An introduction to t-SNE

Weekly AI pills

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Summary

1. Entropy and Kullback–Leibler divergence
2. From SNE to t-SNE
3. Application for Visualization
4. Issues

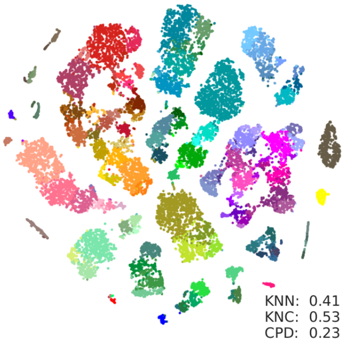
(t)-Stochastic Neighborhood Embedding

Main Papers

- Stochastic Neighbor Embedding - Hinton & Roweis - 2002
- Visualizing Data using t-SNE - Maaten & Hinton - 2008

Aims

- Dimensionality Reduction
- Data Visualization
  1. Exploration
  2. Clusters Visualization



Example of Data Visualization taken from (Tasic et al., 2018)

SNE Algorithm

SNE algorithm: Workflow

1. Represent each sample $x_i \in \mathcal{X}$ with $y_i \in \mathcal{Y}$ in a low-dimensional space
$$\Phi : \underset{\subseteq \mathbb{R}^n}{\mathcal{X}} \longrightarrow \underset{\subseteq \mathbb{R}^2}{\mathcal{Y}}$$
2. Convert **Geometrical Information** to **Probabilistic Distribution**
$$p_{i|j} : \text{“Probability that } x_i \text{ is } \textit{similar} \text{ to } x_j\text{”}$$
$$q_{i|j} : \text{“Probability that } y_i \text{ is } \textit{similar} \text{ to } y_j\text{”}$$
3. Compare distribution $\mathcal{P}$ of $\mathcal{X}$ to distribution $\mathcal{Q}$ of $\mathcal{X}$
4. Adjust the representation Φ to make distributions closer.

Observation

The embedding Φ is defined **point-wise**, i.e Φ is only defined over $\mathcal{X}$ through the definition $\Phi(x_i) = y_i$. Another way to say “y_i are the parameters of Φ”.

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SNE algorithm: Similarity and Probability Distribution

Definition (Similarity with Gaussian Kernel)

For each x_i we consider the similarity

$$\forall j \neq i, \quad p_{i|j} = \frac{\exp\left(-\|x_i - x_j\|^2/(2\sigma_i)^2\right)}{\sum_{k\neq i} \exp\left(-\|x_i - x_k\|^2/(2\sigma_i)^2\right)} \qquad (\mathcal{P}_i)$$

where σ_i is an hyper-parameter depending on x_i.

How σ_i impacts on $p_{i|j}$?

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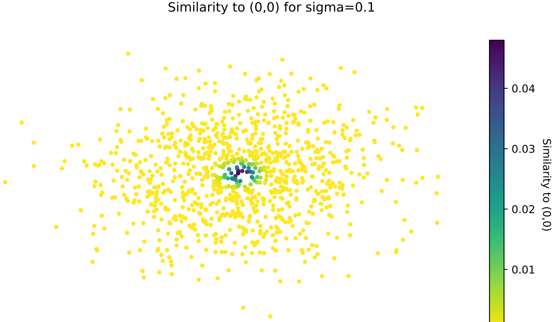

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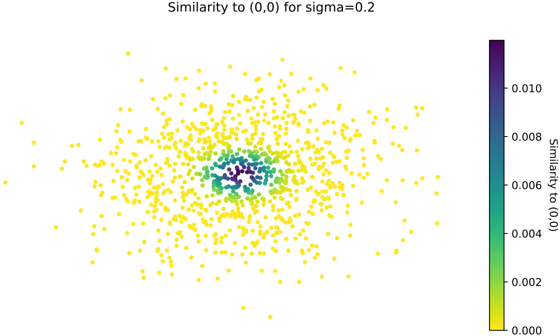

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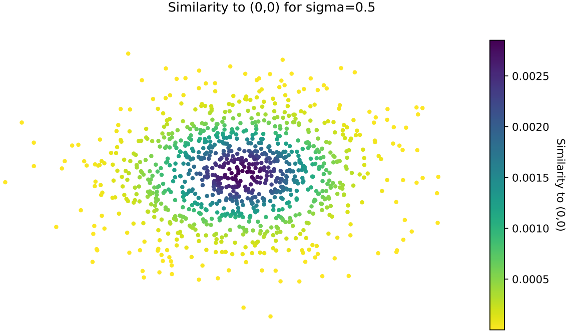

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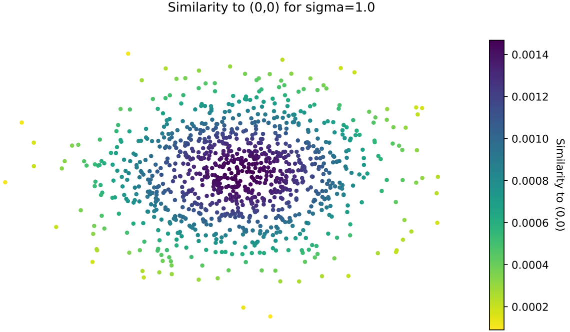

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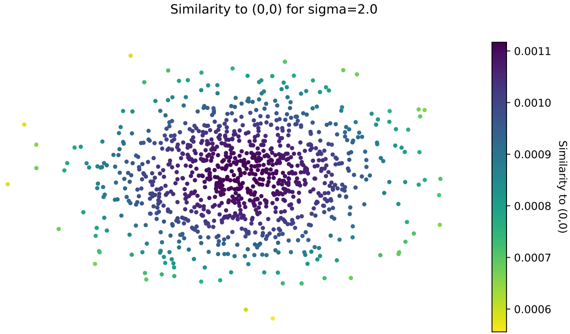

SNE algorithm: Similarity and Probability Distribution

In the same manner we can define similarity in $\mathcal{Y}$.

$$\forall j \neq i, \quad q_{i|j} = \frac{\exp\left(-\|y_i - y_j\|^2\right)}{\sum_{k \neq i} \exp\left(-\|y_i - y_k\|^2\right)} \tag{$\mathcal{Q}_i$}$$

Observation

$\mathcal{P}_i$ and $\mathcal{Q}_i$ are probability distributions for each i.

1. $0 \leq p_{i|j}, q_{i|j} \leq 1$ for each $j \neq i$
2. $\sum_{j \neq i} p_{i|j} = \sum_{j \neq i} q_{i|j} = 1$

SNE algorithm: Kullback-Leibler Divergence

Definition (K.L Divergence)

Let $\mathcal{P} = \{p_1, \cdots, p_n\}$ and $\mathcal{Q} = \{q_1, \cdots, q_n\}$ distributions

$$KL(\mathcal{P}, \mathcal{Q}) = \sum_i p_i \log_2 \left(\frac{p_i}{q_i} \right) \tag{1}$$

We can compare $\mathcal{P}_i$, $\mathcal{Q}_i$ for each i by taking

$$C(\mathcal{Y}) := \sum_i KL(\mathcal{P}_i, \mathcal{Q}_i) \tag{2}$$

Observation: The cost function C is differentiable in y_i

$$\frac{\partial C}{\partial y_i} = 2 \sum_{j \neq i} \underbrace{\left[\left(p_{i|j} + p_{j|i} \right) \left(y_i - y_j \right) \right]}_{\text{Attractive}} - \underbrace{\left[\left(q_{i|j} + q_{j|i} \right) \left(y_i - y_j \right) \right]}_{\text{Repulsive}} \tag{3}$$

Intepretation: C penalizes close x_i, x_j and far y_i, y_j.

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SNE Algorithm

1. Choose $\Phi^{(0)}$ embedding, i.e choose $\{y_i^{(0)}\}$
2. Compute $\mathcal{P}_i$ and $\mathcal{Q}_i$ distributions.
3. Minimize $C(\mathcal{Y})$ through Gradient Descent with momentum

$$y_i^{(t+1)} = y_i^{(t)} - \eta \frac{\partial C}{\partial y_i} + \alpha \left(y_i^{(t)} - y_i^{(t-1)} \right), \quad \forall i$$

How to find σ_i?

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Perplexity

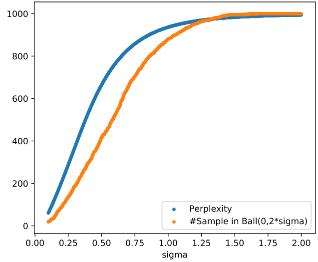
Perplexity: Shannon Entropy and Neighborhood

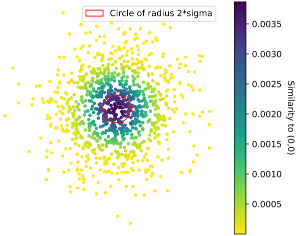
Let $\mathcal{P} = \{p_1, \cdots, p_n\}$ be a distribution

Shannon Entropy $\qquad \mathbb{H}(\mathcal{P}) = -\sum_i p_i \log_2(p_i)$

Perplexity $\qquad Perp(\mathcal{P}) = 2^{\mathbb{H}(\mathcal{P})}$

How σ_i and Perplexity are related to each other?





Perplexity measures the number of samples in a neighborhood.[a]

[a] Original paper doesn't provide a proof, let us take it as an intuition.

Perplexity: Derivation of σ

Observation

Perplexity of $\mathcal{P}_i$ is continuous monotonic in σ_i.

Binary Search: Find σ_i such that $Perp(\mathcal{P}_i(\sigma_i)) = K$

$\sigma^{(l)}$ such that $Perp(\mathcal{P}_i(\sigma^{(l)})) < K$;
$\sigma^{(r)}$ such that $Perp(\mathcal{P}_i(\sigma^{(r)})) > K$;
while $|\sigma^{(r)} - \sigma^{(l)}| < \varepsilon$ **do**
    $\bar{\sigma} \leftarrow (\sigma^{(l)} + \sigma^{(l)})/2$;
    $p \leftarrow Perp(\mathcal{P}_i(\bar{\sigma}))$;
    if $p < K$ **then**
        $\sigma^{(l)} \leftarrow \bar{\sigma}$;
    else
        $\sigma^{(r)} \leftarrow \bar{\sigma}$;
    end
end
return $\bar{\sigma}$

t-SNE is t+SNE

In order to achieve better results Maaten & Hinton modified SNE by

1. Using Student t-distribution for $\mathcal{Y}$

$$\forall i, \quad q_{i|j} = \frac{(1 + \|y_i - y_j\|^2)^{-1}}{\sum_{k \neq i} \left(1 + \|y_i + y_j\|^2\right)^{-1}}, \quad \forall j \neq i$$

2. Using symmetric versions of $p_{i|j}$, $q_{i|j}$ by defining

$$p_{ij} = \left(p_{i|j} + p_{j|i}\right)/(2n), \quad q_{ij} = \left(q_{i|j} + q_{j|i}\right)/(2n)$$

   so that $\mathcal{P} = \{p_{ij}\}$ and $\mathcal{Q} = \{q_{ij}\}$ are joint probabilities.

3. The cost function becomes

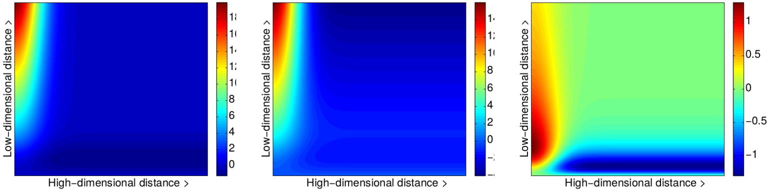
$$C(\mathcal{Y}) = KL(\mathcal{P}, \mathcal{Q})$$

t-SNE: Cost Interpretation

Let we consider a dummy case $\mathcal{X} = \{x_1, x_2\}$. Then

$$
\begin{aligned}
\text{SNE} \quad & (\nabla C)_1 = 2(p_{1|2} + p_{2|1} - q_{1|2} - q_{2|1})(y_1 - y_2) \\
\text{t-SNE} \quad & (\nabla C)_1 = 4(p_{12} - q_{12})\,(y_1 - y_2)\left(1 + \|y_1 - y_2\|^2\right)^{-1}
\end{aligned}
\tag{4}
$$

Observation: Both depends only on $\|x_1 - x_2\|$ and $\|y_1 - y_2\|$.



(a) Gradient of SNE. (b) Gradient of UNI-SNE. (c) Gradient of t-SNE.

Image taken from Maaten & Hinton's paper representing $\|\nabla C\|$ for different distances in the input-space and in the embedding space.

Examples

t-SNE on cortex's cells

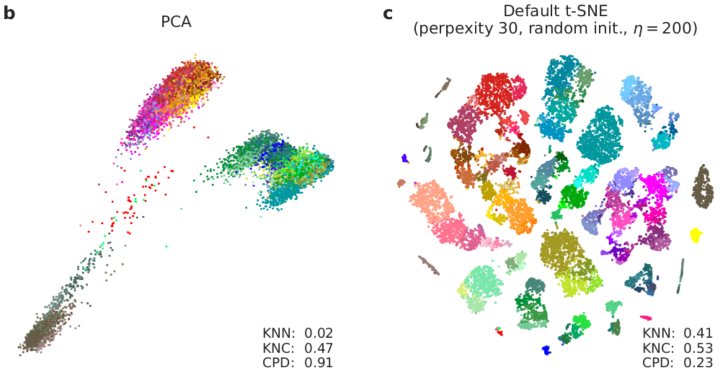


Image taken from Kobak-Barens paper.

An hand made hierarchical clustering of cortex's cell is visualized through t-SNE. PCA is able to find the main three clusters but not to distinguish the sub-clusters.

t-SNE on cortex’ cells: Metrics Evaluations

- **KNN:** local metric. For each samples $x_i \in \mathcal{X}$ and its image $y_i \in \mathcal{Y}$ we take the first k-closest points K_i and H_i and we evaluate

$$KNN := \frac{1}{|\mathcal{X}|} \sum_i \frac{|H_i \cap \Phi(K_i)|}{k}$$

- **KNC:** Cluster metric. The same as KNN but applied to $c_1, \cdots, c_s$ cluster’s centroids.
- **CPD:** Global metric. Defined as the Spearmen correlation.

These metrics in the figure 4 shows that t-SNE performs better in preserving local structures and worst in preserving the global structure of the data[1].

[1] Kobak-Barens paper for more details.

t-SNE on MNIST

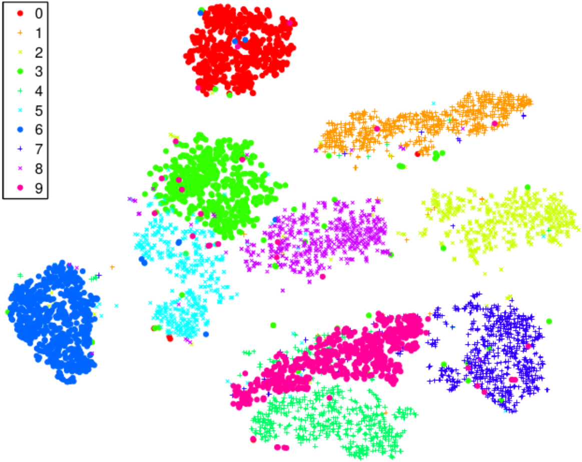
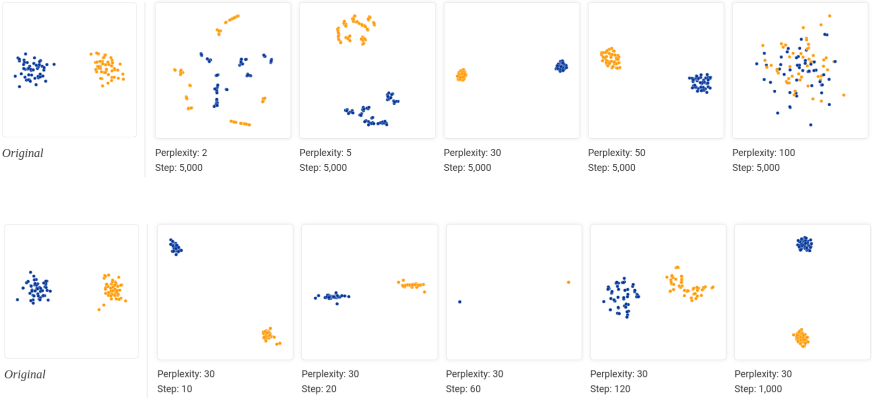


Image taken from Maaten - Hinton paper

t-SNE Warnings

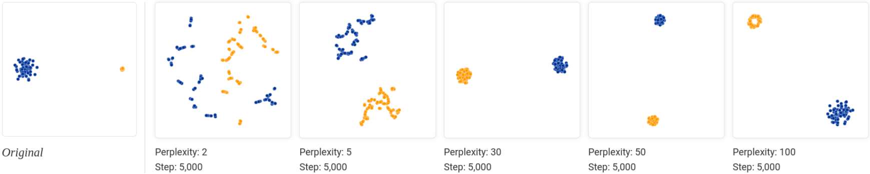
How to use t-SNE[2]

Hyper-Parameters really matter.



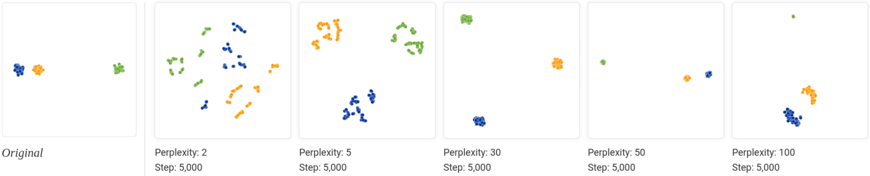
[2] In this section we will show the results in Wattenberg - online paper.

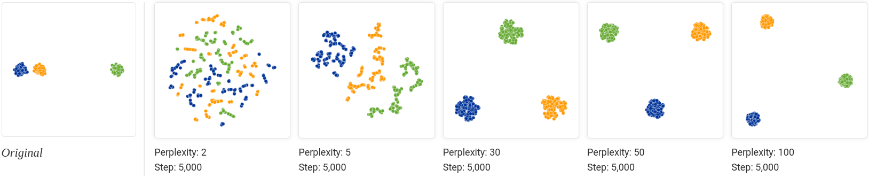
Cluster sizes in a t-SNE plot has no meaning.



How to use t-SNE

There is not control of the distances between clusters.

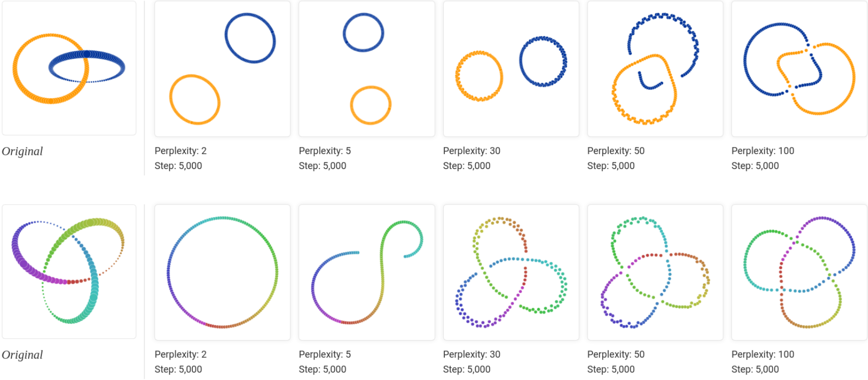




Different initializations produce visualizations within clusters at different distances.

How to use t-SNE

Sometimes topology is not preserved.



Conclusion

What is t-SNE good for

1. Exploring data making associations based on geometrical informations in the original space.
2. Providing intuition over the data that can be established with different techniques.

How to not use t-SNE

1. For evaluate distances between clusters.
2. For evaluate density of clusters.
3. Establish topological property.

Conclusion

Thanks for the attention.