Visualizing Data using t-SNE

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Data Visualization and Manifold Learning

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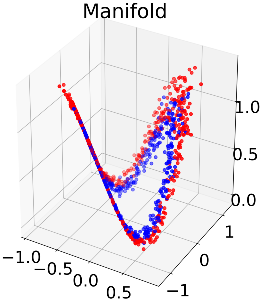
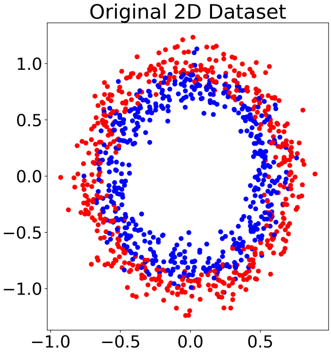
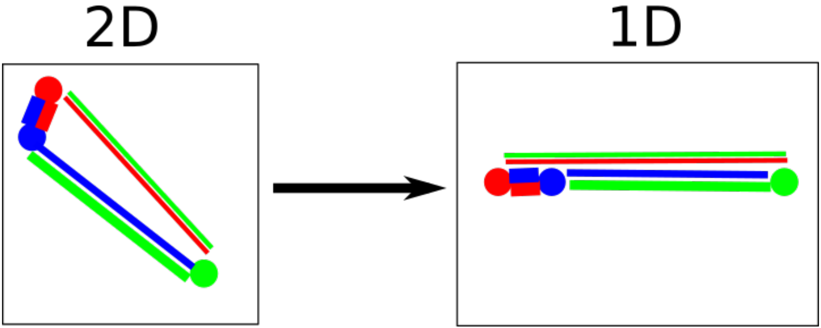




Stochastic Neighbor Embedding (SNE)

High-Level Overview

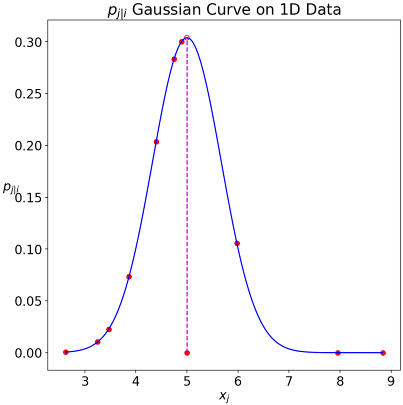
1. Each pair of data points has a measurable neighbor relationship with every other point
2. This relationship is non-symmetric
3. Stochastic neighbor embedding tries to preserve this relationship



Stochastic Neighbor Embedding (SNE)

What is $p_{j|i}$?

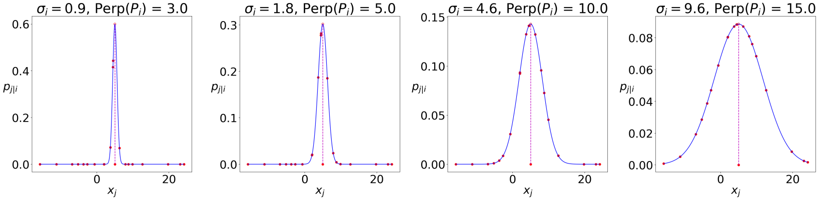
1. $p_{j|i} = \frac{\exp\left(-||x_i - x_j||^2/2\sigma_i^2\right)}{\sum_{k\neq i}\exp\left(-||x_i - x_k||^2/2\sigma_i^2\right)}$
2. Probability datapoint x_i views x_j as its neighbor given Gaussian with variance σ_i



Stochastic Neighbor Embedding (SNE)

Determining σ_i

σ_i	Determined via binary search on perplexity
Perplexity	Smooth approximation of number of neighbors $Perp(P_i) = 2^{H(P_i)}$
Shannon Entropy	Information present in probability space $H(P_i) = -\sum_j p_{j\|i} \log_2 p_{j\|i}$



Stochastic Neighbor Embedding (SNE)

Cost Function

1. $q_{j|i}$ is analogous to $p_{j|i}$ for lower dimension points y_i and y_j. $\sigma = 1/\sqrt{2}$ for all $q_{j|i}$
2. Cost function is $C = \sum_i KL(P_i||Q_i) = \sum_i \sum_j p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}$
3. Cost function uses Kullbeck-Leibler divergence to measure the difference between the set of $q_{j|i}$ and $p_{j|i}$

Stochastic Neighbor Embedding (SNE)

Gradient Descent Optimization

1. $\frac{\partial C}{\partial y_i} = 2 \sum_j \left(p_{j|i} - q_{j|i} + p_{i|j} - q_{i|j} \right) (y_i - y_j)$
2. $Y^{(t)} = Y^{(t-1)} + \nu \frac{\partial C}{\partial Y} + \alpha(t) \left(Y^{(t-1)} - Y^{(t-2)} \right)$
3. Simulated annealing through decaying Gaussian noise

Problems with SNE

- Cost function is not convex
  - Possible to get stuck on local minima
- Computational inefficiency
  - Must compute $p_{j|i}$ many times, especially when estimating σ_i
  - Simulated annealing is slow. Suffers compared to convex optimization
- Overcrowding