Stochastic Neighborhood Embedding

Weekly AI pills

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Summary

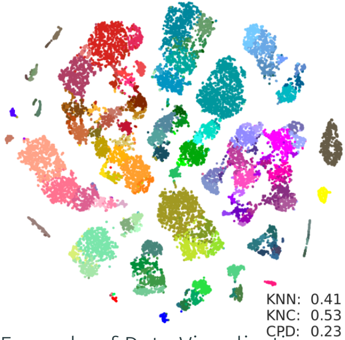
1. Entropy and Kullback–Leibler divergence
2. From SNE to t-SNE
3. Application for Visualization
4. Issues

Introduction

(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” (Future works?).

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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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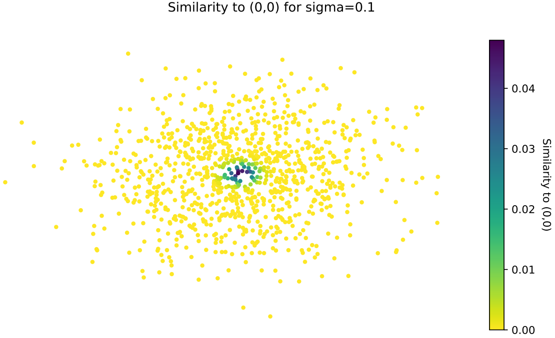

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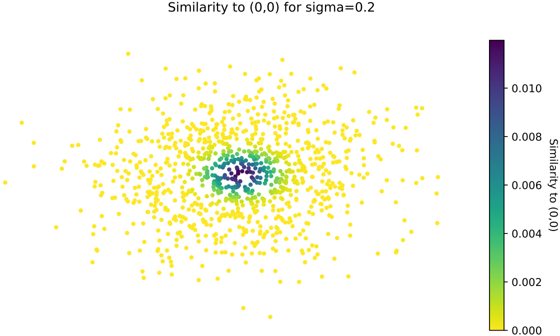

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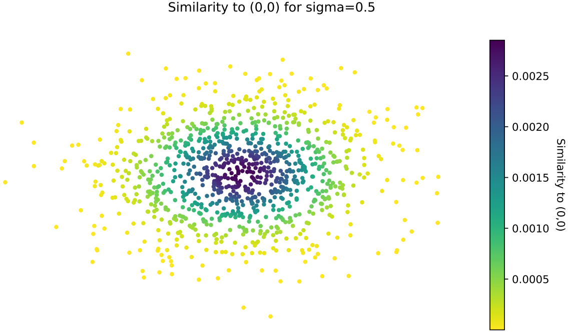

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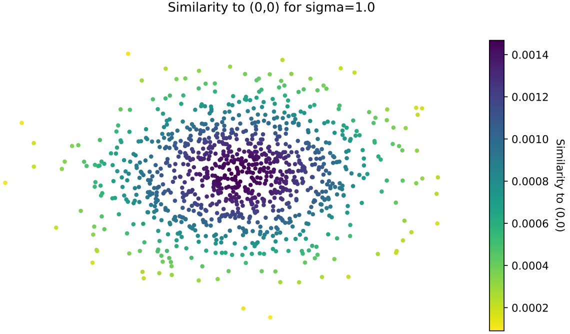

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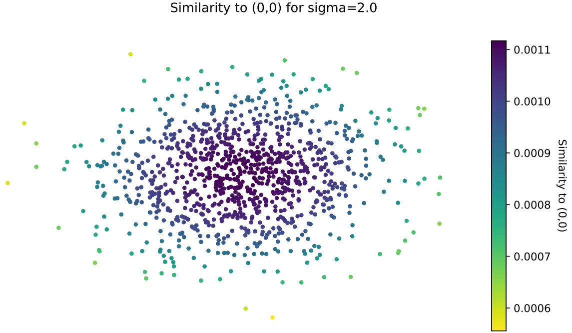

Algorithm: Similarity and Probability Distribution

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

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

Algorithm: Summary

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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How to find σ_i?

Shannon Entropy

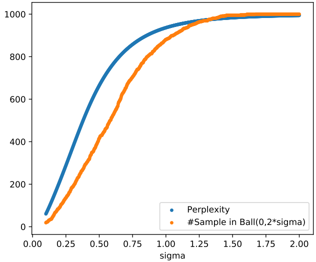
Shannon Entropy, Perplexity

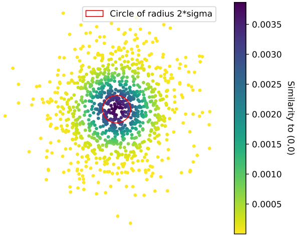
Let $\mathcal{P} = \{p_1, \cdots, p_n\}$ and $\mathcal{Q} = \{q_1, \cdots, q_n\}$ distributions

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

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

How σ_i and Perplexity are related?





Perplexity measures the number of samples in a neighborhood.