

# Data Visualization

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March 26, 2018

# 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

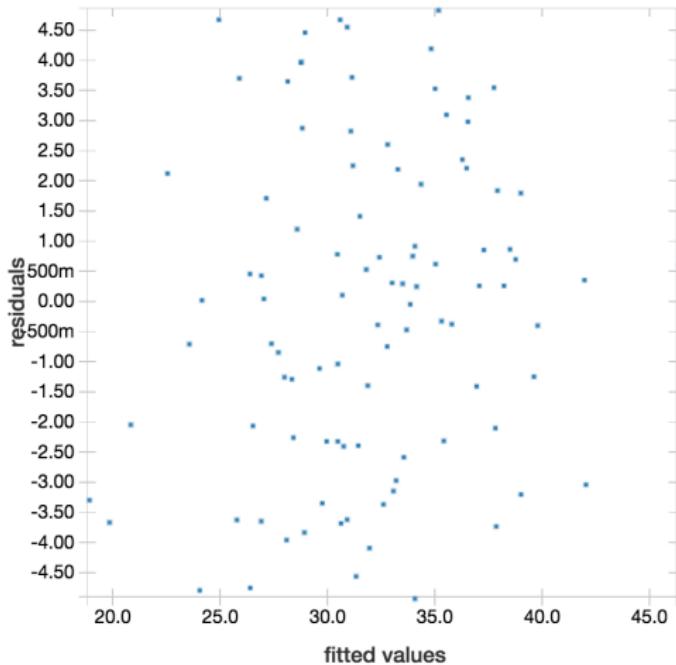


Figure: Source - Databricks blog

# Plotting Residuals: Systematic errors in prediction

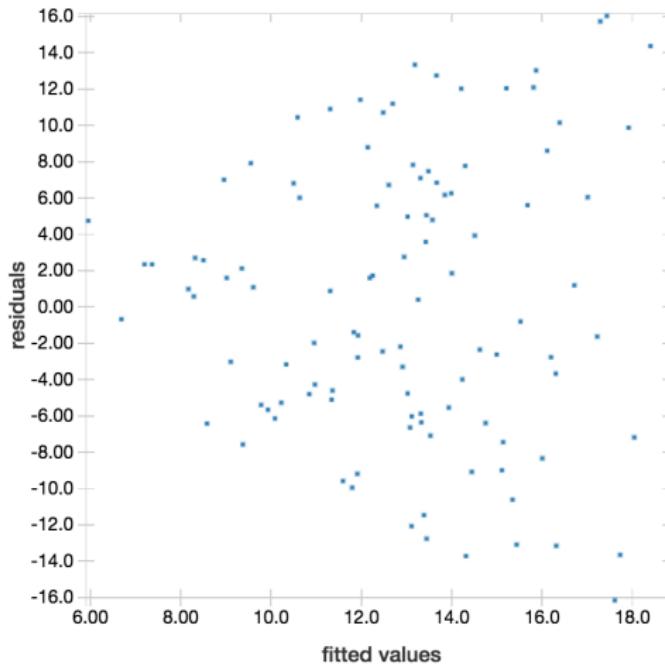


Figure: Source - Databricks blog

# Visualizing KMeans fit

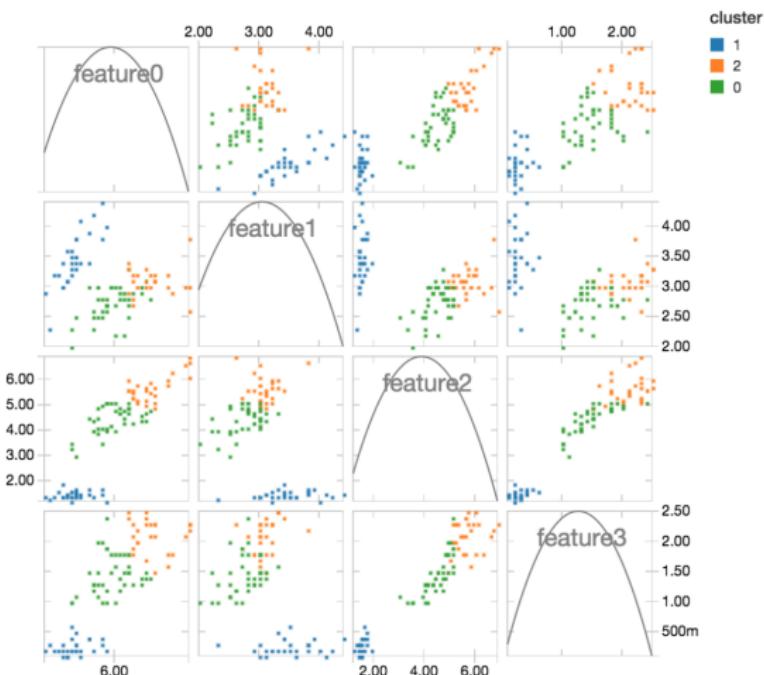
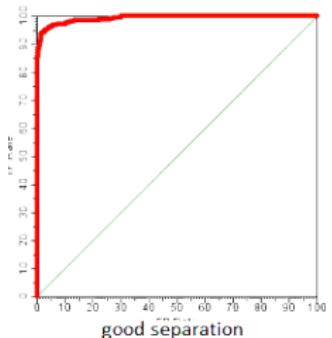
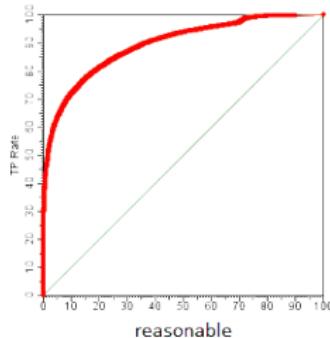


Figure: Source - Databricks blog

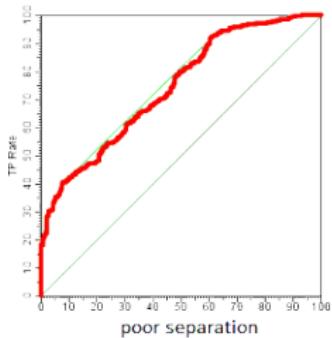
# ROC Curve examples



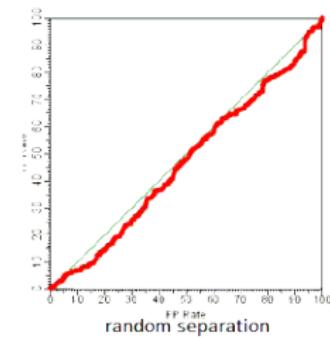
good separation



reasonable



poor separation



random separation

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

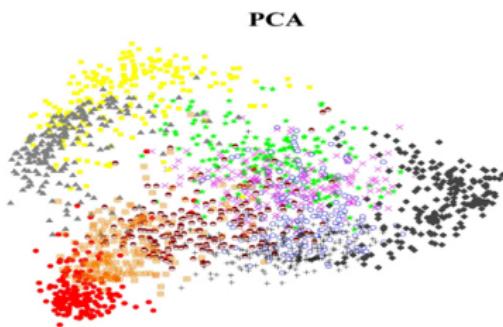


Figure: Source: Xiaofei He

# ISOMAP

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

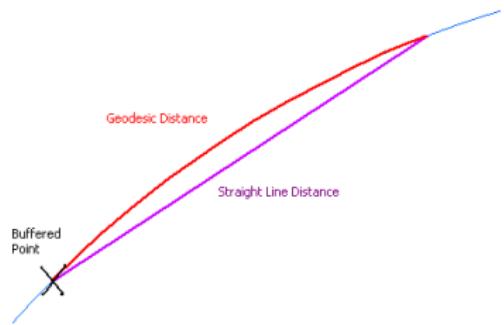


Figure: Source: ESRI

# Locally Linear Embedding

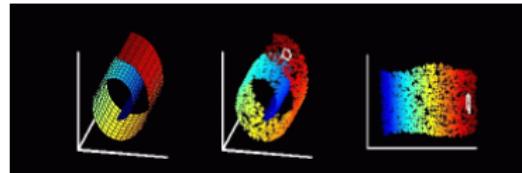


Figure: Source: Roweis and Saul

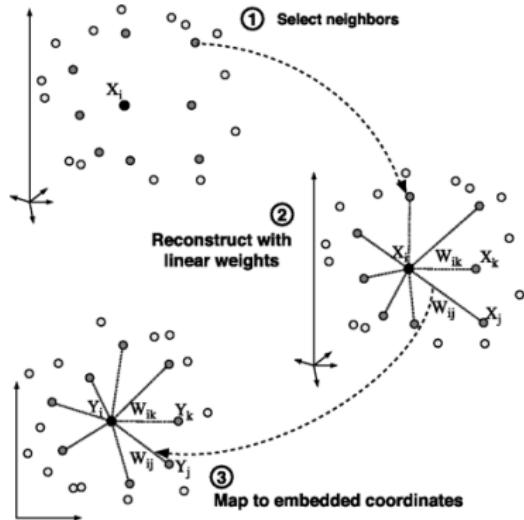


Figure: Source: Roweis and Saul

# SNE Algorithm

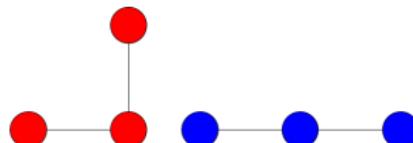
- Similar to LLE but use probabilities instead of distances
- Compute  $p_{j|i}$ , conditional probability that  $x_i$  would pick  $x_j$  as neighbor under a locally modeled pdf
- Formally 
$$p_{j|i} = \frac{\exp(-\frac{|x_i - x_j|^2}{2\sigma_i^2})}{\sum_{k \neq i} \exp(-\frac{|x_i - x_k|^2}{2\sigma_i^2})}$$
- 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 ( $\text{large } p_{j|i}$ ) weigh more than far-away points ( $\text{low } p_{j|i}$ )
- 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



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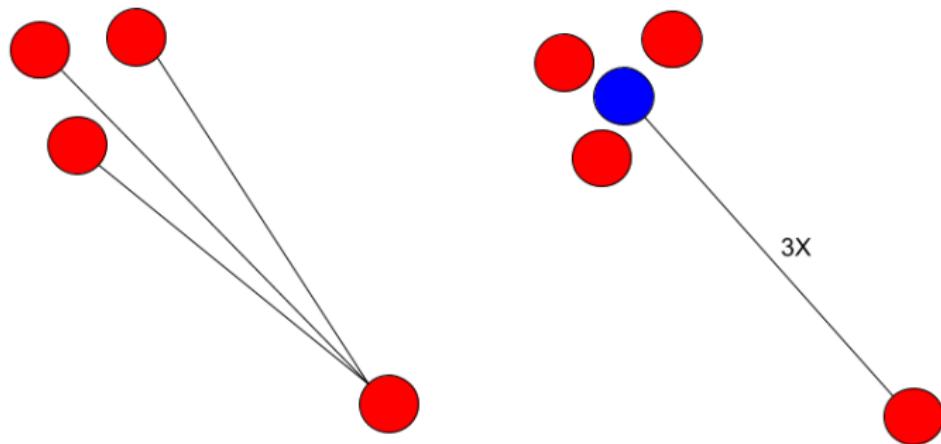
- As formulated,  $O(n^2)$  algorithm
- Doesn't work for really large datasets
- What can we do to reduce the cost?
- **Insight:** Can we approximate roughly equally distance far away points?

# t-SNE with Barnes-Hut approximation

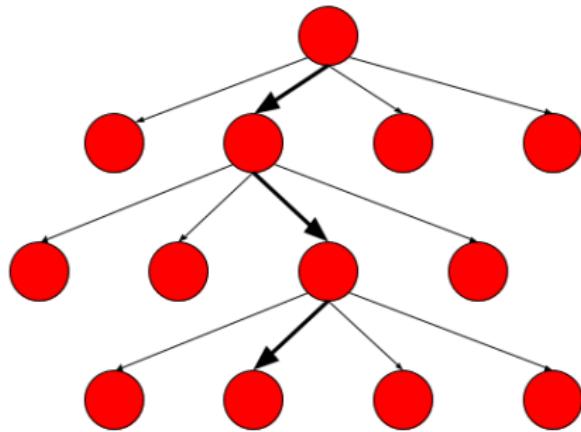
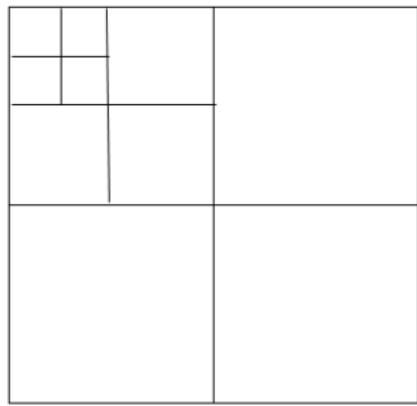
## Barnes-Hut approximation

Barnes-Hut is an approximation algorithm used in Astronomy to simulate n-body problem. It uses a 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

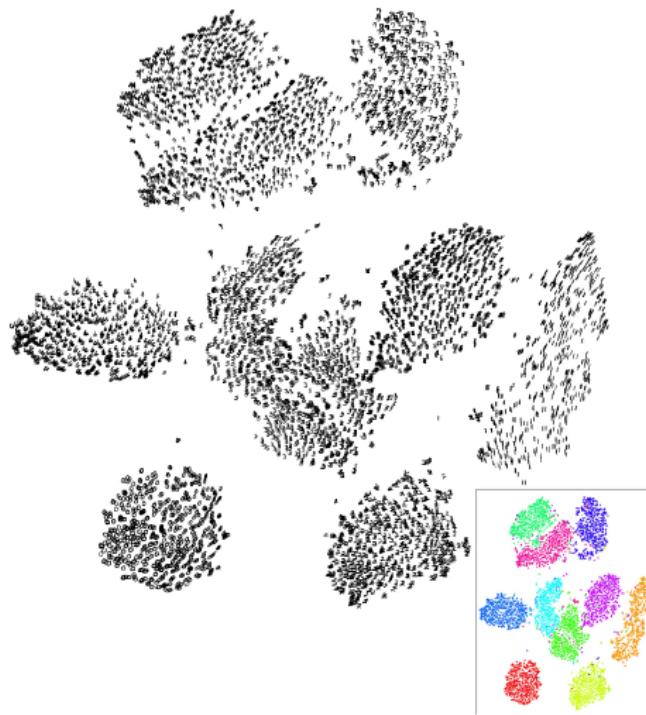


Figure: Source: Laurens van der Maaten

## t-SNE examples: Netflix movies



**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

A word cloud visualization centered around the phrase "thank you". The word "thank" is at the bottom center in red, "you" is to its right in green, and "thank you" is repeated above it in large blue. Numerous other words in different colors (blue, red, green, yellow, orange) represent the phrase in various languages. Some examples include "спасибо" (blue), "obrigado" (green), "dziekuje" (yellow), "bedankt" (orange), "merci" (red), "gracias" (green), "tesekkür ederim" (blue), "ngiyabonga" (blue), "go raibh maith agat" (purple), "dakujem" (red), and "mercs" (red). The background is white.