

# An introduction to t-SNE

## Weekly AI pills

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2020-11-13

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ISTITUTO  
DI TECNOLOGIE DELLA  
COMUNICAZIONE,  
DELL'INFORMAZIONE  
E DELLA  
PERCEZIONE



Scuola Superiore  
Sant'Anna



# Summary

SNE Algorithm

Perplexity

t-SNE is t+SNE

Examples

t-SNE Warnings



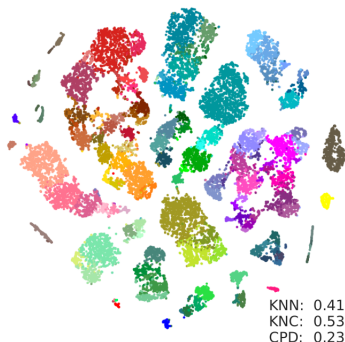
## (t)-Stochastic Neighborhood Embedding

### 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

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# 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**

$p_{ij}$  : “Probability that  $x_i$  is *similar* to  $x_j$ ”

$q_{ij}$  : “Probability that  $y_i$  is *similar* to  $y_j$ ”

3. Compare distribution  $\mathcal{P}$  of  $\mathcal{X}$  to distribution  $\mathcal{Q}$  of  $\mathcal{Y}$
4. Adjust the representation  $\Phi$  to make distributions closer.

## Observation

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

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# SNE algorithm: Similarity and Probability Distribution

## Definition (Similarity with Gaussian Kernel)

For each  $x_i$  we consider the similarity

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

where  $\sigma_i$  is an hyper-parameter depending on  $x_i$ .

How  $\sigma_i$  impacts on  $p_{ij}$ ?

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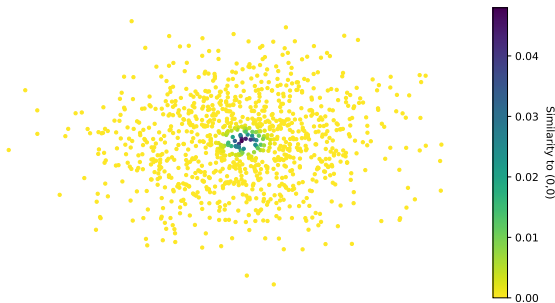
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Similarity to (0,0) for sigma=0.1





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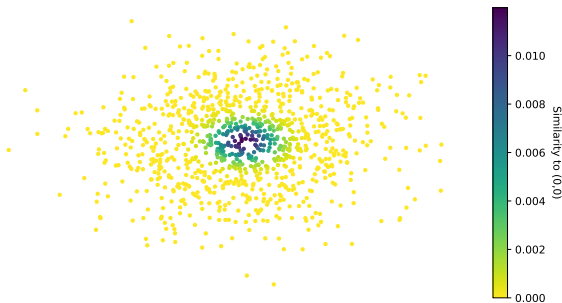
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Similarity to (0,0) for sigma=0.2



# SNE algorithm: Similarity and Probability Distribution

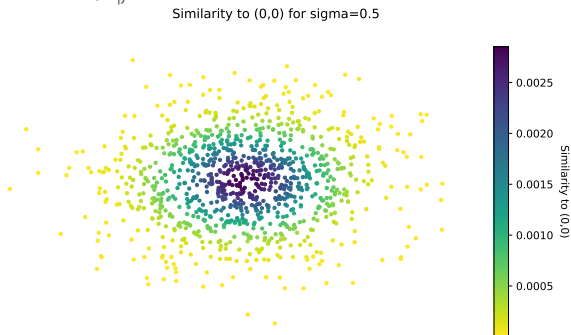
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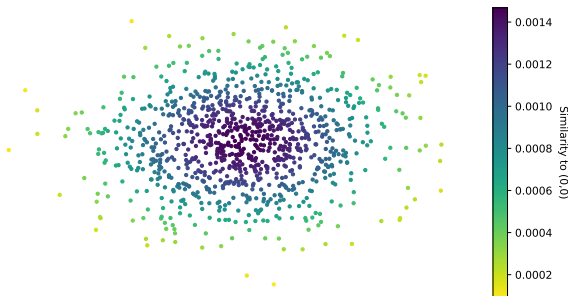
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# SNE algorithm: Similarity and Probability Distribution

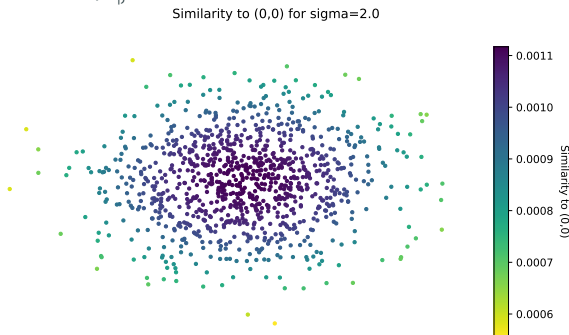
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# SNE algorithm: Similarity and Probability Distribution

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

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

## 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  $\mathcal{P} = \{p_1, \dots, p_n\}$  and  $\mathcal{Q} = \{q_1, \dots, q_n\}$  distributions

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

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

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

Observation: The cost function  $C$  is differentiable in  $y_i$

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

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  $\sigma_i$ ?



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# Perplexity

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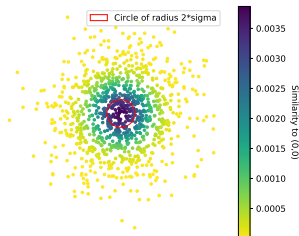
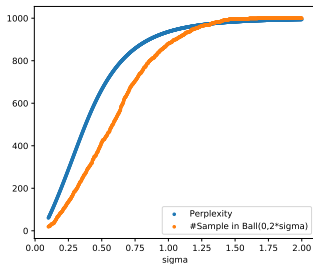
# Perplexity: Shannon Entropy and Neighborhood

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

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

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

How  $\sigma_i$  and Perplexity are related to each other?



Perplexity measures the number of samples in a neighborhood.<sup>a</sup>

<sup>a</sup>Original paper doesn't provide a proof, let us take it as an intuition.

# Perplexity: Derivation of $\sigma$

## Observation

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

**Binary Search:** Find  $\sigma_i$  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**

$\bar{\sigma} \leftarrow (\sigma^{(l)} + \sigma^{(r)})/2$ ;

$p \leftarrow Perp(\mathcal{P}_i(\bar{\sigma}))$ ;

**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

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# t-SNE: Symmetric + Student

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

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

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

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

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

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

3. The cost function becomes

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

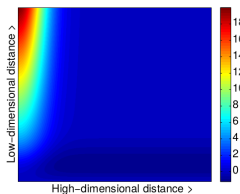
# t-SNE: Cost Interpretation

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

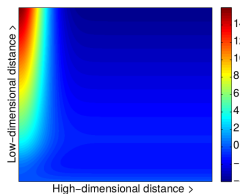
$$\text{SNE} \quad (\nabla C)_1 = 2(p_{1|2} + p_{2|1} - q_{1|2} - q_{2|1})(y_1 - y_2) \quad (4)$$

$$\text{t-SNE} \quad (\nabla C)_1 = 4(p_{12} - q_{12})(y_1 - y_2)(1 + \|y_1 - y_2\|^2)^{-1}$$

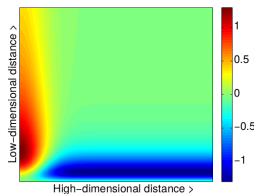
Observation: Both depend only on  $\|x_1 - x_2\|$  and  $\|y_1 - y_2\|$ .



(a) Gradient of SNE.



(b) Gradient of UNI-SNE.



(c) Gradient of t-SNE.

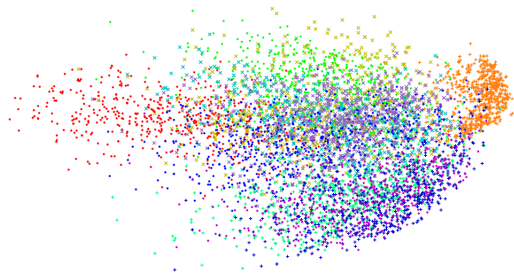
Image taken from Maaten & Hinton's paper representing  $\|\nabla C\|$  for different distances in the input-space and in the embedding space.

## Examples

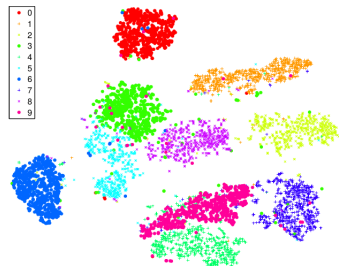
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PCA visualization. First two principal components.



t-SNE visualization. Image taken from Maaten - Hinton paper

# t-SNE on cortex's cells

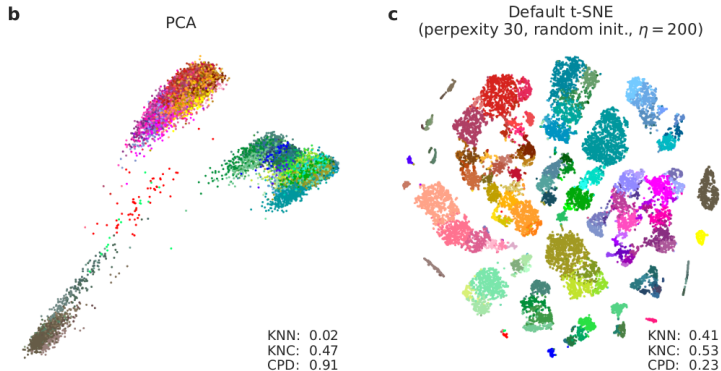


Image taken from Kobak-Barens paper.

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  $c_1, \dots, c_s$  cluster's centroids.
- **CPD:** Global metric. Defined as the Spearmen correlation.

These metrics in the figure 6 shows that t-SNE performs better in preserving local structures and worst in preserving the global structure of the data<sup>1</sup>.

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<sup>1</sup>Kobak-Barens paper for more details.

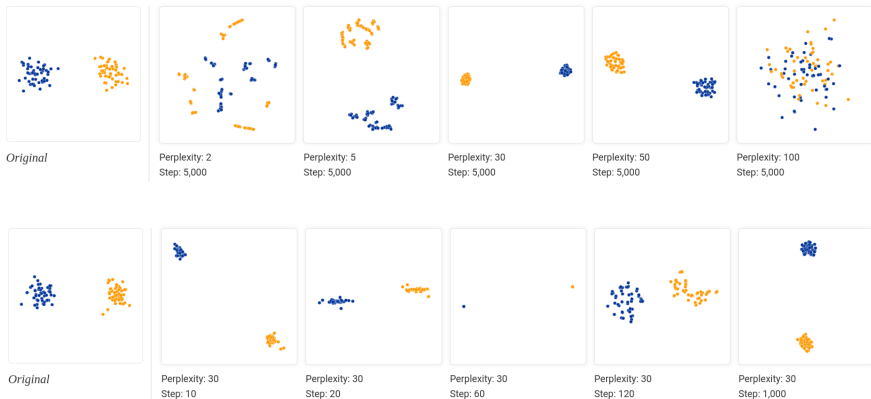
## t-SNE Warnings

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# How to use t-SNE<sup>2</sup>

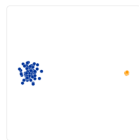
Hyper-Parameters really matter.



<sup>2</sup>In this section we will show the results in [Wattenberg - online paper](#).

# How to use t-SNE

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



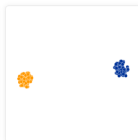
*Original*



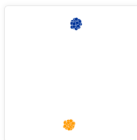
Perplexity: 2  
Step: 5,000



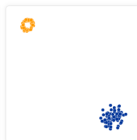
Perplexity: 5  
Step: 5,000



Perplexity: 30  
Step: 5,000



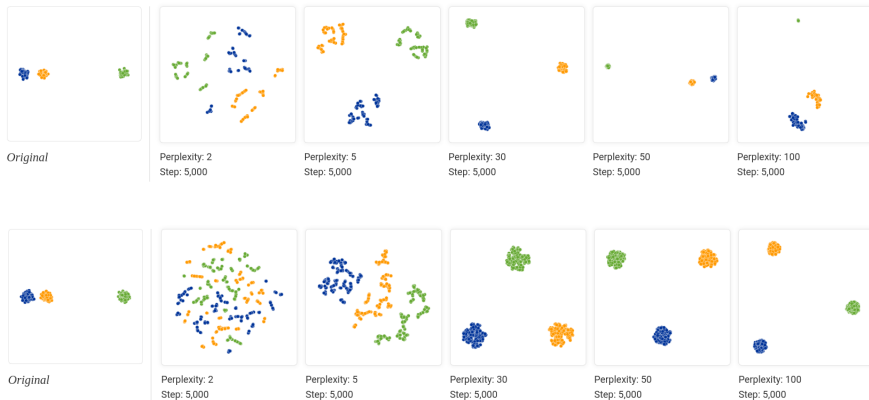
Perplexity: 50  
Step: 5,000



Perplexity: 100  
Step: 5,000

# 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

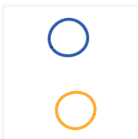
Sometimes topology is not preserved.



*Original*



Perplexity: 2  
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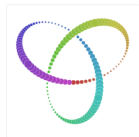
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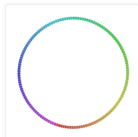
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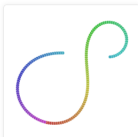
Perplexity: 100  
Step: 5,000



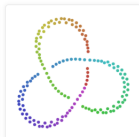
*Original*



Perplexity: 2  
Step: 5,000



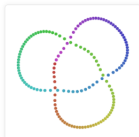
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Step: 5,000



## 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. To evaluate distances between clusters.
2. To evaluate density of clusters.
3. Establish topological property.

Thanks for the attention.