Stochastic Neighborhood Embedding

Weekly AI pills

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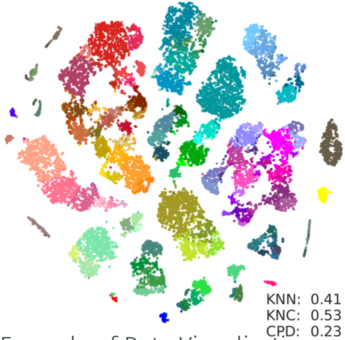
Summary

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

(t)-Stochastic Neighborhood Embedding

Aims

- Dimensionality Reduction
- Data Visualization
  1. Exploration
  2. Visual Clustering



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

Algorithm

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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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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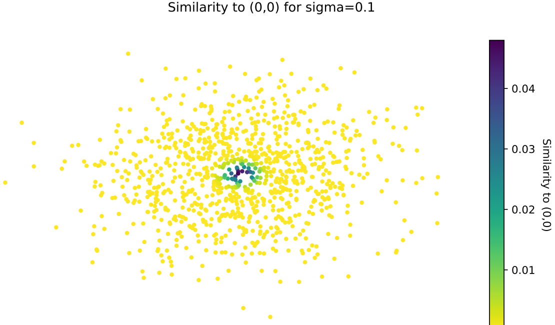

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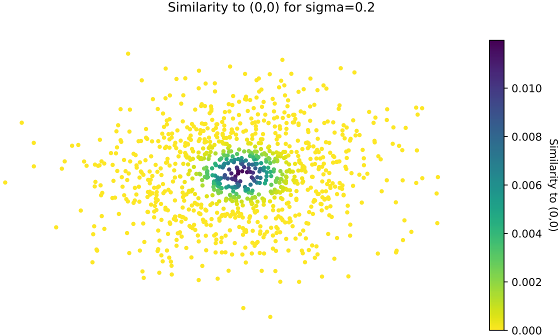

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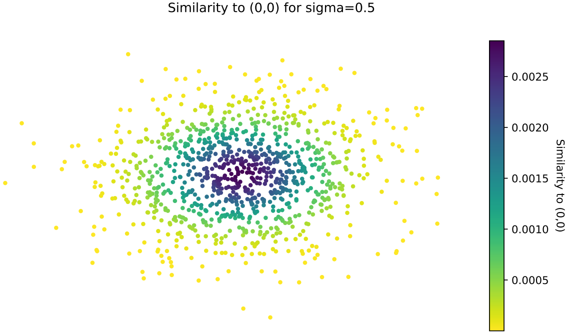

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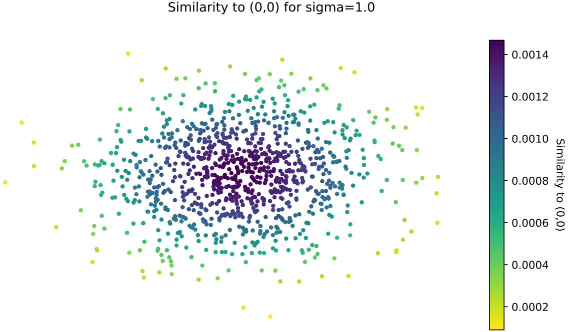

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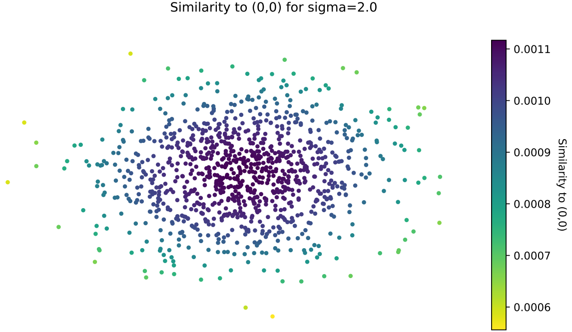

Algorithm: Similarity and Probability Distribution

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. $\sum_{j \neq i} p_{i|j} = \sum_{j \neq i} q_{i|j} = 1$

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

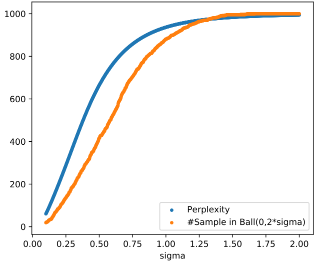
Perplexity: Shannon Entropy and Neighborhood

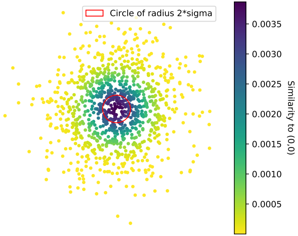
Let $\mathcal{P} = \{p_1, \cdots, p_n\}$ be a distribution

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

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

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.

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

t-SNE: Symmetric + Student

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

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

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

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

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

Examples

t-SNE on cortex's cells

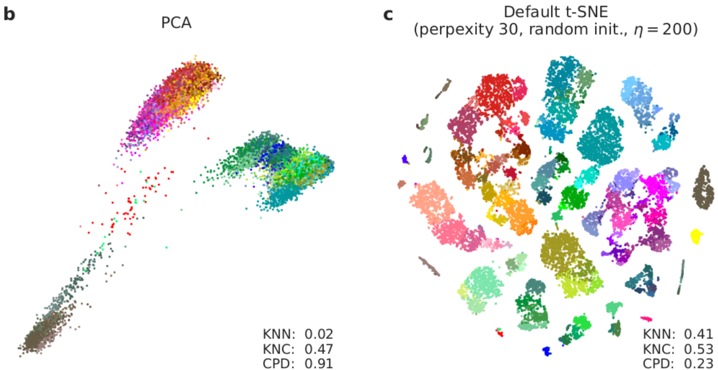


Image taken from Kobak-Barens paper.

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.

Looking at figure 3 locally t-SNE performs better, globally PCA performs better.

t-SNE on MNIST

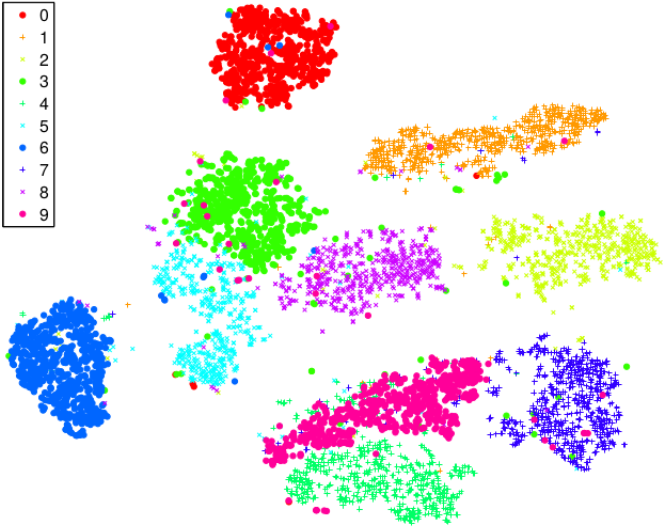


Image taken from Maaten - Hinton paper