Manifold learning

t-SNE, UMAP, LLE, etc

Readings

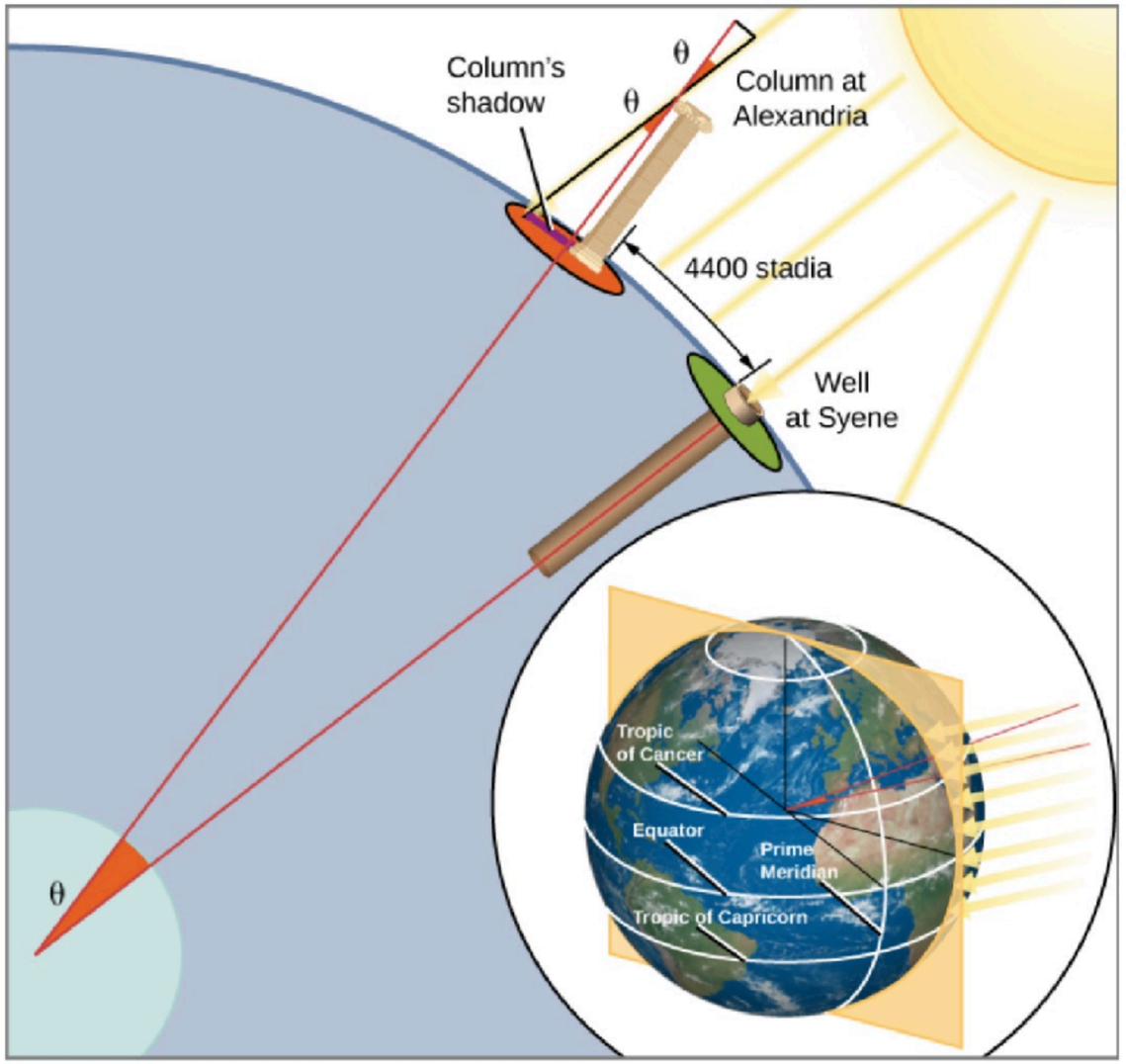
- https://jmlr.org/papers/volume9/vandermaaten08a/vandermaaten08a.pdf
- https://distill.pub/2016/misread-tsne/
- https://pair-code.github.io/understanding-umap/index.html
- https://umap-learn.readthedocs.io/en/latest/how_umap_works.html

Manifolds

- A manifold is a topological space that is locally Euclidean
- Consider the existence of FLAT EARTHERS
- On the small scales that we see daily the Earth does indeed look flat.
- Any object that is nearly "flat" on small scales is a manifold, and so manifolds constitute a generalization of objects we could live on :)

Manifolds
SIDE BAR

- A manifold is a topological space that is locally Euclidean
- Flat earth is not some ancient belief… the ancient Greeks and others were generally aware of the curvature of the Earth.
- Eratosthenes of Cyrene (3rd century BCE) was chief librarian at the Library of Alexandria & calculated the Earth's circumference with an error of ~2%



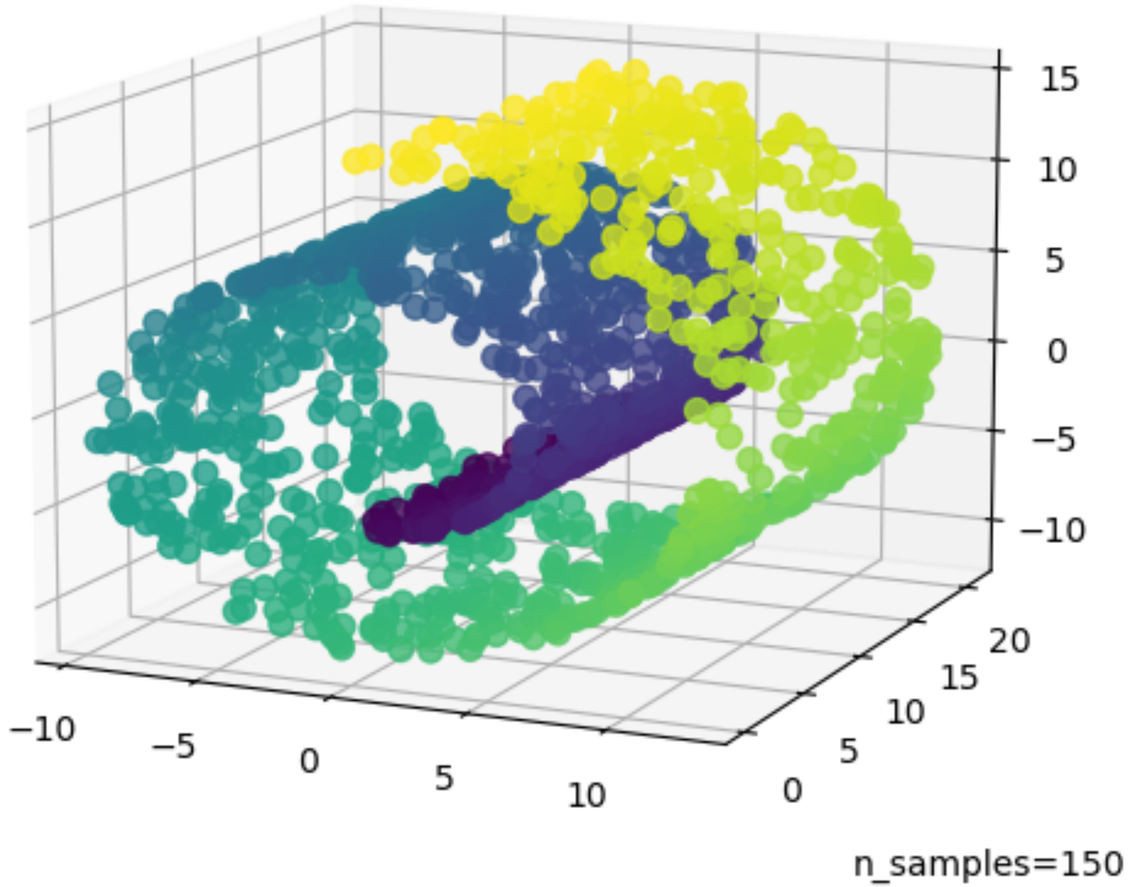
Topology
SIDE BAR

- One of the goals of topology is to find ways of distinguishing manifolds, e.g….
  - A circle is topologically the same as any closed loop
  - The surface of a coffee mug with a handle is topologically the same as the surface of the donut

Manifold learning

- Manifold learning is an approach to dimensionality reduction where the problem is only locally linear/Euclidean
- Algorithms for this task are based on the idea that the dimensionality of many data sets is only artificially high if you allow curved manifolds

Swiss roll dataset



Manifold learning

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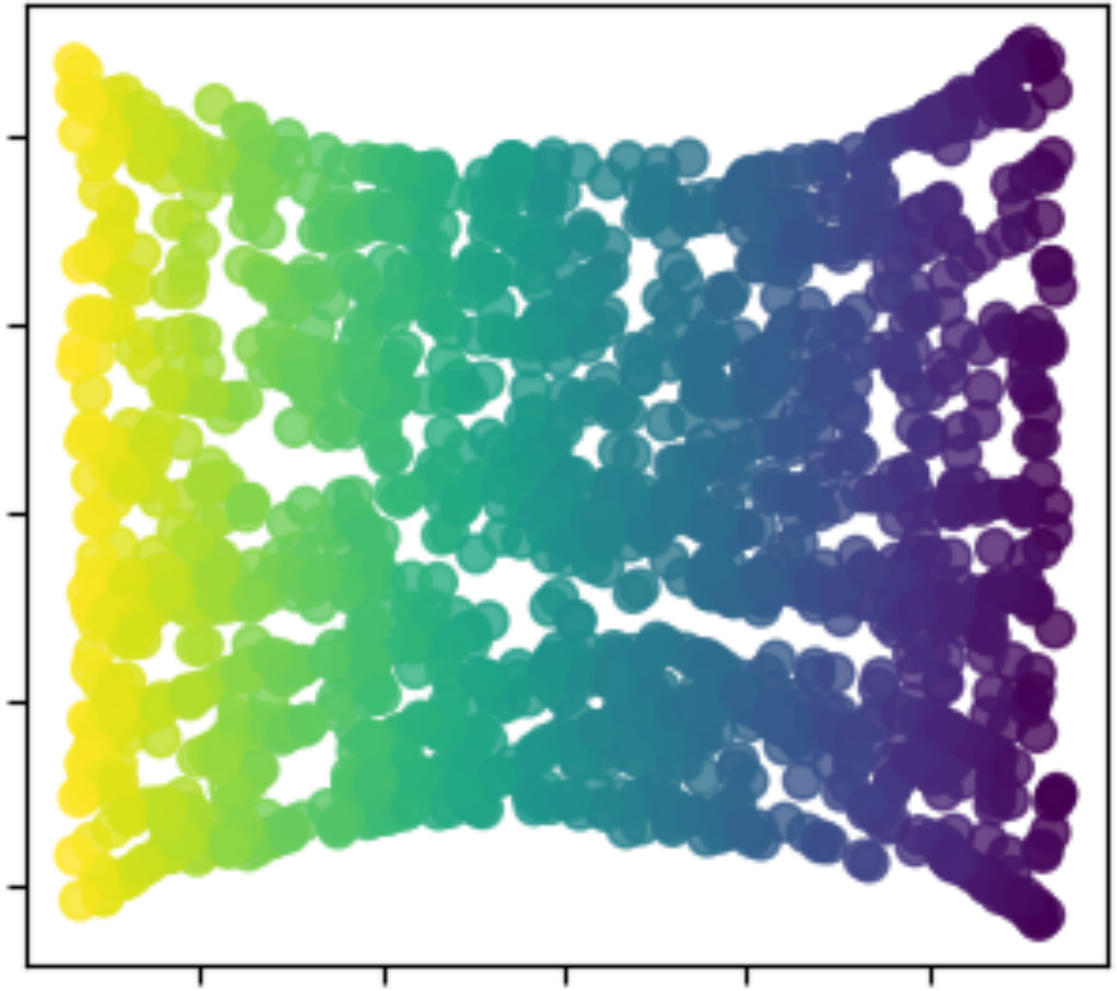
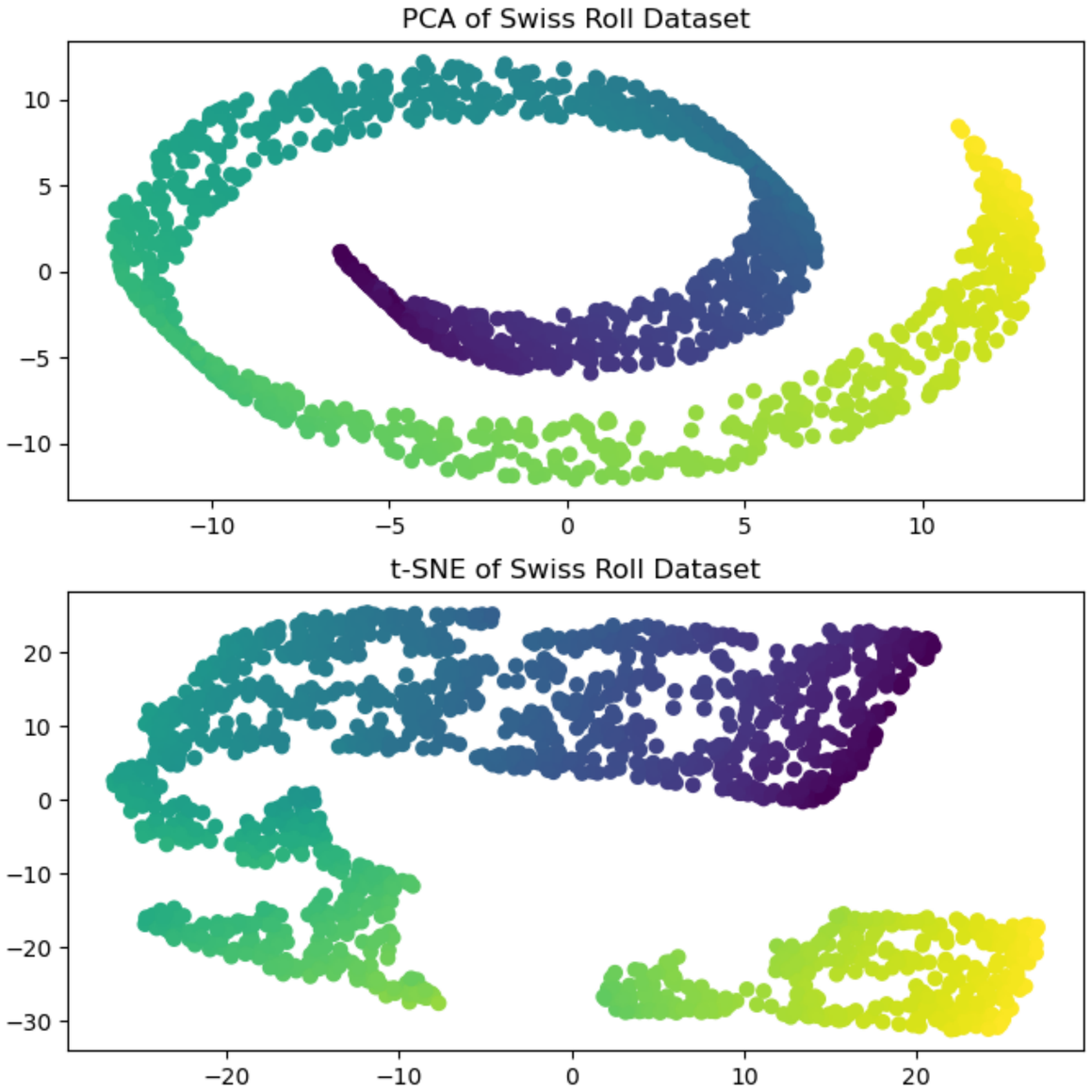
"Idealized" 2D manifold for Swiss Roll

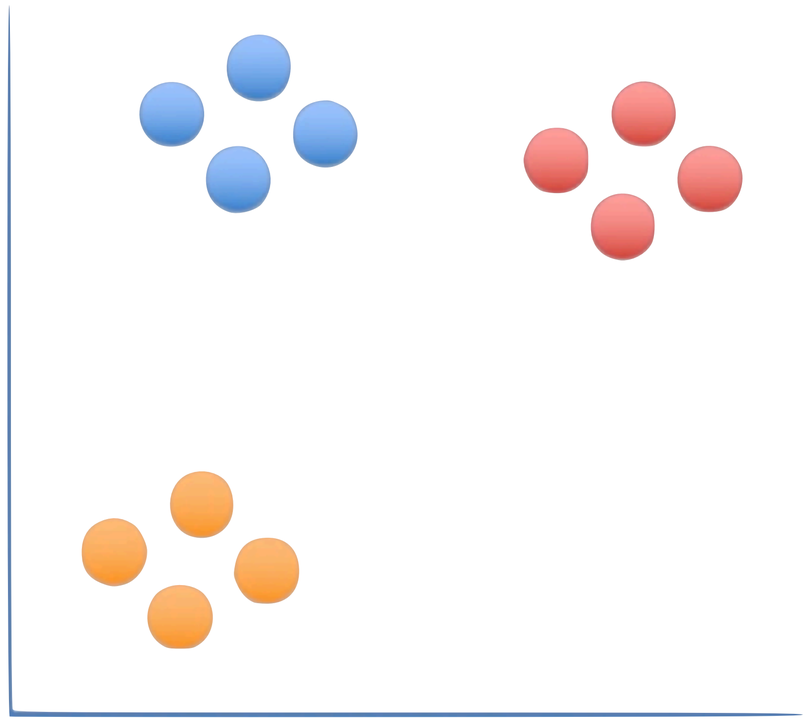


t-SNE

t-distributed Stochastic Neighbor Embedding

- PCA tries to find a global structure
  - Can lead to local inconsistencies in a subspace…far away points can become nearest neighbors
- t-SNE tries to preserve local structure
  - “For high-dimensional data that lies on or near a low-dimensional, non-linear manifold it is usually more important to keep the low-dimensional representations of very similar datapoints close together, which is typically not possible with a linear mapping”





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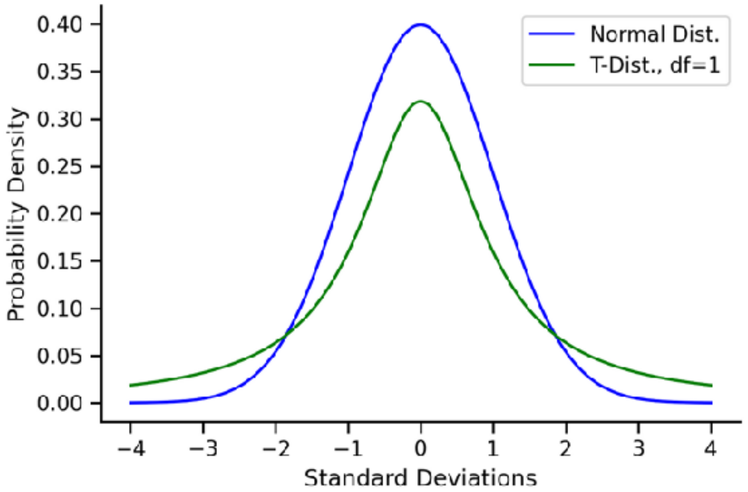

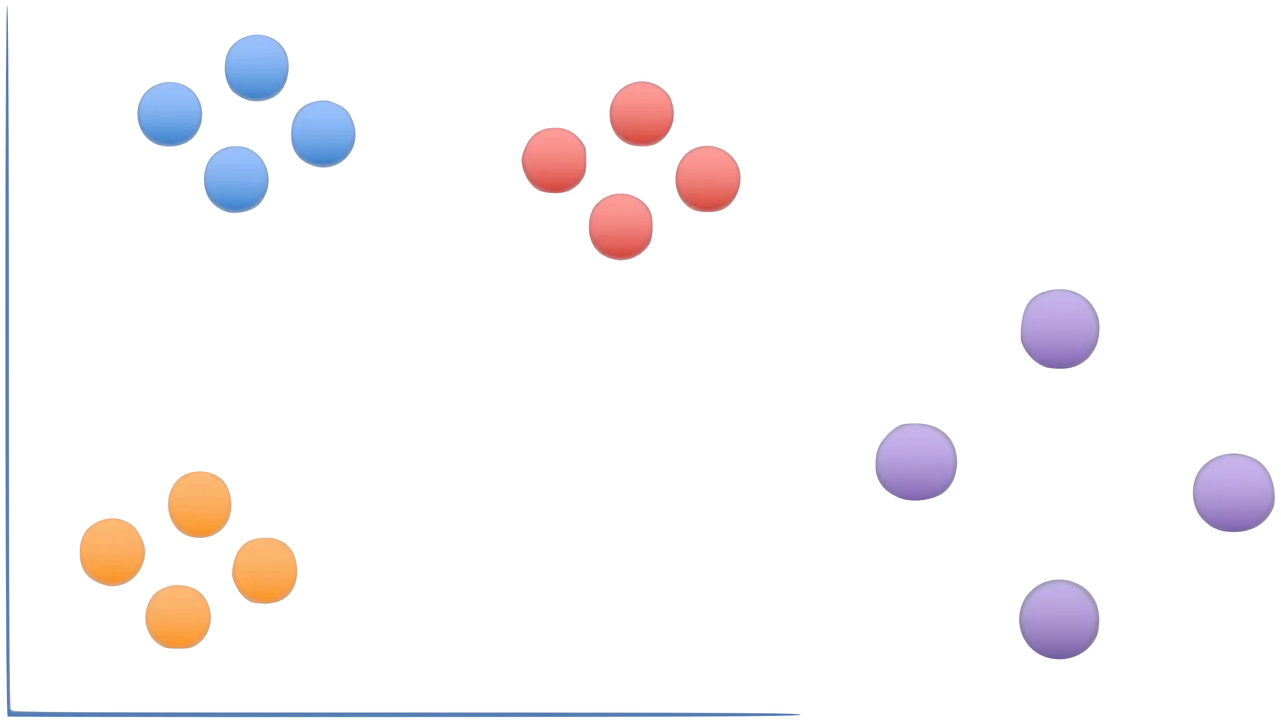

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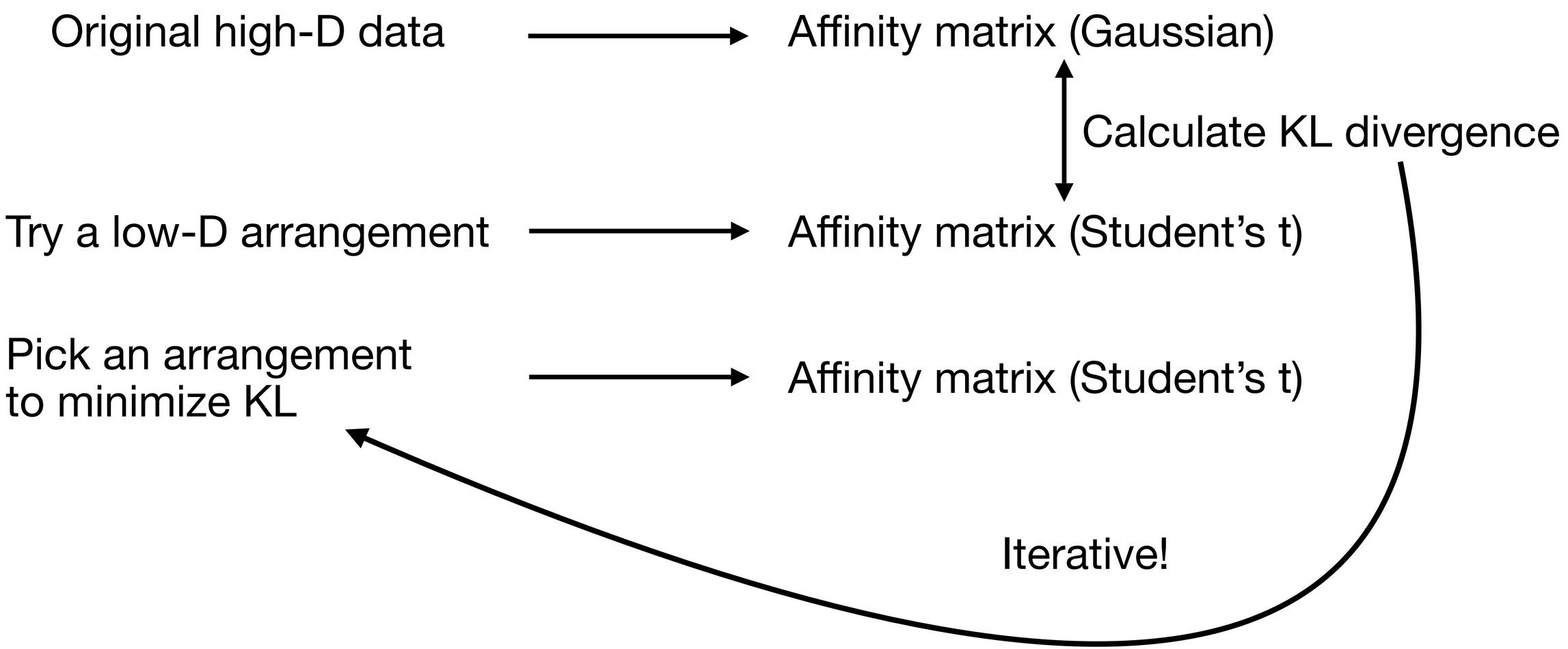
t-SNE concepts



https://lvdmaaten.github.io/publications/papers/JMLR_2014.pdf

t-SNE algorithm

points in the embedding. Assume we are given a data set of (high-dimensional) input objects $\mathcal{D} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\}$ and a function $d(\mathbf{x}_i, \mathbf{x}_j)$ that computes a distance between a pair of objects, *e.g.*, the Euclidean distance $d(\mathbf{x}_i, \mathbf{x}_j) = \|\mathbf{x}_i - \mathbf{x}_j\|$. Our aim is to learn an s-dimensional embedding in which each object is represented by a point, $\mathcal{E} = \{\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_N\}$ with $\mathbf{y}_i \in \mathbb{R}^s$ (typical values for s are 2 or 3). To this end, t-SNE defines joint probabilities

$$p_{j|i} = \frac{\exp(-d(\mathbf{x}_i, \mathbf{x}_j)^2/2\sigma_i^2)}{\sum_{k \neq i} \exp(-d(\mathbf{x}_i, \mathbf{x}_k)^2/2\sigma_i^2)}, \qquad p_{i|i} = 0$$

$$p_{ij} = \frac{p_{j|i} + p_{i|j}}{2N}.$$

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t-SNE algorithm

In the s-dimensional embedding $\mathcal{E}$, the similarities between two points $\mathbf{y}_i$ and $\mathbf{y}_j$ (*i.e.*, the low-dimensional models of $\mathbf{x}_i$ and $\mathbf{x}_j$) are measured using a normalized heavy-tailed kernel. Specifically, the embedding similarity q_{ij} between the two points $\mathbf{y}_i$ and $\mathbf{y}_j$ is computed as a normalized Student-t kernel with a single degree of freedom:

$$q_{ij} = \frac{(1 + \|\mathbf{y}_i - \mathbf{y}_j\|^2)^{-1}}{\sum_{k \neq l}(1 + \|\mathbf{y}_k - \mathbf{y}_l\|^2)^{-1}}, \qquad q_{ii} = 0. \tag{3}$$

The heavy tails of the normalized Student-t kernel allow dissimilar input objects $\mathbf{x}_i$ and $\mathbf{x}_j$ to be modeled by low-dimensional counterparts $\mathbf{y}_i$ and $\mathbf{y}_j$ that are too far apart. This is desirable because it creates more space to accurately model the small pairwise distances (*i.e.*, the local data structure) in the low-dimensional embedding.

The locations of the embedding points $\mathbf{y}_i$ are determined by minimizing the Kullback-Leibler divergence between the joint distributions P and Q:

$$C(\mathcal{E}) = KL(P||Q) = \sum_{i \neq j} p_{ij} \log \frac{p_{ij}}{q_{ij}}. \tag{4}$$

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t-SNE algorithm

Due to the asymmetry of the Kullback-Leibler divergence, the objective function focuses on modeling high values of p_{ij} (similar objects) by high values of q_{ij} (nearby points in the embedding space). The objective function is non-convex in the embedding $\mathcal{E}$. It is typically minimized by descending along the gradient:

$$\frac{\partial C}{\partial \mathbf{y}_i} = 4 \sum_{j \neq i} (p_{ij} - q_{ij}) q_{ij} Z (\mathbf{y}_i - \mathbf{y}_j), \tag{5}$$

where we defined the normalization term $Z = \sum_{k \neq l} (1 + \|\mathbf{y}_k - \mathbf{y}_l\|^2)^{-1}$.

It is straightforward to see that the evaluation of the joint distributions P and Q is $\mathcal{O}(N^2)$, because both distributions involve a normalization term that sum over all $N(N-1)$ pairs of unique objects. Since t-SNE scales quadratically in the number of objects N, its applicability is limited to data sets with only a few thousand input objects; beyond that, learning becomes too slow to be practical (and the memory requirements become too large).

https://lvdmaaten.github.io/publications/papers/JMLR_2014.pdf

t-SNE algorithm

One last thing we have not yet mentioned how to set the bandwidths σ_i for the Gaussian kernels centered over each data point in the input space. It is unlikely that one single value of σ_i is optimal for all data points because the density of the data is likely to vary. In dense regions, a smaller value of σ_i is usually more appropriate than in sparser regions. Perplexity is defined as

$$\text{Perplexity}(\mathbf{p}_i) = 2^{H(\mathbf{p}_i)}$$

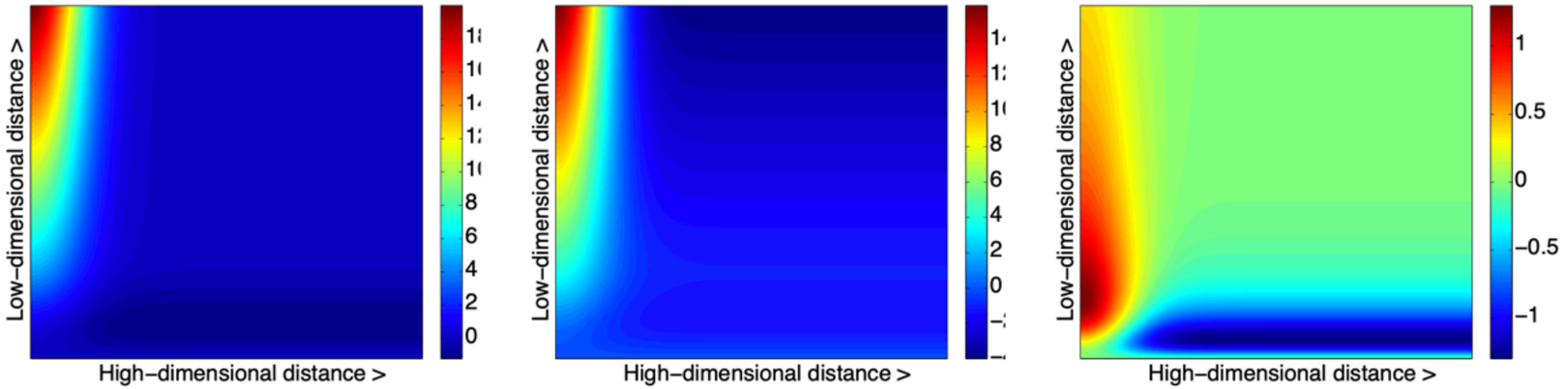
where H is the Shannon entropy of a discrete distribution

$$H(\mathbf{p}_i) = -\sum_i p_{j|i} \log_2(p_{j|i})$$

Perplexity can be thought of as a continuous analogue to the k nearest neighbours, to which t-SNE will attempt to preserve distances. More concretely, the bandwidths σ_i are set such that each Gaussian kernel fits k nearest neighbors within one standard deviation of the probability density.

- Low Perplexity is small σ_i
- High Perplexity is large σ_i

Mismatched Tails can Compensate for Mismatched Dimensionalities



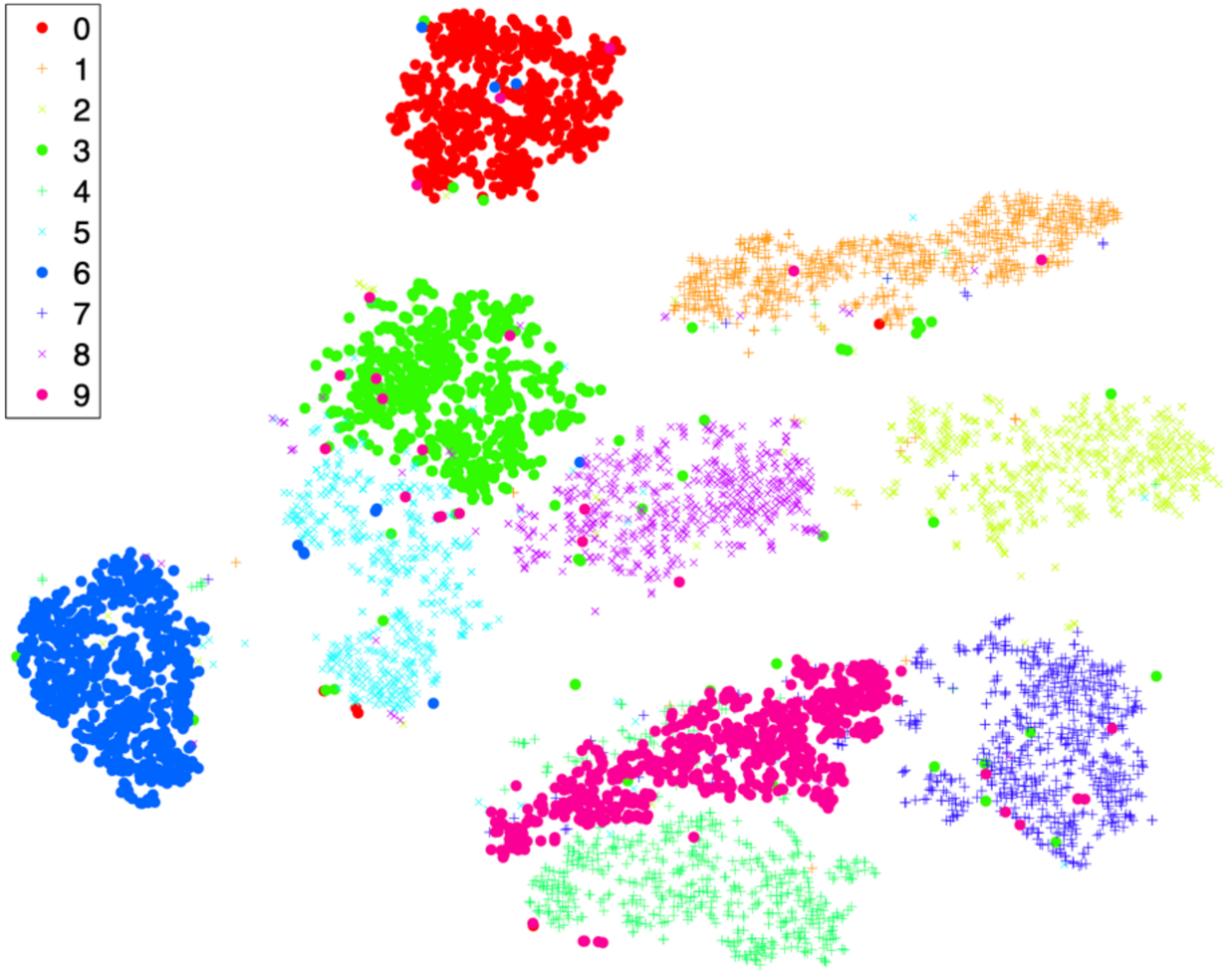
(a) Gradient of SNE. (b) Gradient of UNI-SNE. (c) Gradient of t-SNE.

Figure 1: Gradients of three types of SNE as a function of the pairwise Euclidean distance between two points in the high-dimensional and the pairwise distance between the points in the low-dimensional data representation.

Algorithm 1: Simple version of t-Distributed Stochastic Neighbor Embedding.

Data: data set $\mathcal{X} = \{x_1, x_2, ..., x_n\}$,
cost function parameters: perplexity $Perp$,
optimization parameters: number of iterations T, learning rate η, momentum $\alpha(t)$.
Result: low-dimensional data representation $\mathcal{Y}^{(T)} = \{y_1, y_2, ..., y_n\}$.
begin
    compute pairwise affinities $p_{j|i}$ with perplexity $Perp$ (using Equation 1)
    set $p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}$
    sample initial solution $\mathcal{Y}^{(0)} = \{y_1, y_2, ..., y_n\}$ from $\mathcal{N}(0, 10^{-4}I)$
    for *t=1* **to** T **do**
        compute low-dimensional affinities q_{ij} (using Equation 4)
        compute gradient $\frac{\delta C}{\delta \mathcal{Y}}$ (using Equation 5)
        set $\mathcal{Y}^{(t)} = \mathcal{Y}^{(t-1)} + \eta \frac{\delta C}{\delta \mathcal{Y}} + \alpha(t) \left(\mathcal{Y}^{(t-1)} - \mathcal{Y}^{(t-2)} \right)$
    end
end

MNIST



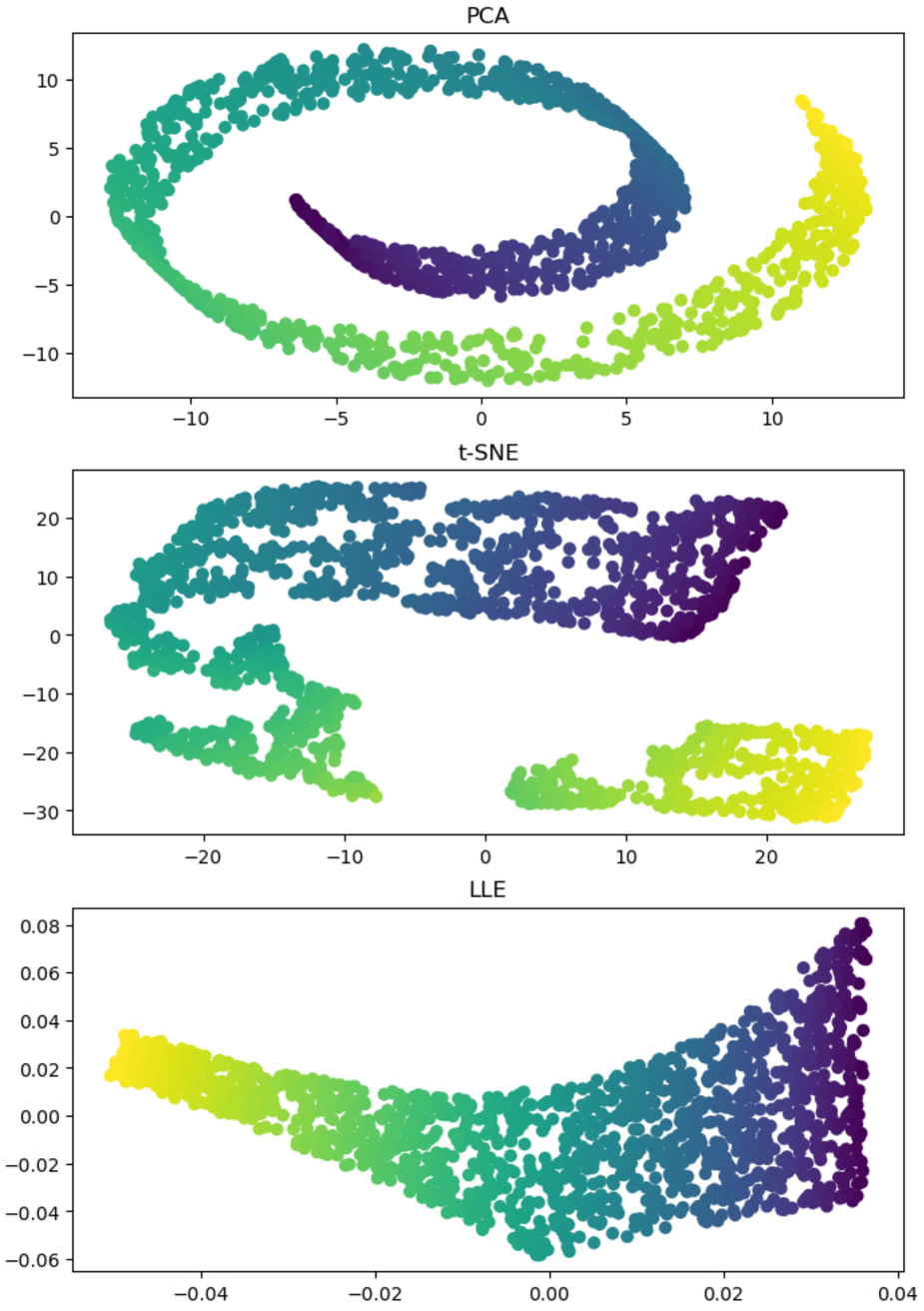
(a) Visualization by t-SNE.

t-SNE limitations

- Computationally expensive!
  - $\mathcal{O}(N^2)$ because of affinity matrix calculations… and worse than that because we have to do this iteratively on the lower-d embedding
  - Barnes-Hut approximation to gradient descent on KL (a spanning tree style algorithm) compares points to “cells” in $\mathcal{O}(N \log N)$.
    - Can only go up to 3D! Only works with dense input data!
    - Can go up to ~10^5 to 10^6 samples
- Only has .fit_transform() because there’s no way to .transform() separately from a .fit()! You’d have to redo from scratch to calculate where a new data point should go!
  - This technique is for visualization, not for building cross-validated classifiers on top of

Procrustes alignment

- Can measure the stability of the overall structure of the embedding.
- Considering the normalized Procrustes distance between the embedding of a sub-sample, and the corresponding sub-sample of an embedding of the full dataset
- As the size of the sub-sample increases the average distance per point between the sub- sampled embeddings should decrease, potentially toward some asymptote of maximal agreement under repeated runs. Ideally this asymptotic value would be zero error, but for stochastic embeddings such as UMAP and t- SNE this is not achievable.


PCA
10
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LLE
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