Analyzing Visualization and Dimensionality-Reduction Algorithms

Oliver Hayman
Mentor: Ashwin Narayan
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Motivation

Algorithms are needed to spot patterns in high dimensional data sets

Not perfect at preserving relationships

Expression patterns from different mouse brain cells
**t-distributed Stochastic Neighbor Embedding**

Probability distribution on points in high-dimensional space:

\[
p_{j|i} = \frac{\exp\left(-\frac{||x_i - x_j||^2}{2\sigma^2}\right)}{\sum_{k \neq i} \exp\left(-\frac{||x_i - x_k||^2}{2\sigma^2}\right)}
\]

- probability of picking \( x_j \) in Gaussian distribution centered at \( x_i \)

\[
p_{ij} = \frac{p_{ij} + p_{ji}}{2n}
\]

- modified probability of picking points in joint Gaussian distribution

similarly in the embedded space:

\[
q_{ij} = \frac{1 + ||y_i - y_j||^2}{\sum_{k \neq i} \left(1 + ||y_i - y_k||^2\right)}
\]

- probability of picking points in joint Student’s t-Distribution

t-SNE minimizes the distance b/w these two distributions
Choice of *perplexity* is key

Choose $\sigma_i$ so that it is bigger in sparse regions and smaller in dense regions.

Governed by a parameter called perplexity - can be thought of as number of neighbors for each point grouped together.

Example

![Example plots with different perplexities](image)
Example runs

Perplexity: 80

Perplexity: 30

Perplexity: 10

Perplexity: 50

Perplexity: 30
What makes a visualization “good”?

Need metric to measure clustering

\[ \alpha(x_i, a) - \text{distance from } x_i \text{ to } a \text{th closest data point} \]

\[ \beta(x_i, a) - \text{number of points whose distance from } x_i \text{ is less than } a \]

For set X, metric is

\[ \frac{1}{n} \sum_{x_i \in X} \beta \left( x_i, \left( \frac{2\alpha(x_i, c)}{c} \right)^\frac{1}{d} \right) \]

- 2 hyperspheres, metric based on number of points in smaller one
Perplexity choice affects clustering

Fit to equation $F(x) = ae^{-bx} + c$
Towards theoretical results

For uniform distributions in unit hypercube,

\[ v(r) \] - volume of hypersphere

\[ f(x,r) \] - volume of hypersphere cut a distance \( x \) from center

Formulas for \( P(\text{larger hypersphere having radius } r) \), \( P(\text{point in smaller hypersphere } | \text{ larger hypersphere has radius } r) \) used to determine expected value

Made assumption that hypersphere will only intersect one edge of hypercube (gives an approximation)
Future work

Find and prove relationship between perplexity and clustering

Find modification to algorithm

Apply methods to other algorithms

Define other metrics for different properties
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References
