

Data Visualization

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Overview

1 Overview

2 t-SNE

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Agenda

- Are the models working as expected?
- Do the metrics make sense?
- Visualizing multi-dimensional data
- Trying to understand DL models

Plotting Residuals

Residual Errors

In a good model, it is expected that the errors that the model makes will not have any *systematic* nature to them. That is, the errors should be essentially *random*.

Plotting Residuals: No systematic errors in prediction

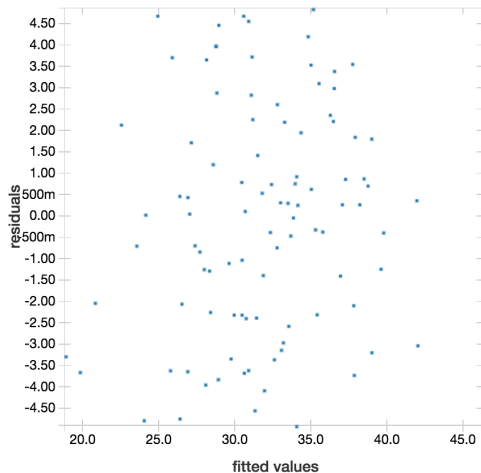


Figure: Source - Databricks blog

Plotting Residuals: Systematic errors in prediction

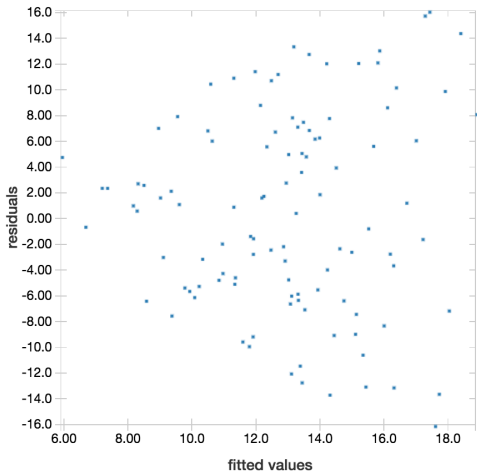


Figure: Source - Databricks blog

Visualizing KMeans fit

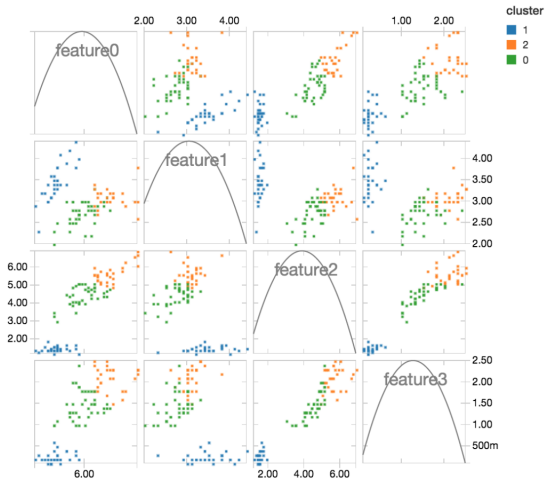


Figure: Source - Databricks blog

ROC Curve examples

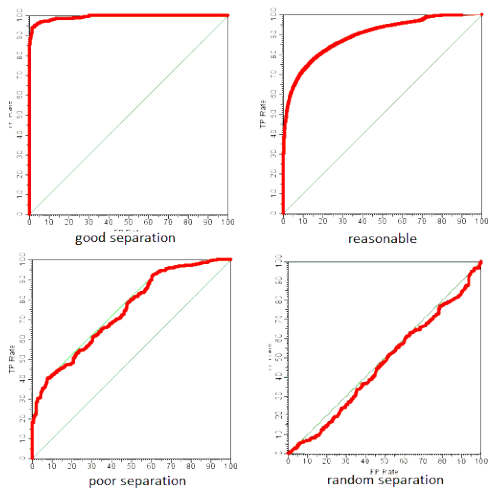


Figure: Source - MLWiki

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t-distributed Stochastic Neighbor Embedding (t-SNE)

t-SNE

t-Distributed Stochastic Neighbor Embedding (t-SNE) is a (prize-winning) technique for dimensionality reduction that is particularly well suited for the visualization of high-dimensional datasets. The technique can be implemented via Barnes-Hut approximations, allowing it to be applied on large real-world datasets. It has been applied on data sets with up to 30 million examples [1].

Visualizing/reducing dimensions of high-dimensional data

- PCA - preserves large distances
- ISOMAP - changes similarity function and then applies PCA
- Locally linear embedding

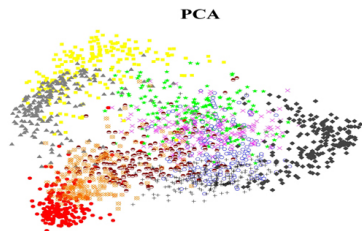


Figure: Source: Xiaofei He

ISOMAP

- ISOMAP reduces dimensions non-linearly
- Related to kernel PCA
- Instead of Euclidean distance, use a geodesic / manifold distance

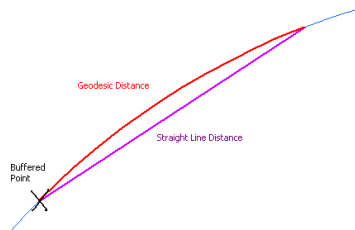


Figure: Source: ESRI

Locally Linear Embedding

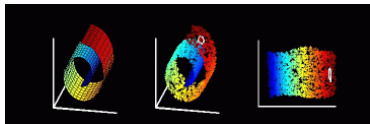


Figure: Source: Roweis and Saul

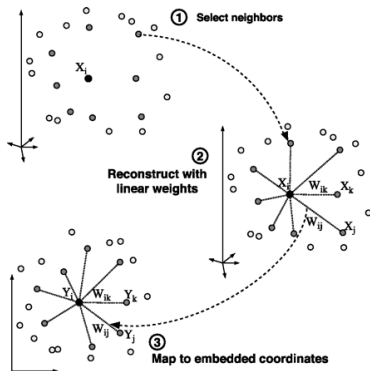


Figure: Source: Roweis and Saul

SNE Algorithm

- Similar to LLE but use probabilities instead of distances
- Compute $p_{j|i}$, conditional probability that x_i would pick x_j as neighbor under a locally modeled pdf

- Formally
$$p_{j|i} = \frac{\exp(-\frac{|x_i - x_j|^2}{2\sigma_i^2})}{\sum_{k \neq i} \exp(-\frac{|x_i - x_k|^2}{2\sigma_i^2})}$$

- Define
$$q_{j|i} = \frac{\exp(-|y_i - y_j|^2)}{\sum_{k \neq i} \exp(-|y_k - y_j|^2)}$$

- Define $C = \sum_i \sum_j p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}$, the KL Divergence

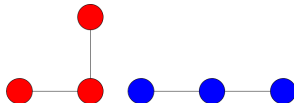
- Perform gradient descent to minimize C

SNE Algorithm: KL Divergence

- KL Divergence is asymmetric
- Nearby points (large $p_{j|i}$) weigh more than far-away points (low $p_{j|i}$)
- Objective function strongly favors preserving distances between nearby points over far away points

t-SNE Algorithm

- Use $p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}$ instead
- Use $q_{ij} = \frac{(1 + |y_i - y_j|^2)^{-1}}{\sum_{k \neq i} (1 + |y_i - y_k|^2)^{-1}}$,
the Student-t distribution
- Student-t distribution is heavy-tailed. Allows for a small probability for far-away points, forcing them to move further away in low-dim space



t-SNE: Barnes-Hut approximation

- As formulated, $O(n^2)$ algorithm

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t-SNE: Barnes-Hut approximation

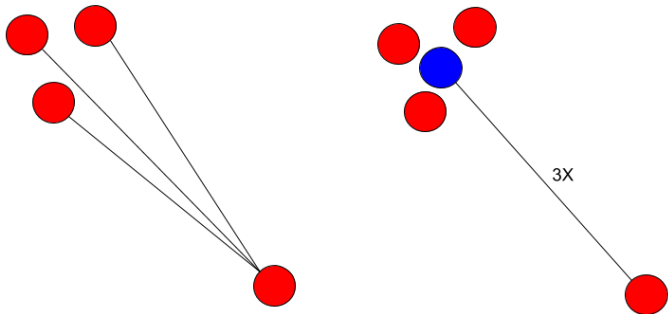
- As formulated, $O(n^2)$ algorithm
- Doesn't work for really large datasets
- What can we do to reduce the cost?
- **Insight:** Can we approximate roughly equally distance far away points?

t-SNE with Barnes-Hut approximation

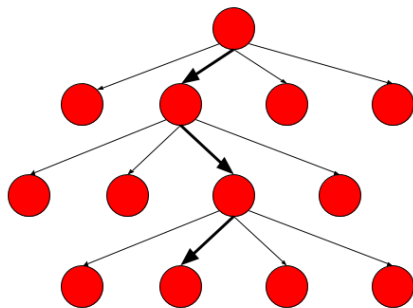
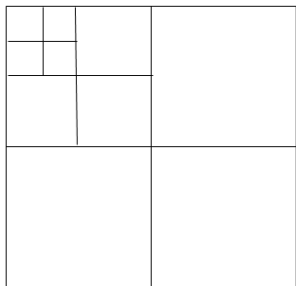
Barnes-Hut approximation

Barnes-Hut is an approximation algorithm used in Astronomy to simulate n -body problem. It uses an octree representation to model bodies in a 3-D space and recursively groups them in this octree. In 2D, we replace octree with quadtree. Converts the n^2 search into an $n \log n$ search.

Barnes-Hut Approximation



Quadtree representation



t-SNE examples: MNIST Digits

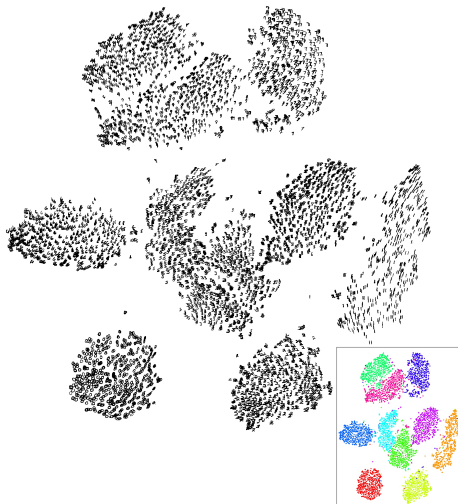


Figure: Source: Laurens van der Maaten

t-SNE examples: Words

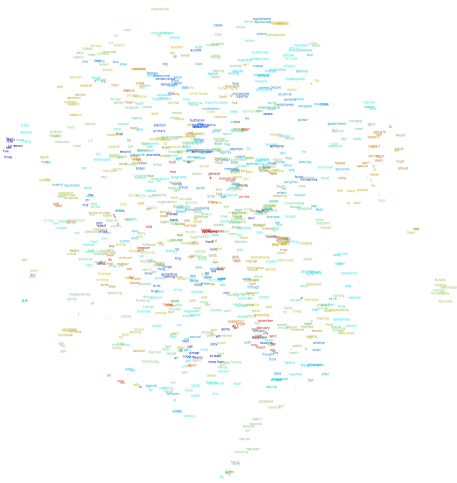


Figure: Source: Laurens van der Maaten

t-SNE Multiple Map extension

- Multiple word senses: e.g. (River, Bank, Bailout)
- In general, how do we deal with non-metric similarities?
- Extend $q_{ij} = \frac{\sum_m \pi_i^m \pi_j^m (1 + |y_i^m - y_j^m|^2)^{-1}}{\sum_k \sum_{m'} \sum_{l \neq k} (1 + |y_k^{m'} - y_l^{m'}|^2)^{-1}}$
- Now, you get multiple maps. Each map models a different similarity between words

