Data Visualization with t-SNE in Theory and Practice

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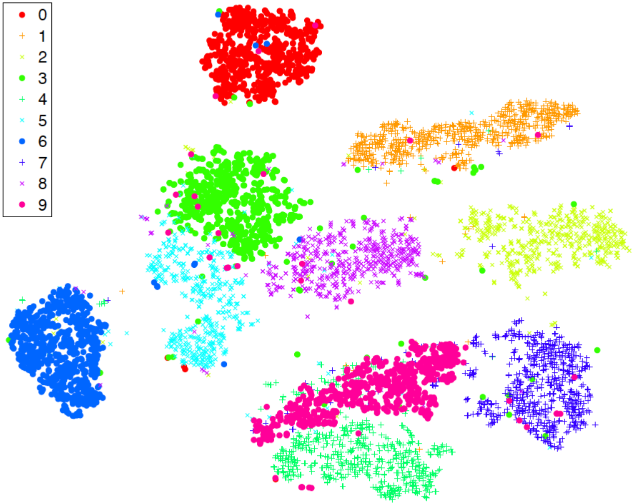
19th December 2024



Outline

Dimensionality Reduction

Goal: Map high-dimensional data to a lower dimension $\mathbb{R}^d \to \mathbb{R}^s$, $s \ll d$ while perserving intrinsic structure.

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Methods

- Linear methods: Principal Component Analysis (PCA), Multidimensional Scaling (MDS)
- Nonlinear methods: Isomap, t-Stochastic Neighbor Embedding (t-SNE)

Challenges of High Dimensions

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Crowding Problem

- High-dimensional points cannot be faithfully embedded in two or three dimensions
- Intrinsically distant points may cluster artificially due to limited space in the embedding

The Main Idea Behind t-SNE

Problem

Given a set of high-dimensional points $\mathcal{X} = \{x_1, x_2, ..., x_n\} \subset \mathbb{R}^d$ *find a "good" lower-dimensional representation* $\mathcal{Y} = \{y_1, y_2, ..., y_n\} \subset \mathbb{R}^s$ *of these points, where* $s = 2, 3$.

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An Informal Overview of t-SNE [MH08, Van der Maaten, Hinton]

- Create an initial set of points $\mathcal{Y}$ in $\mathbb{R}^s$
- Turn $\mathcal{X}$ and $\mathcal{Y}$ into probability distributions reflecting pairwise similarities between datapoints
- Force these distributions to be as similar as possible by moving points in the lower dimension around

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- To avoid overcrowding, we define a similarity measure between points in the low dimensional embedding y_i and y_j $(i \neq j)$ via

$$q_{ij} = \frac{(1 + ||y_i - y_j||^2)^{-1}}{\sum_l \sum_{k \neq l}(1 + ||y_k - y_l||^2)^{-1}}$$

using a Student's t-distribution with one degree of freedom (Cauchy distribution) which is heavy-tailed compared to a Gaussian.

Defining a Loss Function

Definition (Kullback-Leibler divergence)

Let P and Q be discrete probability distributions defined on a sample space $\mathcal{X}$. The Kullback-Leibler divergence between P and Q is defined as

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- KL divergence is asymmetric, i.e. in general $\mathrm{KL}(P||Q) \neq \mathrm{KL}(Q||P)$.

Optimization via Gradient Descent

- We can minimize $C(\mathcal{Y})$ using Gradient Descent, where

$$\frac{\partial C}{\partial y_i} = 4\sum_{j \neq i}(p_{ij} - q_{ij})q_{ij}Z(y_i - y_j) \text{ with } Z = \sum_{l}\sum_{k \neq l}(1 + \|y_k - y_l\|^2)^{-1}.$$

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- Standard optimization techniques for gradient descent can be employed, such as including a momentum term

$$y_i^{(t+1)} = y_i^{(t)} - h \cdot \frac{\partial C}{\partial y_i^{(t)}} + \beta(y_i^{(t)} - y_i^{(t-1)}) \text{ with } 0 \leq \beta < 1, h > 0.$$

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- Rewriting the gradient yields interpretation via attractive and repulsive forces:

$$-\frac{1}{4} \frac{\partial C}{\partial y_i} = \underbrace{\sum_{j \neq i} p_{ij} q_{ij} Z (y_j - y_i)}_{\text{attractive force}} - \underbrace{\sum_{j \neq i} q_{ij}^2 Z (y_j - y_i)}_{\text{repulsive force}}$$

Initialization

- It is best to use "informative initialization" instead of random initialization for t-SNE.
- PCA initialization better preserves global structure.

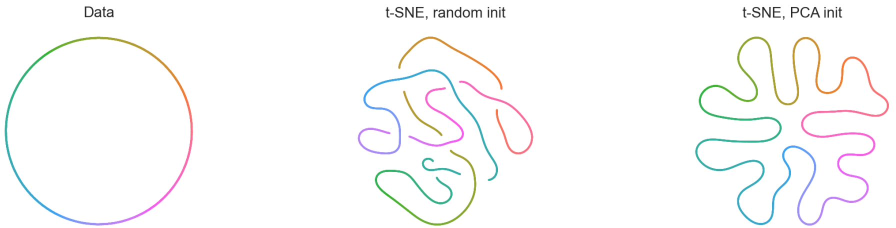

Figure: The t-SNE algorithm only produces a faithful representation of the circle with informative initialization. Visualization reproduced from [KL21]

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Let X be a discrete random variable taking values in $\mathcal{X}$ which is distributed according to $p : \mathcal{X} \to [0,1]$, then the Shannon Entropy is $H(X) = -\sum_{x\in\mathcal{X}} p(x)\log_2(p(x))$.

- We define a constant **perplexity** value

$$\text{Perp}(P_i) = 2^{H(P_i)} = 2^{-\sum_j p_{j|i}\log p_{j|i}}$$

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- Perplexity effectively measures the number of neighbours we wish to consider.

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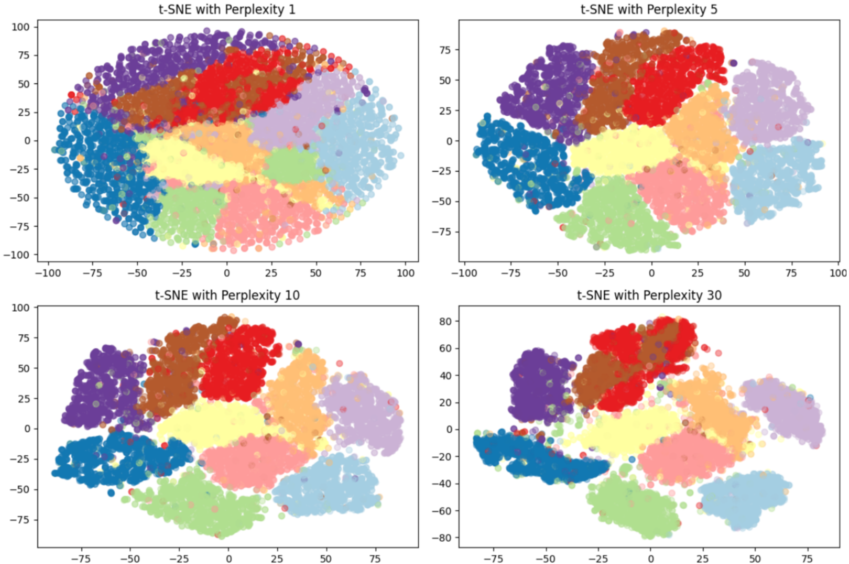

Figure: Different perplexity values on the MNIST dataset.

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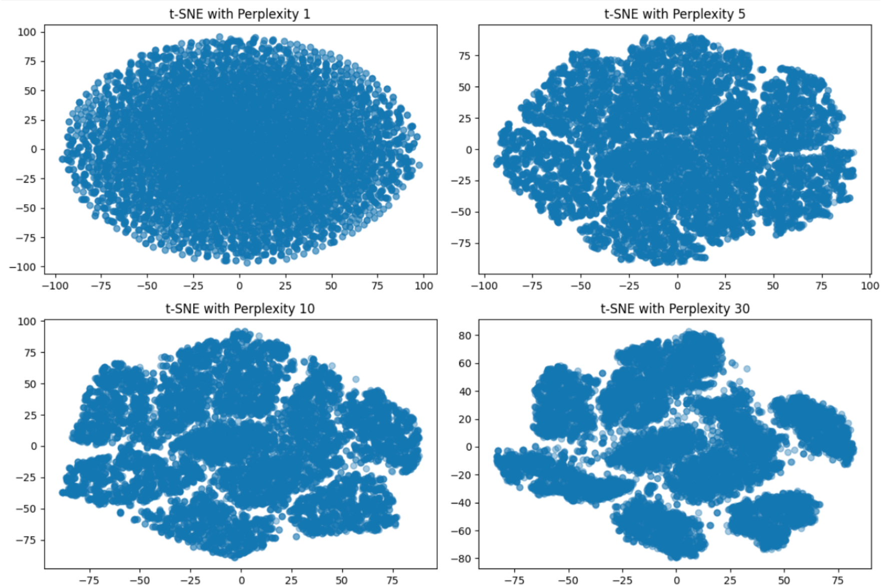

Figure: Different perplexity values on the MNIST dataset without ground truth labels.

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- **Question**: How do we find good values for α and for how many iterations should we keep early exaggeration on?

Automated Optimized Parameters

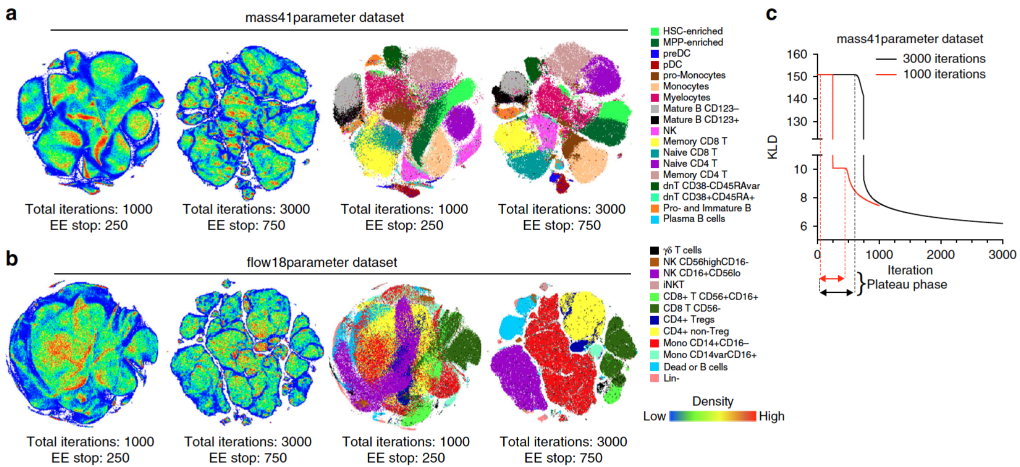

Figure: Performance of t-SNE for cytometry data visualization, see [Bel+19].

Theoretical Work on t-SNE

Theorem (Cluster Formation [LS22])

Let $\mathcal{X}$ be "clustered" and initialize $\mathcal{Y} \subset [-0.01, 0.01]^2$. Choose α and h such that for some $1 \leq i \leq n$

$$0.01 \leq \alpha h \sum_{\substack{j \neq i \\ \text{same cluster}}} p_{ij} \leq 0.9$$

Then, the diameter of the embedded cluster $\{y_i : 1 \leq j \leq n \wedge \pi(j) = \pi(i)\}$ decays exponentially until its diameter satisfies, for some universal $c > 0$,

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- Other theoretical results study connections to spectral clustering ([CM22]) and limiting behaviour for $n \to \infty$ ([MP24]).

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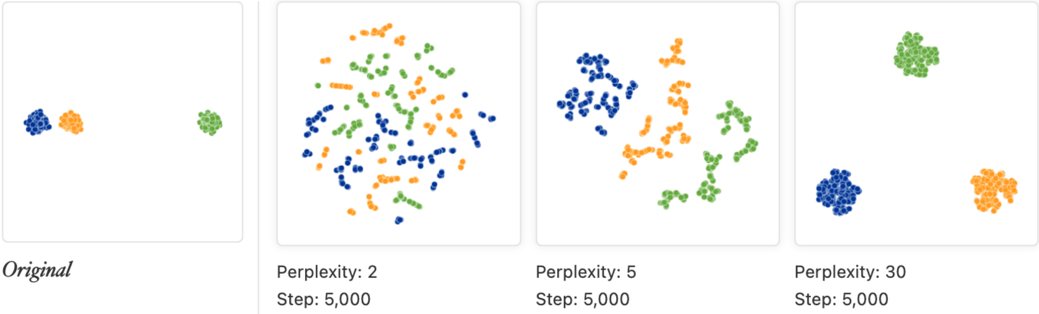

Figure: t-SNE does not preserve distance between clusters, see [WVJ16]

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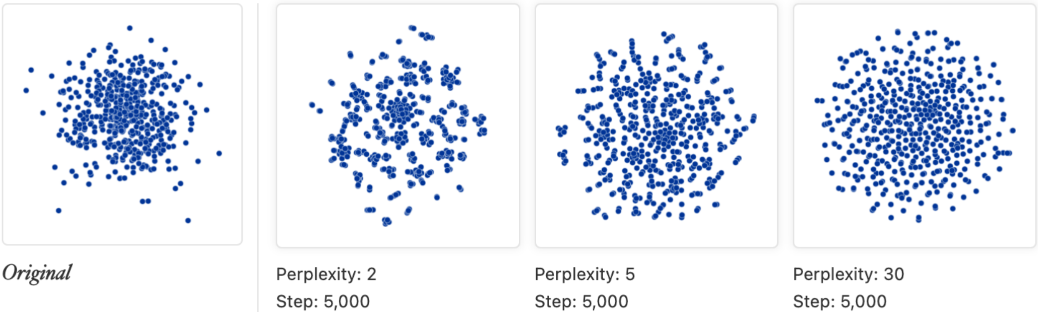

Figure: Random Gaussian noise does not always look random, see [WVJ16]

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- How does initialization impact t-SNE results across different datasets?
- How can we deal with large datasets? Does rescaled t-SNE work in practice?

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