ and $xj$ will be far away from each other in d-dimension space.
- So, now our optimization problem would be to find all the $y_i$s that minimize KL-divergence(P, Q)
- Lastly, since KL-divergence is a measure of dissimilarity, it is always greater than or equal to 0.

## 't' in t-SNE

- For computing $P_{ij}$, we used a Gaussian-like function.
- However, it was found that if we compute $P_{ij}$ using t-distribution with 1 degree of freedom, the results were better.
- t-distributions with $dof$=1 have longer tails than Gaussian distributions
- Gaussian distribution falls exponentially while t-distributions sort of inversely
- So, for our $Qij$s, if we start using t-distribution, two points can go farther away and still get pairwise distance preserved of sort
- Meaning, in t-SNE, we use Gaussian distribution for $P_{ij}$s and t-distribution for $Q_{ij}$s because if two points are far away in lower dimensional space, the probabilities will remain the same

- If we increase $dof$ and keep increasing, it will behave like a Gaussian distribution which will face the problem of crowding
- At, $dof$=∞, it behaves very similarly to a Gaussian distribution
- t-distribution with $dof$=1 is also known as Cauchy Distribution

**Perplexity**

- Perplexity is one of the most parameters that you might want to configure when using t-SNE.
- Perplexity can be interpreted as the effective number of neighbors whose distance we want to preserve
- Typically, we keep the value between [5,50]
- The optimization of t-SNE is very time-consuming as there are no single optima.
- Also, if you add a bunch of newer data points to the dataset, you won't get projections into lower dimensional space automatically.
- You would have to fit the t-SNE model again on the whole dataset.

**Use this blog to play around with t-SNE on different data distributions:**
[https://distill.pub/2016/misread-tsne/](https://distill.pub/2016/misread-tsne/)