CPSC 340:
Machine Learning and Data Mining

Nonlinear Dimensionality Reduction

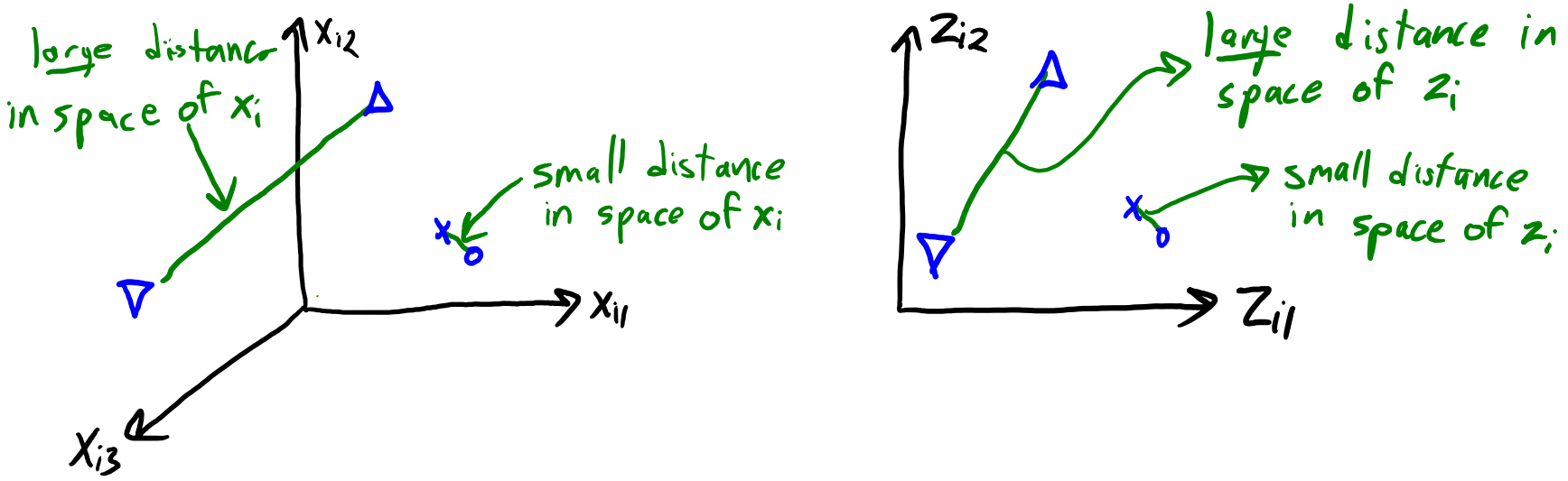
Last week: non-negative matrix factorization

- Another example instead of faces
- You have ‘n’ movies and a review for each movie
  - You use ‘d’ bag-of-word features for the reviews
  - So ‘X’ has size n-by-d
- You want to find “topics” in the reviews (features for the movies)
- You can use NMF for this
  - Interpretation of W: k topics, each with a selection of words
  - Interpretation of Z: each movie is a mixture of the k topics
- NMF makes much more sense than PCA
  - Each topic involves a small number of words
  - Each review has a small number of topics
- PCA would not make sense
  - you could have negative inclusion of a topic for a movie
  - Topics and have negative words
  - all movies are a mixture of every possible topic and all topics involve every possible word
- So here we like the sparsity and the non-negativity

Last Time: Multi-Dimensional Scaling

- Multi-dimensional scaling (MDS):
  - Non-parametric visualization: directly optimize the z_i locations.

$$f(Z) = \sum_{i=1}^{n} \sum_{j=i+1}^{n} d_3(d_2(z_i, z_j) - d_1(x_i, x_j))$$



  - Traditional MDS methods lead to a "crowding" effect.

Different MDS Cost Functions

- MDS default objective: squared difference of Euclidean norm:

$$f(Z) = \sum_{i=1}^{n} \sum_{j=i+1}^{n} \left(\|z_i - z_j\| - \|x_i - x_j\| \right)^2$$

- But we can make z_i match different distances/similarities:

$$f(Z) = \sum_{i=1}^{n} \sum_{j=i+1}^{n} d_3(d_2(z_i, z_j) - d_1(x_i, x_j))$$

  - d_1 is the high-dimensional distance we want to match.
  - d_2 is the low-dimensional distance we can control.
  - d_3 controls how we compare high-/low-dimensional distances.
  - the functions d_1, d_2, d_3 are not necessarily the same

Classic Multi-Dimensional Scaling (MDS)

- MDS default objective function with general distances/similarities:

$$f(Z) = \sum_{i=1}^{n} \sum_{j=i+1}^{n} d_3(d_2(z_i, z_j) - d_1(x_i, x_j))$$

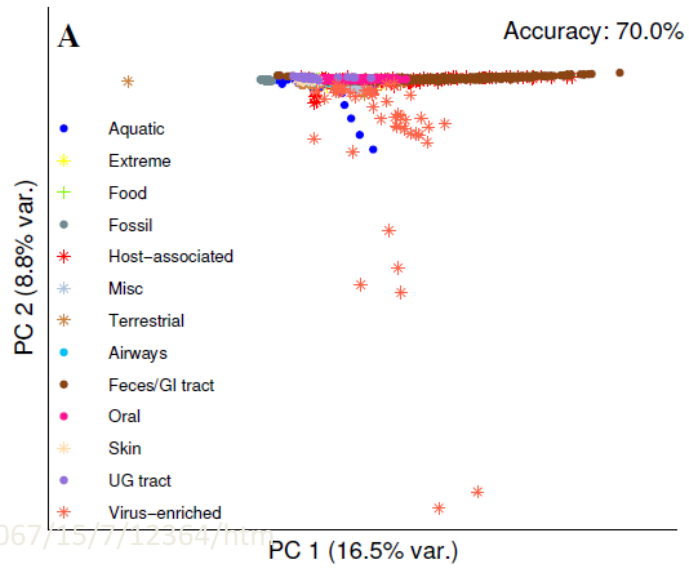
- "Classic" MDS uses $d_1(x_i,x_j) = x_i^T x_j$ and $d_2(z_i,z_j) = z_i^T z_j$.
  - We obtain PCA in this special case (for centered x_i).
  - Not a great choice because it's a linear model.

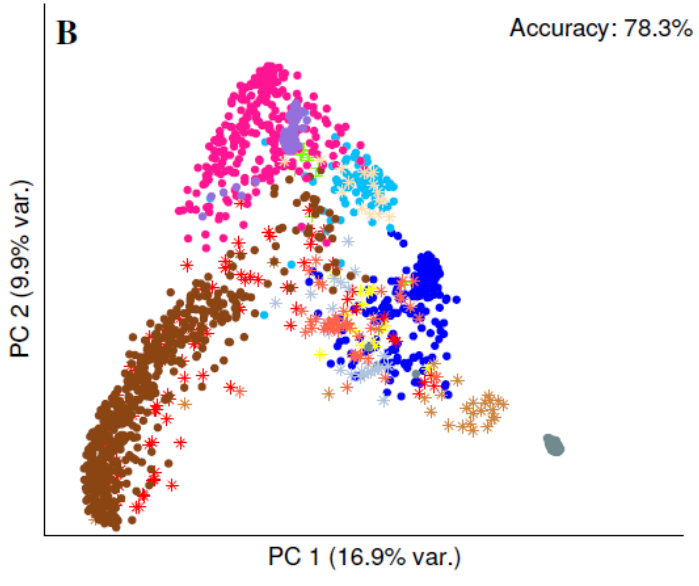
Non-Euclidean Multi-Dimensional Scaling (MDS)

- MDS default objective function with general distances/similarities:

$$f(Z) = \sum_{i=1}^{n} \sum_{j=i+1}^{n} d_3(d_2(z_i, z_j) - d_1(x_i, x_j))$$

- Another possibility: $d_1(x_i,x_j) = ||x_i - x_j||_1$ and $d_2(z_i,z_j) = ||z_i - z_j||$.
  - The z_i approximate the high-dimensional L_1-norm distances.





Sammon's Mapping

- Challenge for most MDS models: they focus on large distances.
  - Leads to "crowding" effect like with PCA.
- Early attempt to address this is Sammon's mapping:
  - Weighted MDS so large/small distances more comparable.

$$f(Z) = \sum_{i=1}^{n} \sum_{j=i+1}^{n} \left(\frac{d_2(z_i, z_j) - d_1(x_i, x_j)}{d_1(x_i, x_j)} \right)^2$$

  - Denominator reduces focus on large distances.

Sammon's Mapping

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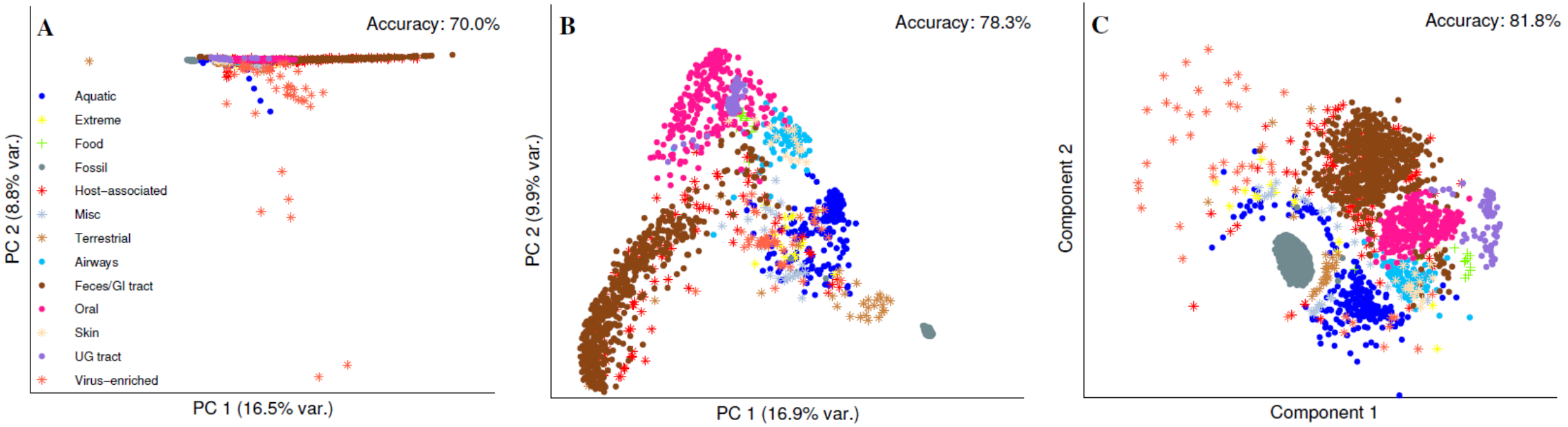
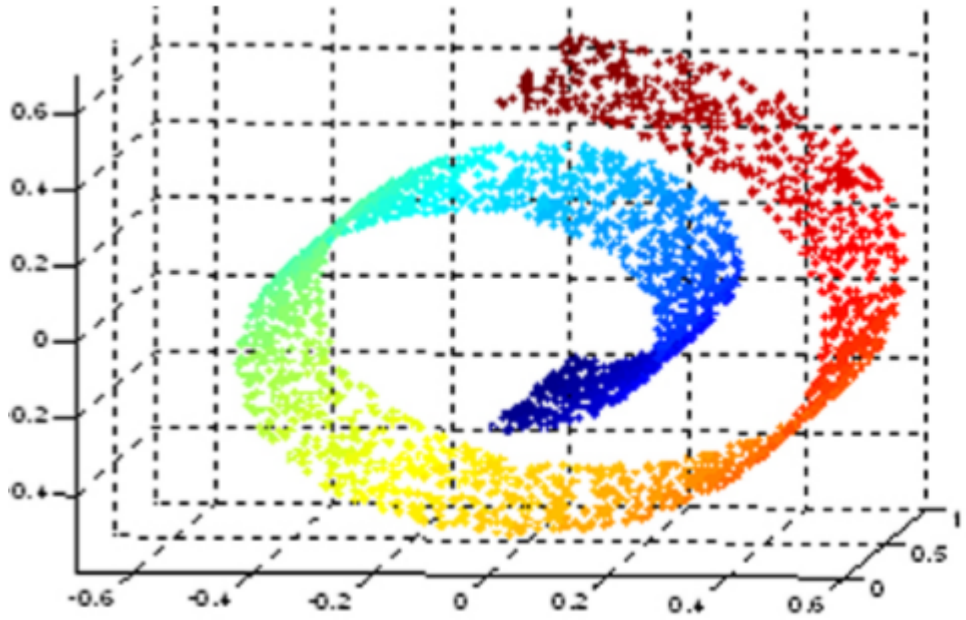


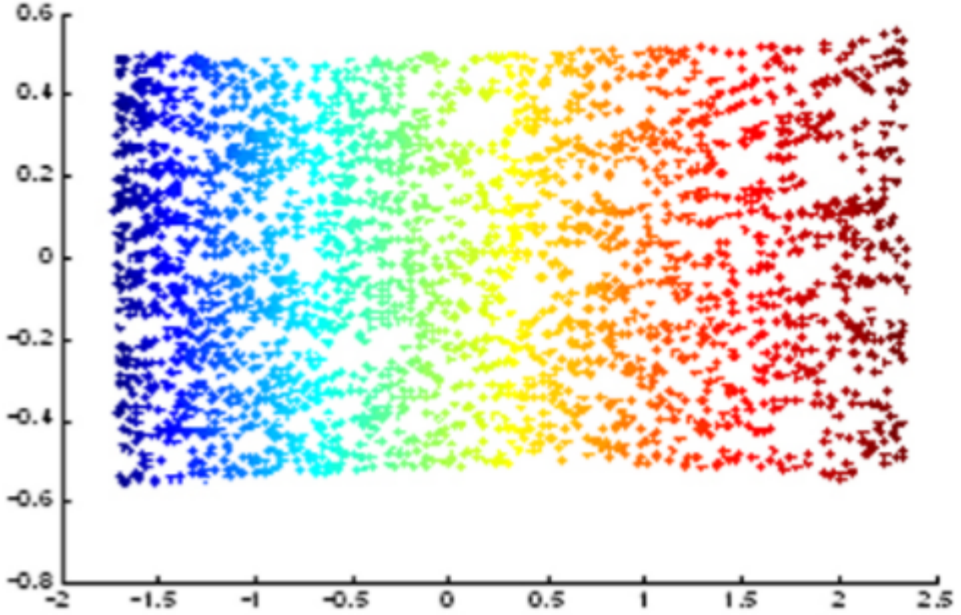
Learning Manifolds

- Consider data that lives on a low-dimensional “manifold”.
- Example is the ‘Swiss roll’:

Original data



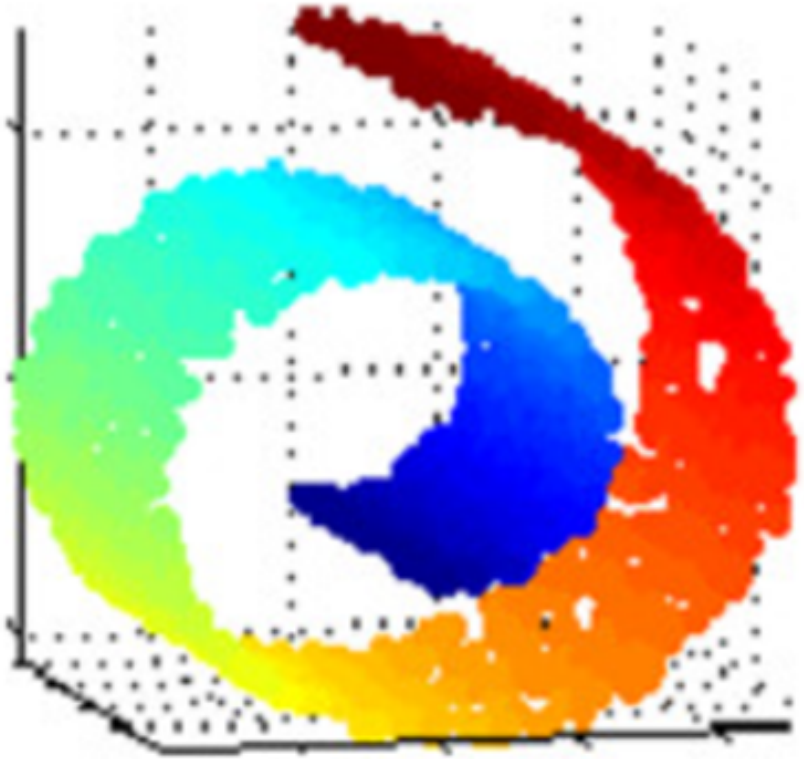
Two-dimensional manifold



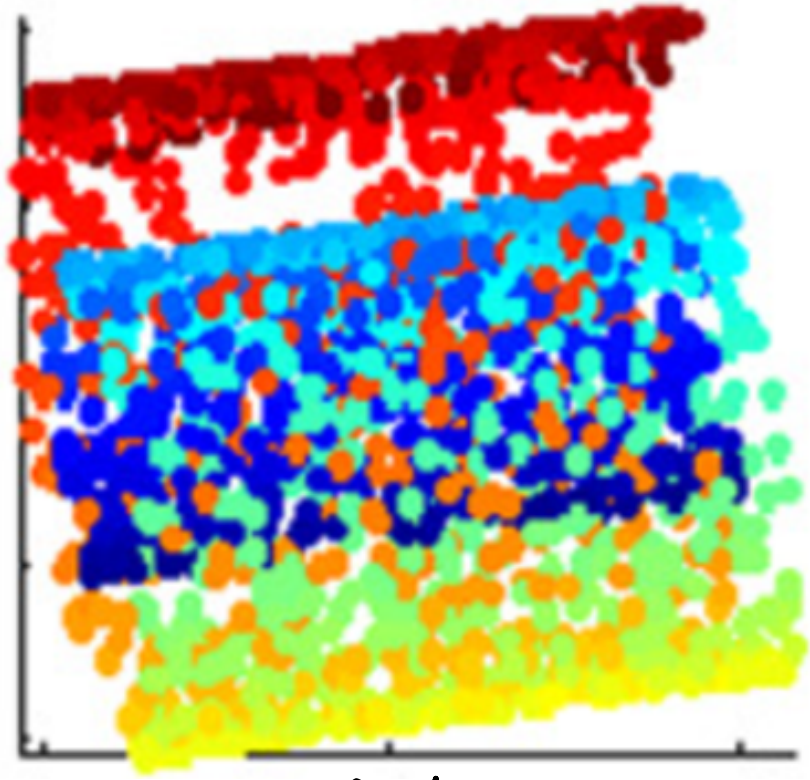
http://www.biomedcentral.com/content/pdf/1471-2105-13-S7-S3.pdf

Learning Manifolds

- Consider data that lives on a low-dimensional "manifold".
  - With usual distances, PCA/MDS will not discover non-linear manifolds.



Original data

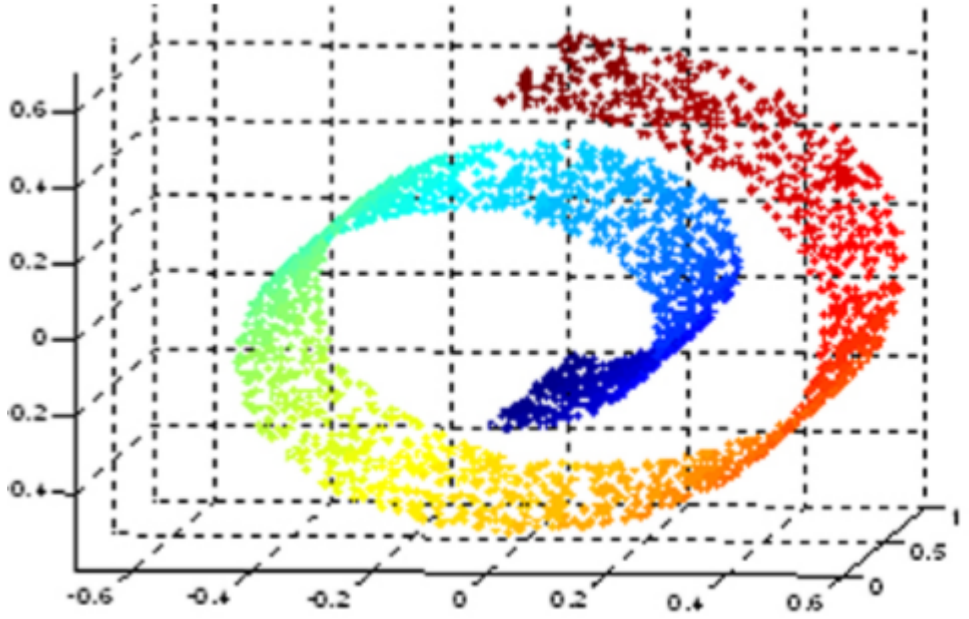


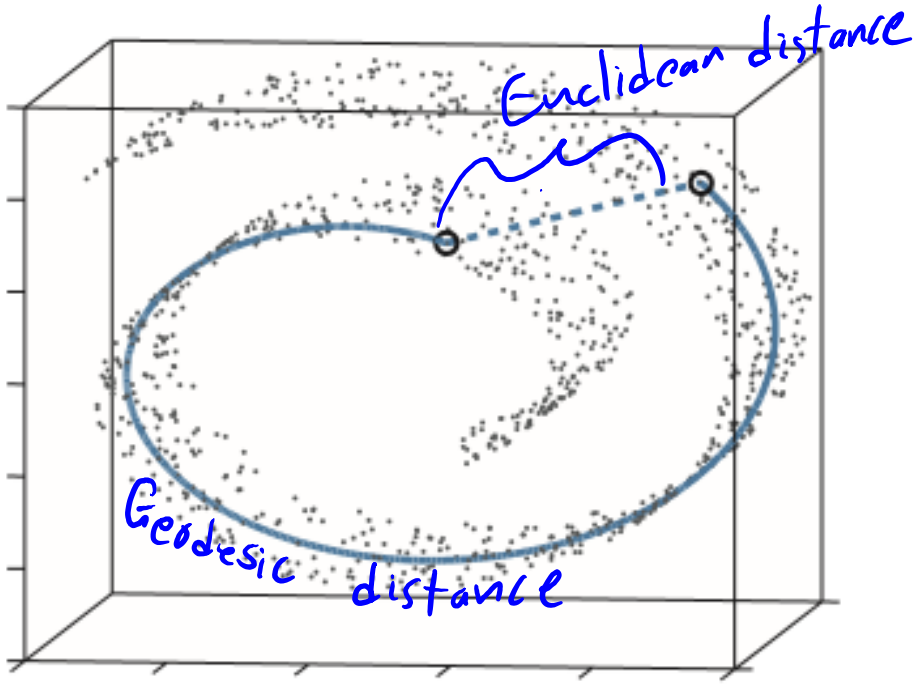
PCA

http://www.peh-med.com/content/9/1/12/figure/F1

Learning Manifolds

- Consider data that lives on a low-dimensional "manifold".
  - With usual distances, PCA/MDS will not discover non-linear manifolds.
- We need geodesic distance: the distance *through* the manifold.

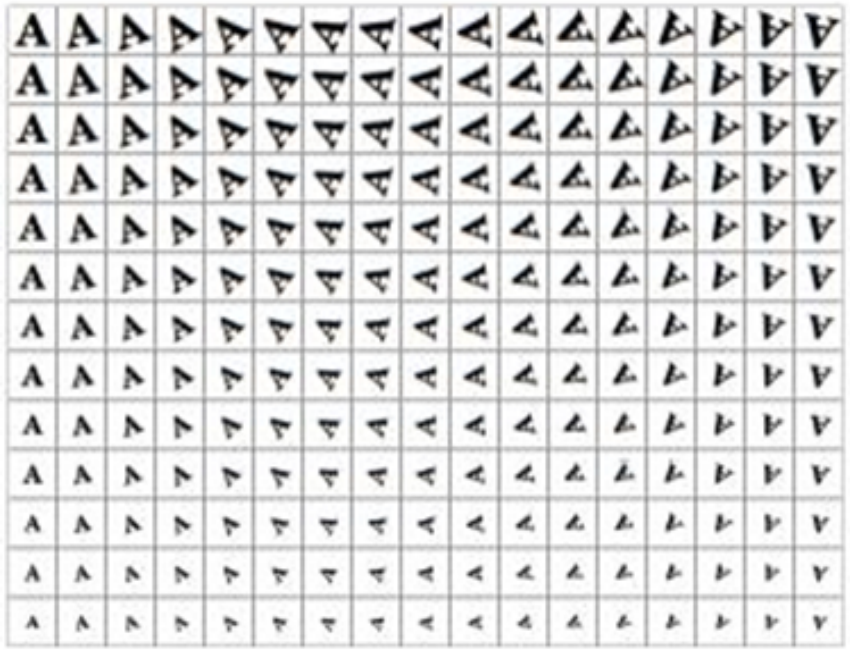




http://www.biomedcentral.com/content/pdf/1471-2105-13-S7-S3.pdf
http://wearables.cc.gatech.edu/paper_of_week/isomap.pdf

Manifolds in Image Space

- Consider slowly-varying transformation of image:

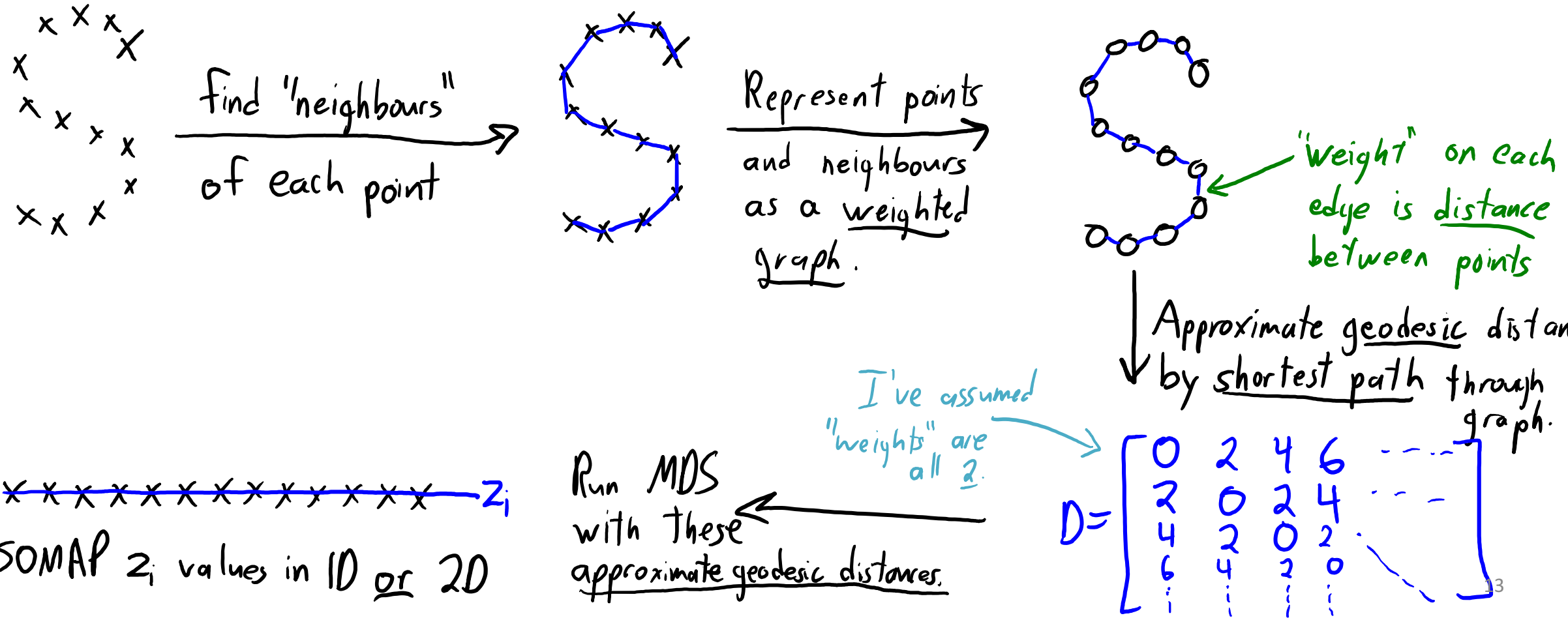


- Images are on a manifold in the high-dimensional space.
  - Euclidean distance doesn't reflect manifold structure.
  - Geodesic distance is distance through space of rotations/resizings.

https://en.wikipedia.org/wiki/Nonlinear_dimensionality_reduction

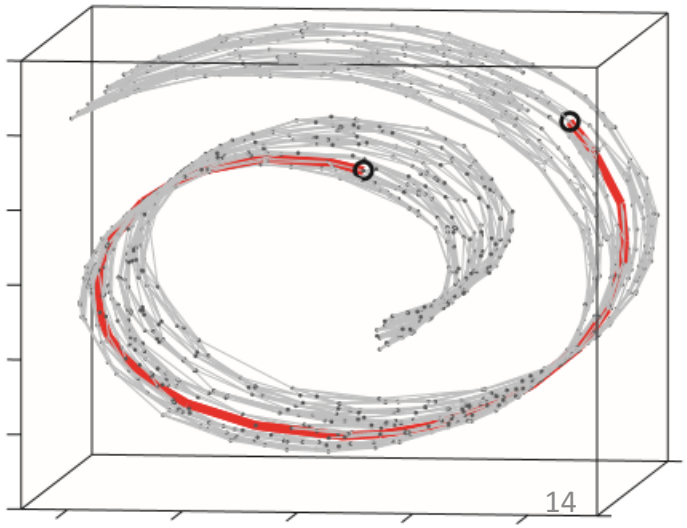
ISOMAP

- ISOMAP is latent-factor model for visualizing data on manifolds:



ISOMAP

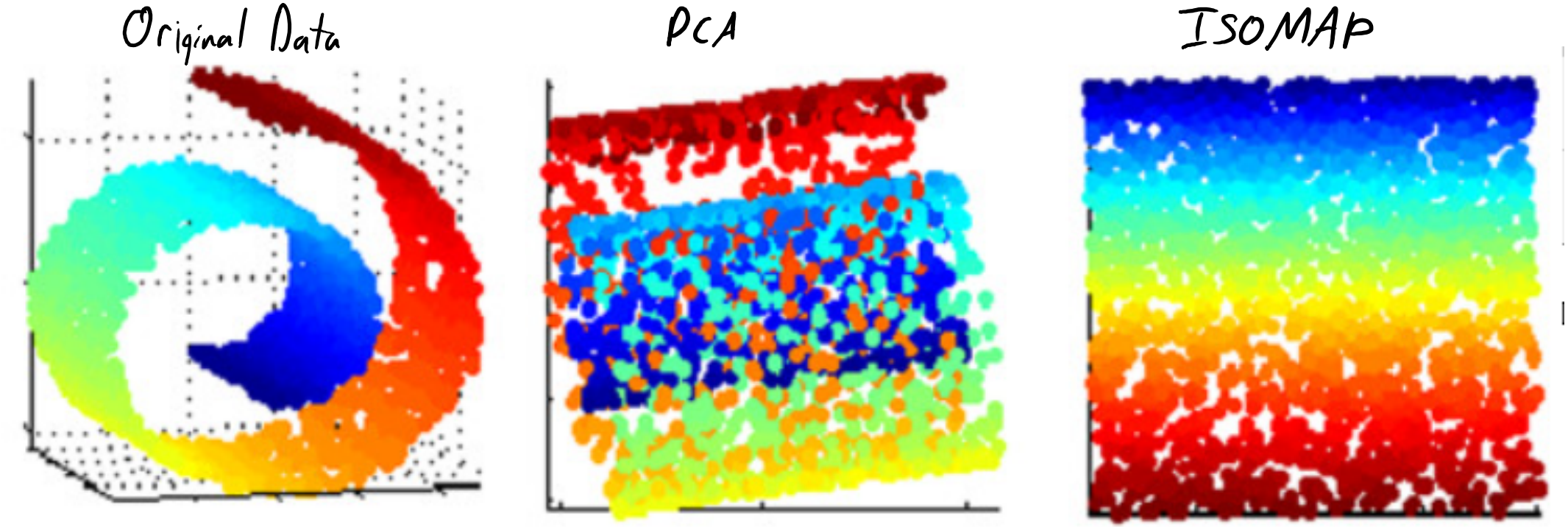
- ISOMAP is latent-factor model for visualizing data on manifolds:
  1. Find the neighbours of each point.
     - Either “k-nearest neighbours graph”, or points within a radius ‘r’.
  2. Compute edge weights:
     - Usually distance between neighbours.
  3. Compute weighted shortest path between all points.
  4. Run MDS using these distances.



K-nearest neighbour graph:
- Find KNN for every point x_i
- "Or"-version: take edge i–j if x_i is neighbour of x_j or vice versa.
- "And"-version: x_i and x_j must be KNNs of each other.

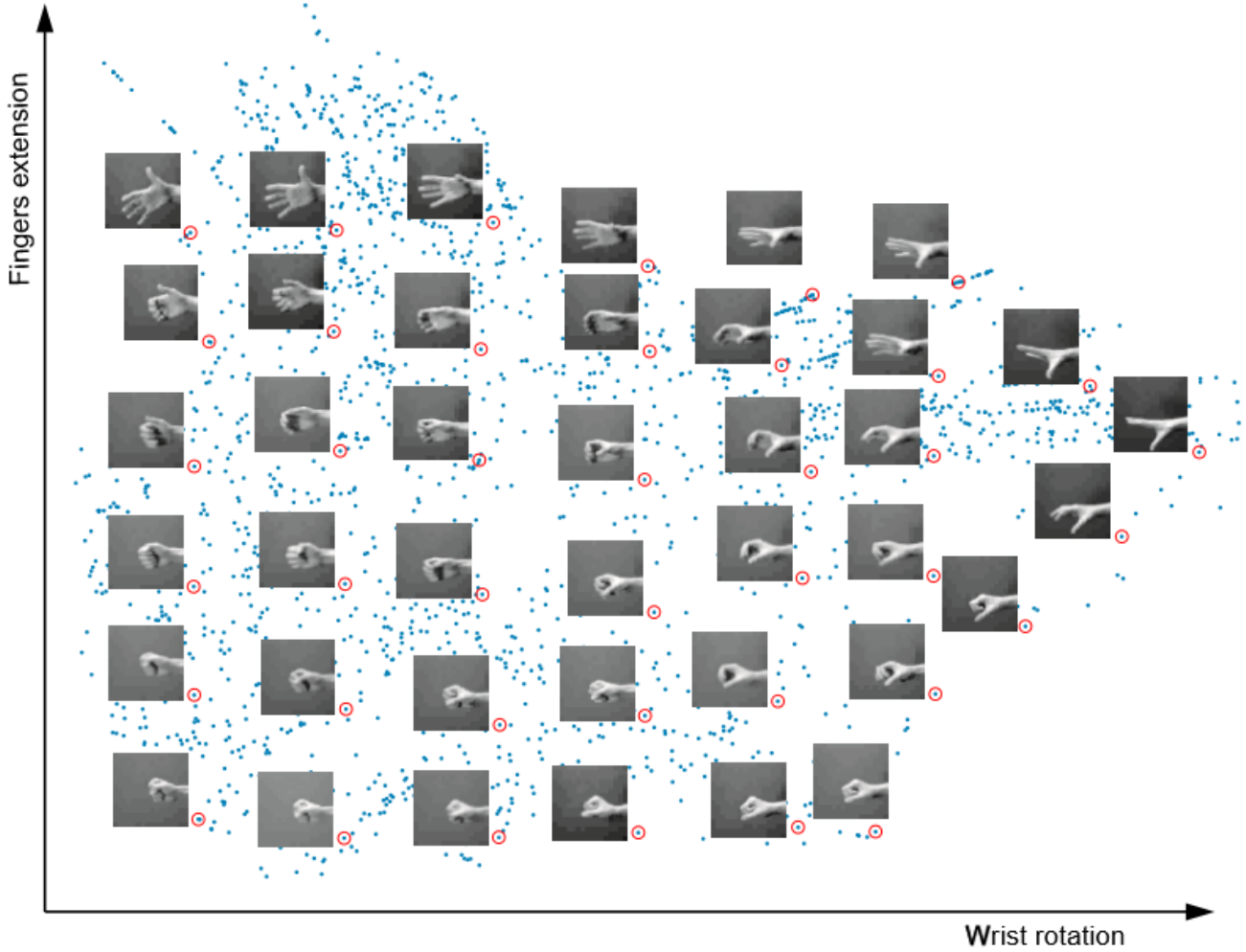
ISOMAP

- ISOMAP can "unwrap" the roll:
  - Shortest paths are approximations to geodesic distances.



- Sensitive to having the right graph:
  - Points off of manifold and gaps in manifold cause problems.

ISOMAP on Hand Images

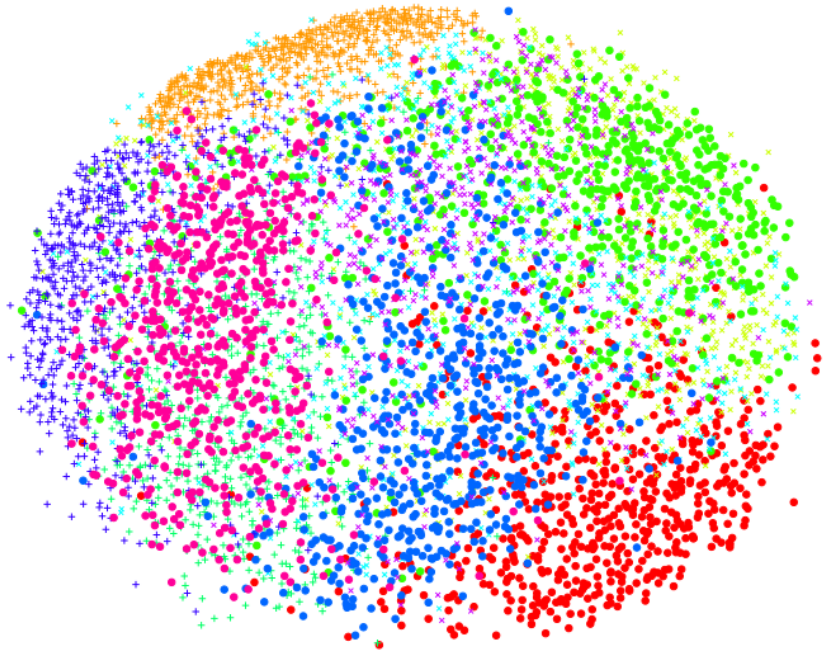


- Related method is “local linear embedding”.

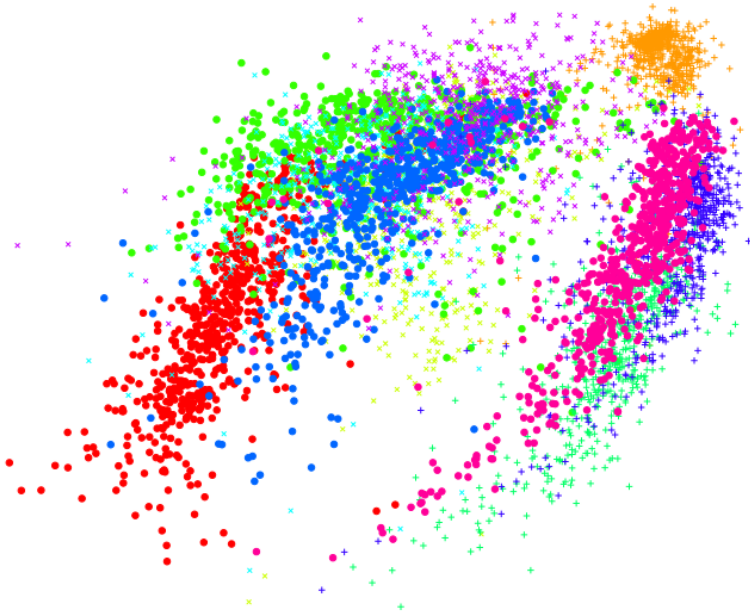
http://wearables.cc.gatech.edu/paper_of_week/isomap.pdf

Sammon's Map vs. ISOMAP vs. PCA

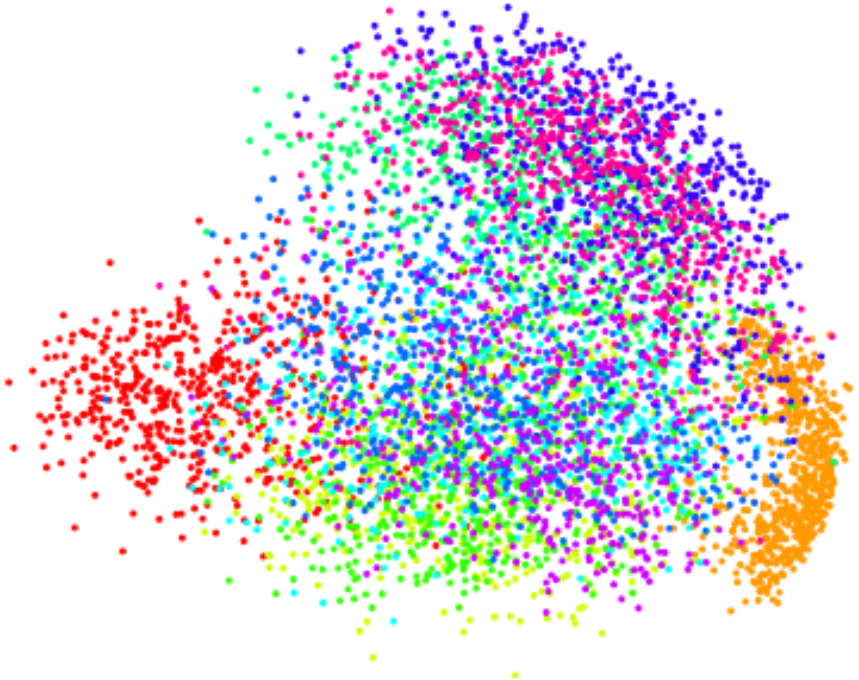
Sammon Map



ISOMAP

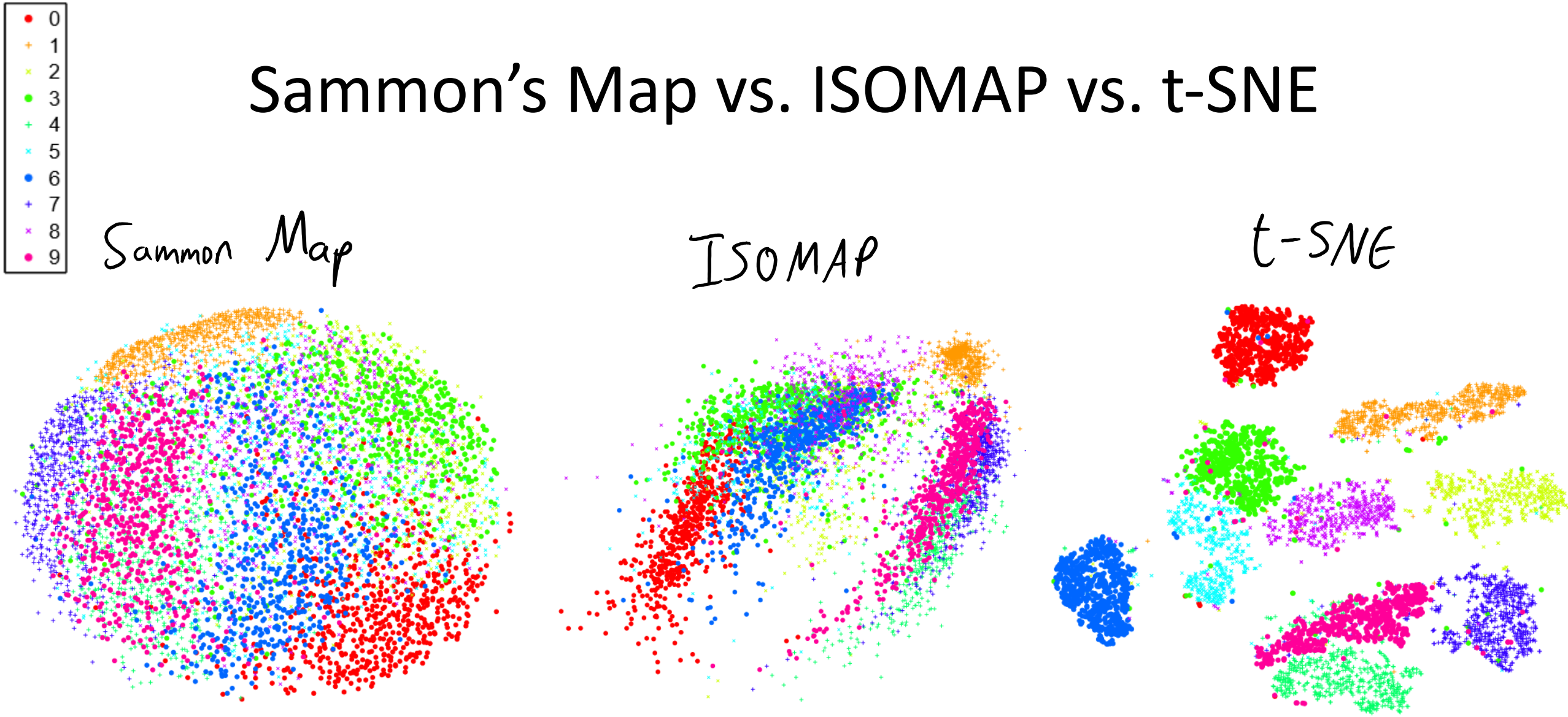


PCA



http://lvdmaaten.github.io/publications/papers/JMLR_2008.pdf

Sammon's Map vs. ISOMAP vs. t-SNE



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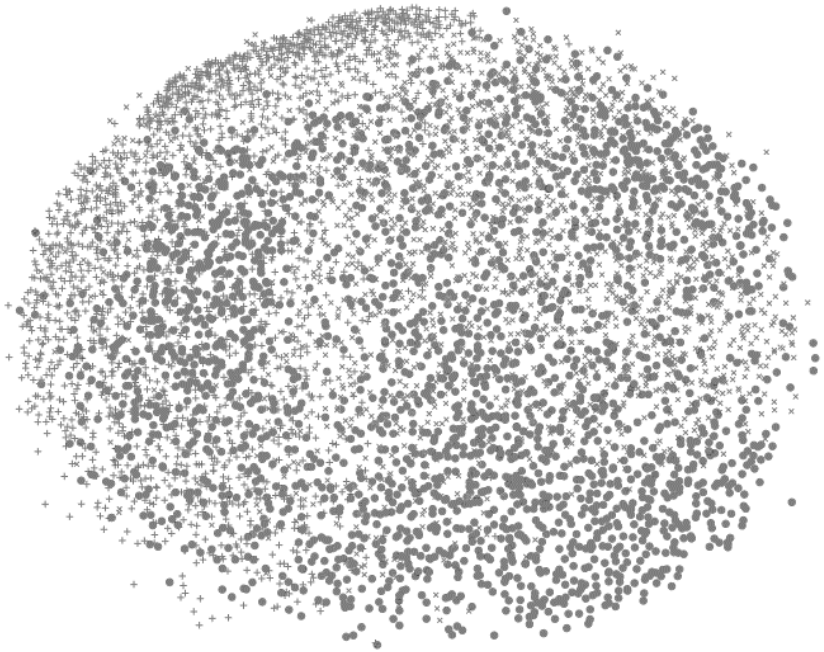
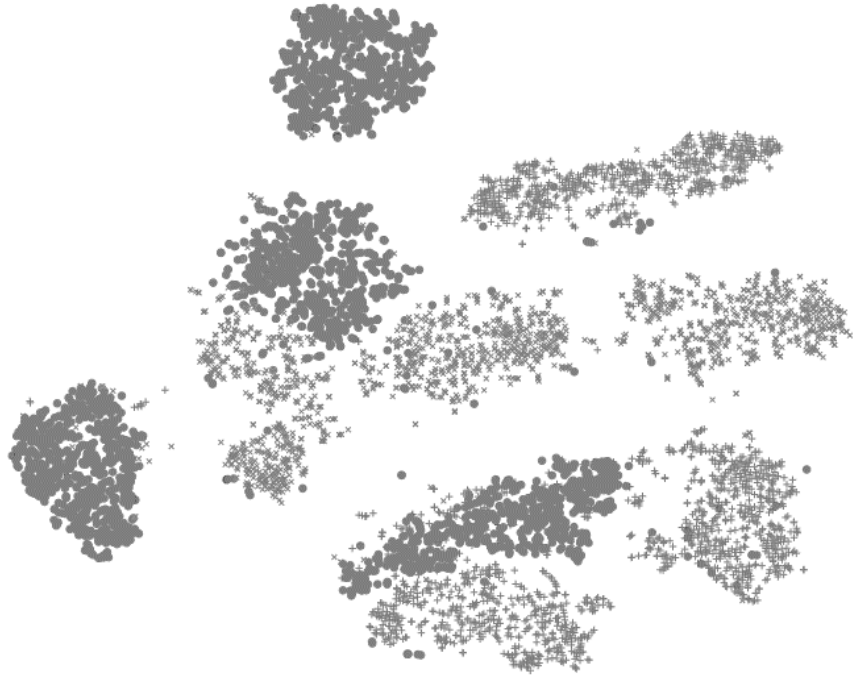
Sammon's Map vs. ISOMAP vs. t-SNE

Sammon Map



ISOMAP

t-SNE



Remember this is unsupervised, algorithms do not know the labels.

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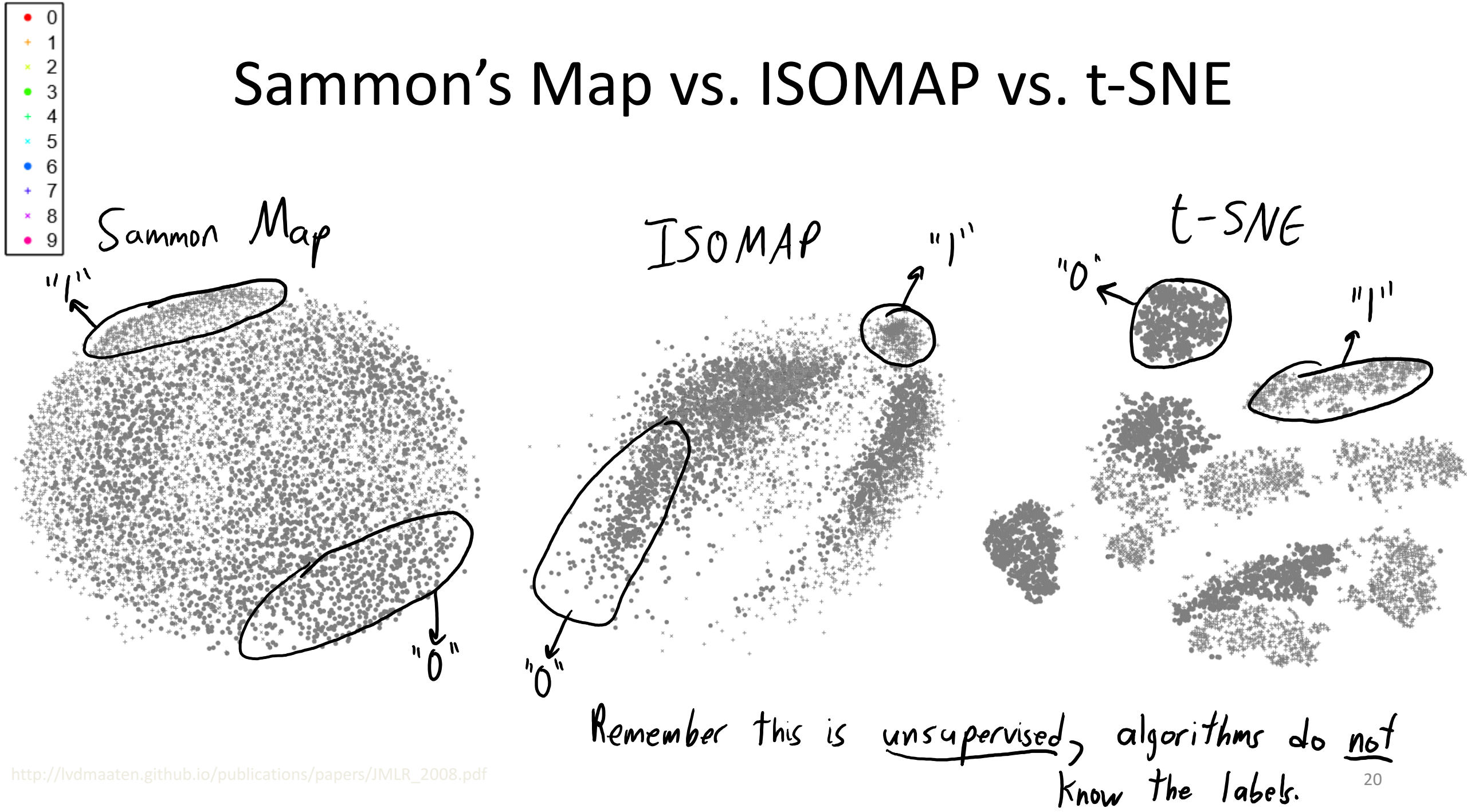
Sammon's Map vs. ISOMAP vs. t-SNE



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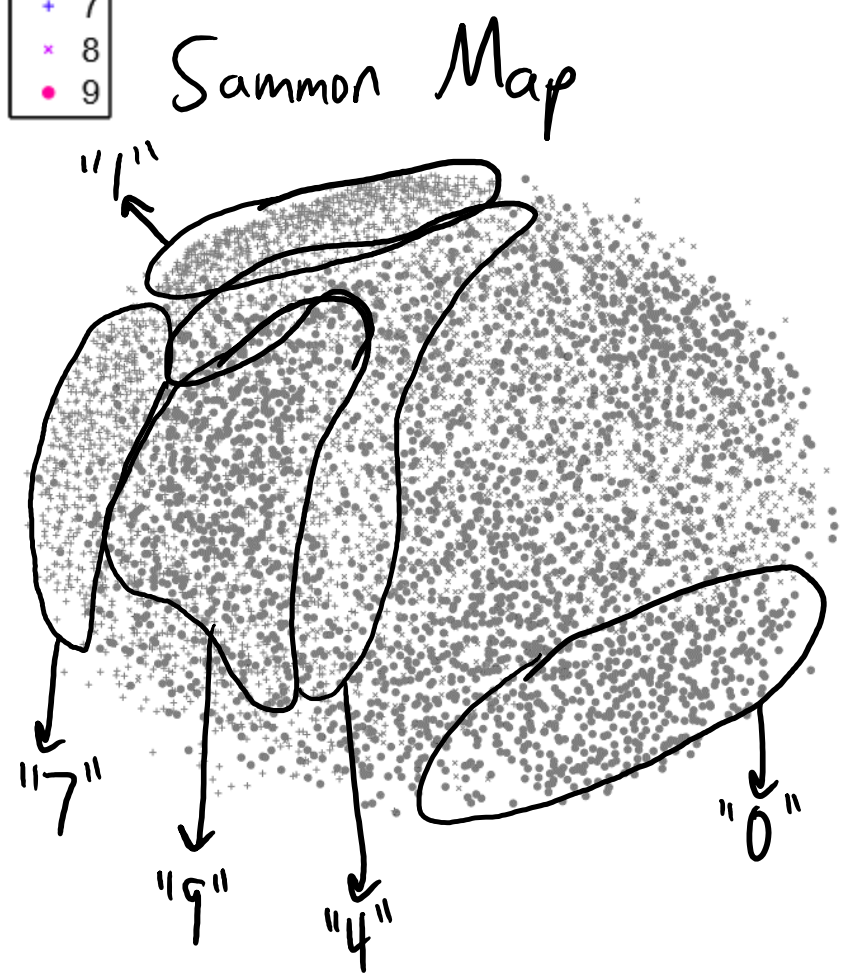

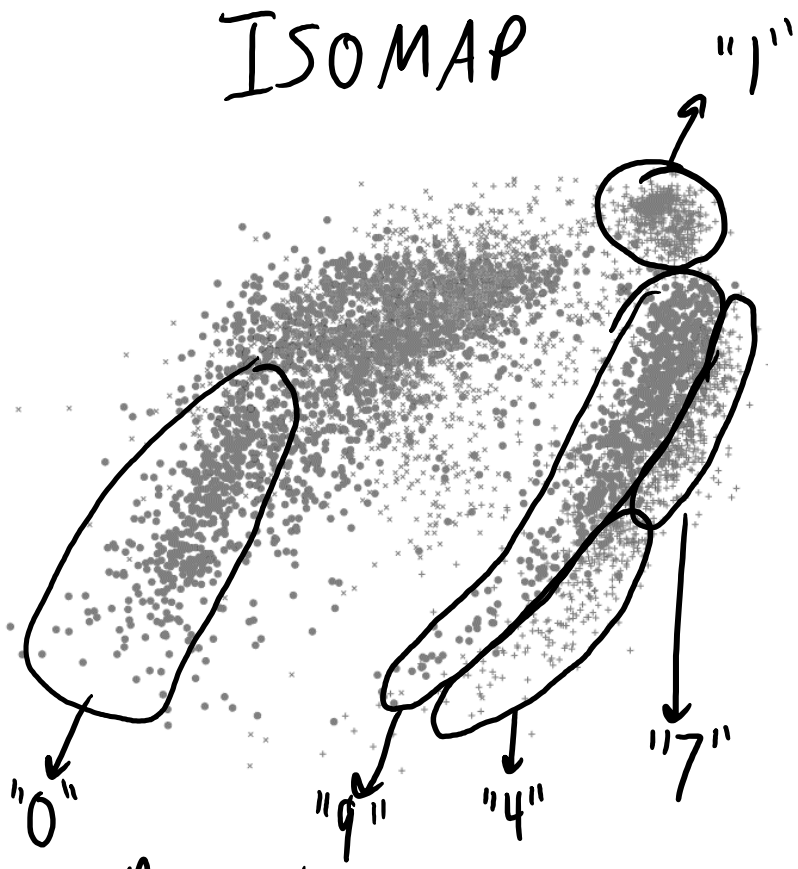

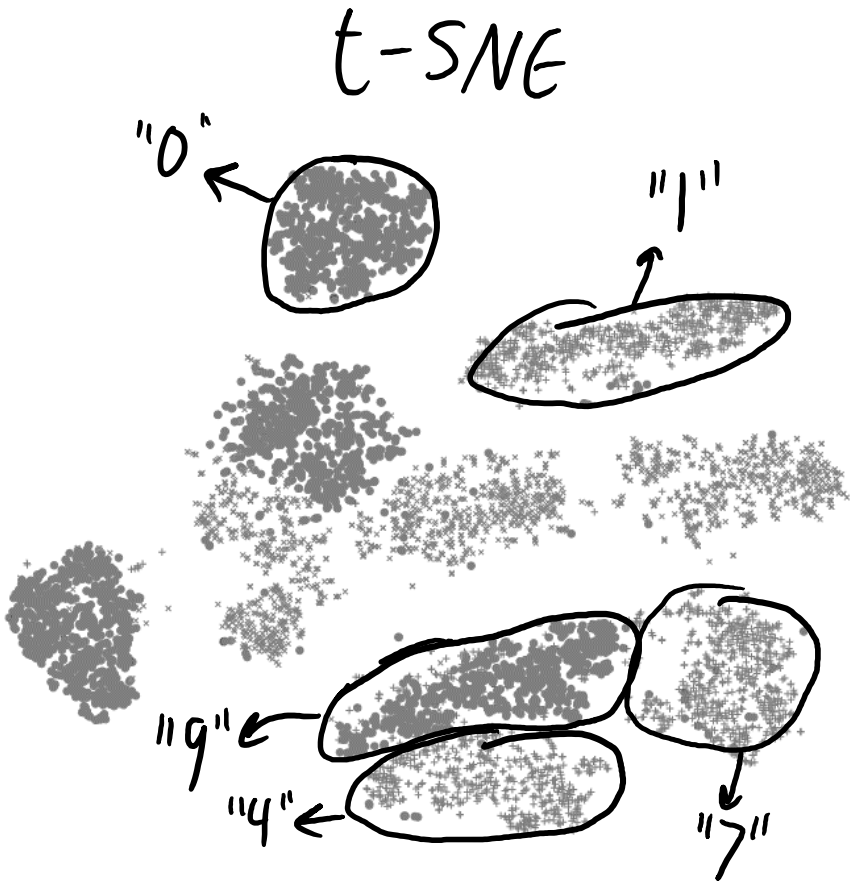

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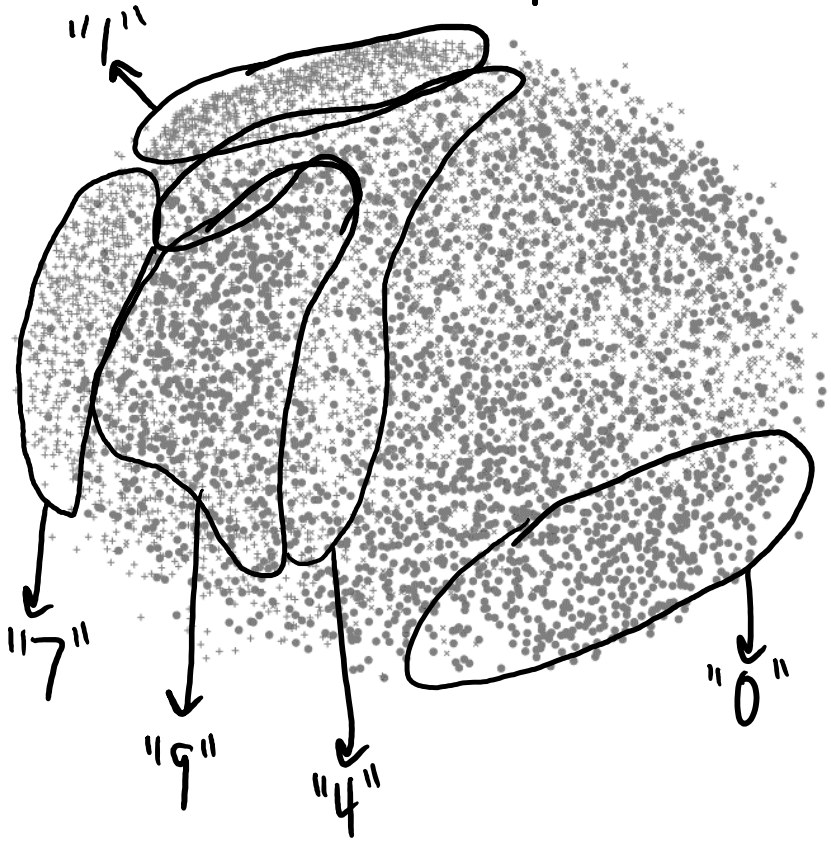
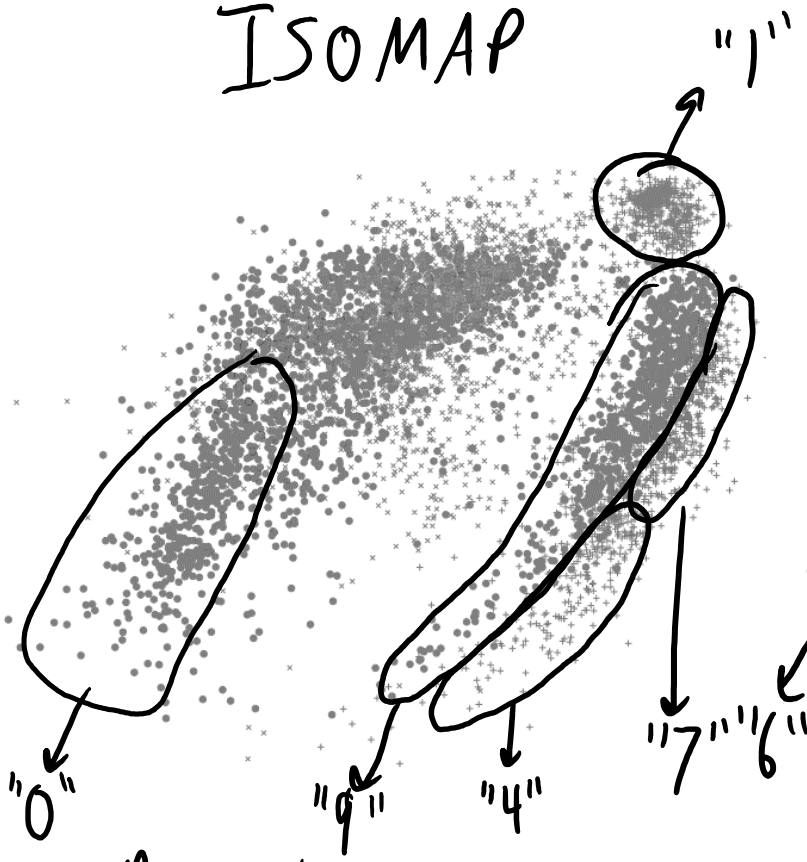
Sammon's Map vs. ISOMAP vs. t-SNE

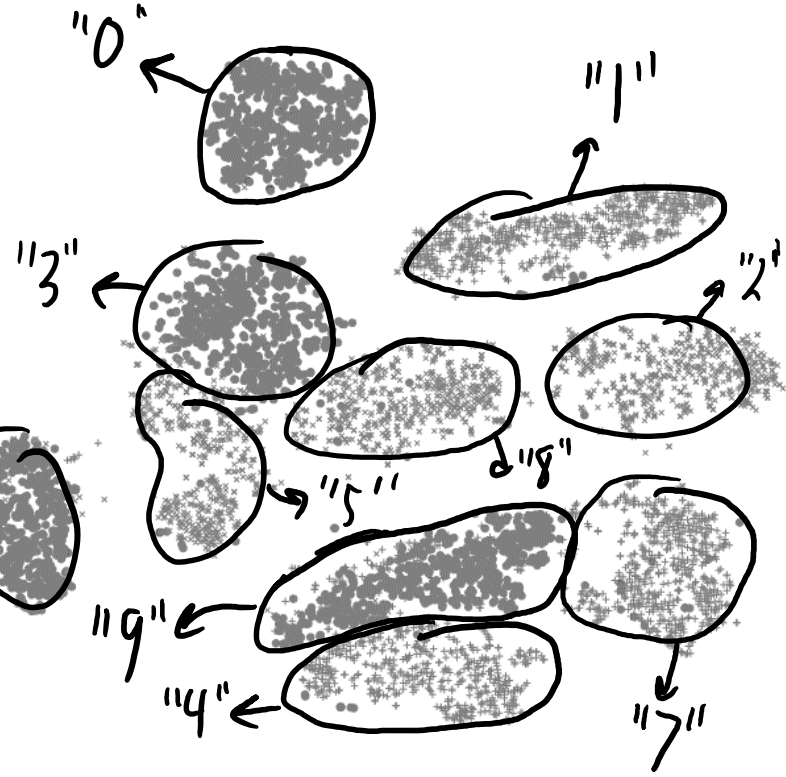
Sammon Map



ISOMAP



t-SNE



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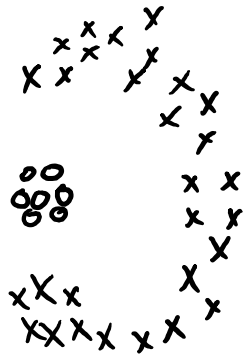
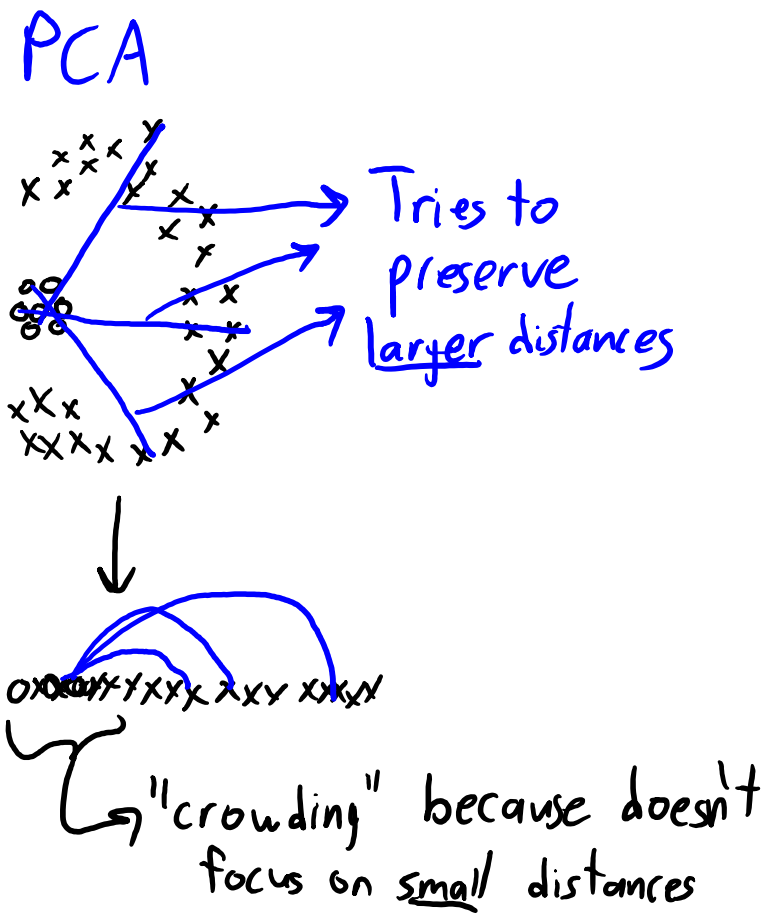
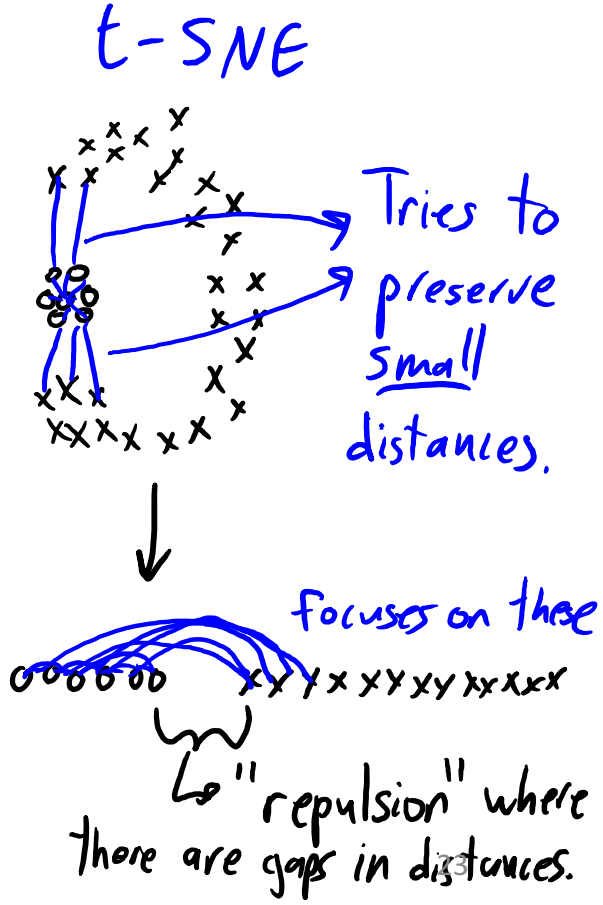
t-Distributed Stochastic Neighbour Embedding

- One key idea in t-SNE:
  - Focus on small distances by allowing large variance in large distances.







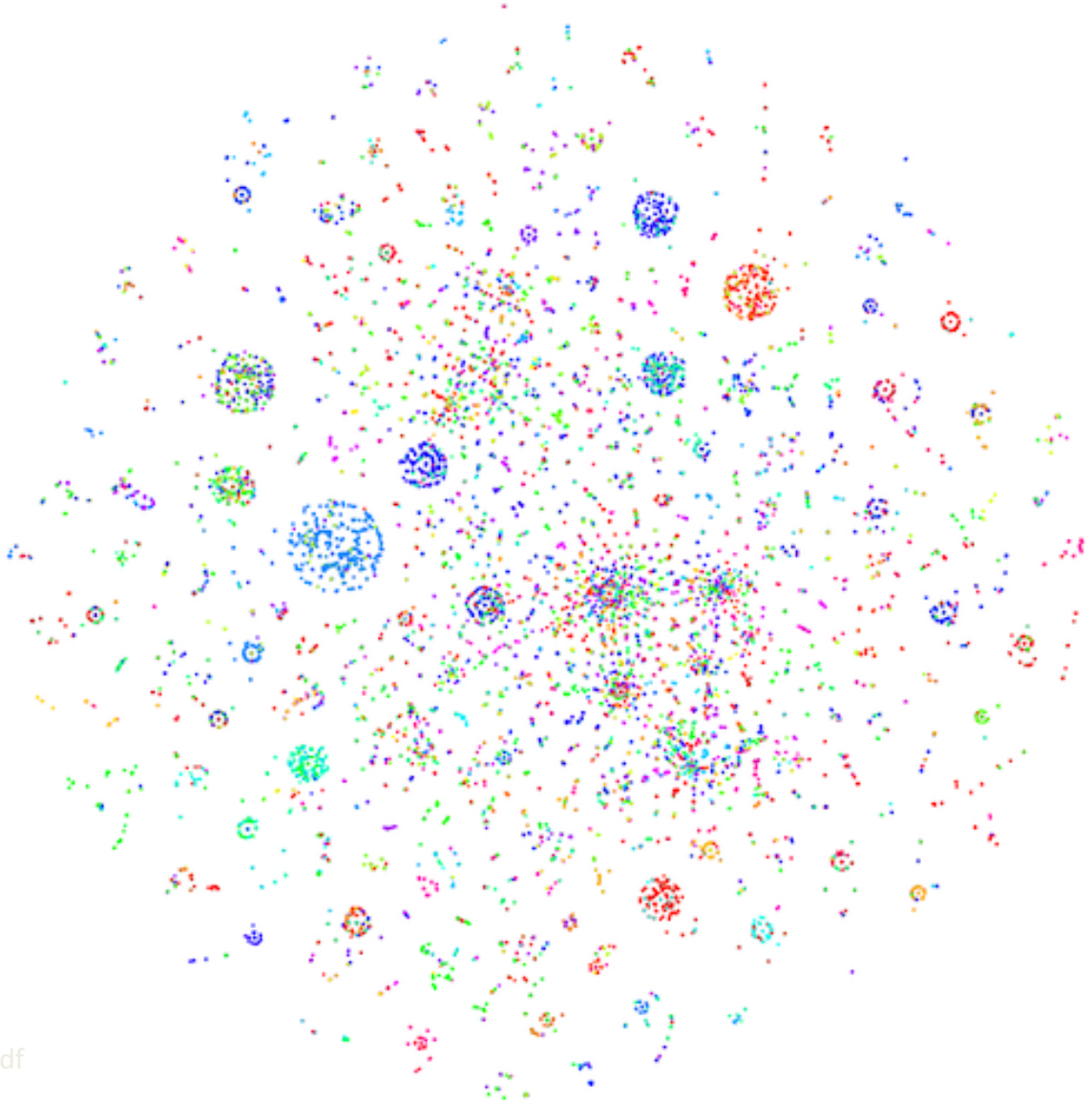
t-Distributed Stochastic Neighbour Embedding

- t-SNE is a special case of MDS (specific d_1, d_2, and d_3 choices):
  - d_1: for each x_i, compute probability that each x_j is a 'neighbour'.
    - Computation is similar to k-means++, but most weight to close points (Gaussian).
    - Doesn't require explicit graph.
  - d_2: for each z_i, compute probability that each z_j is a 'neighbour'.
    - Similar to above, but uses student's t (grows really slowly with distance).
    - Avoids 'crowding', because you have a huge range that large distances can fill.
  - d_3: Compare x_i and z_i using an entropy-like measure:
    - How much 'randomness' is in probabilities of x_i if you know the z_i (and vice versa)?

Interpretation of the “t” in t-SNE

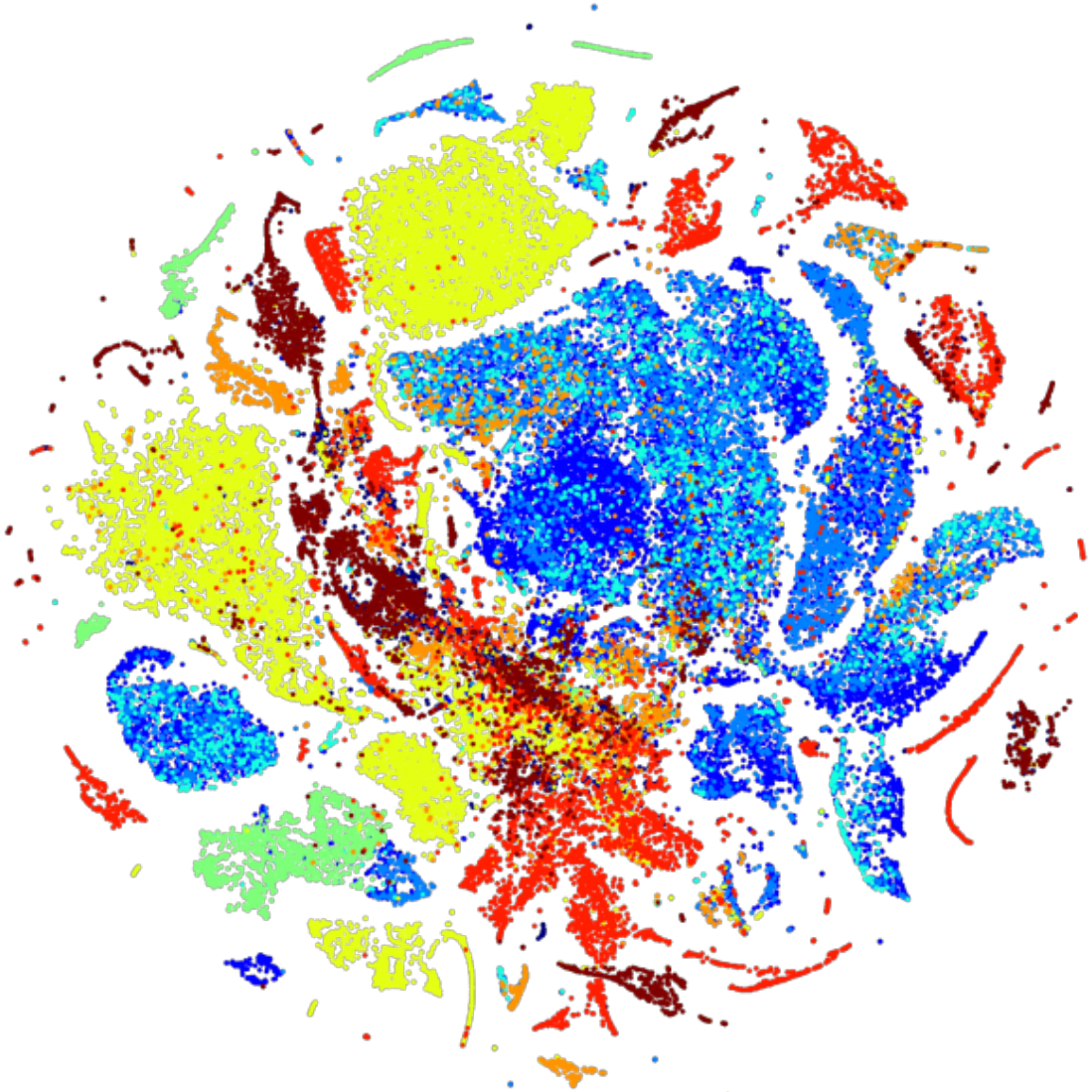
- If two points are close in the z-space, that means something
  - They must have been close in the x-space
- If two points are far apart in the z-space, that might not mean anything
  - They may have been close, or not, in the x-space
  - The ”long tail” of the t-distribution means we don’t take big distances too seriously
- So there’s an asymmetry here and that’s why we use $d_1 \neq d_2$

t-SNE on Wikipedia Articles



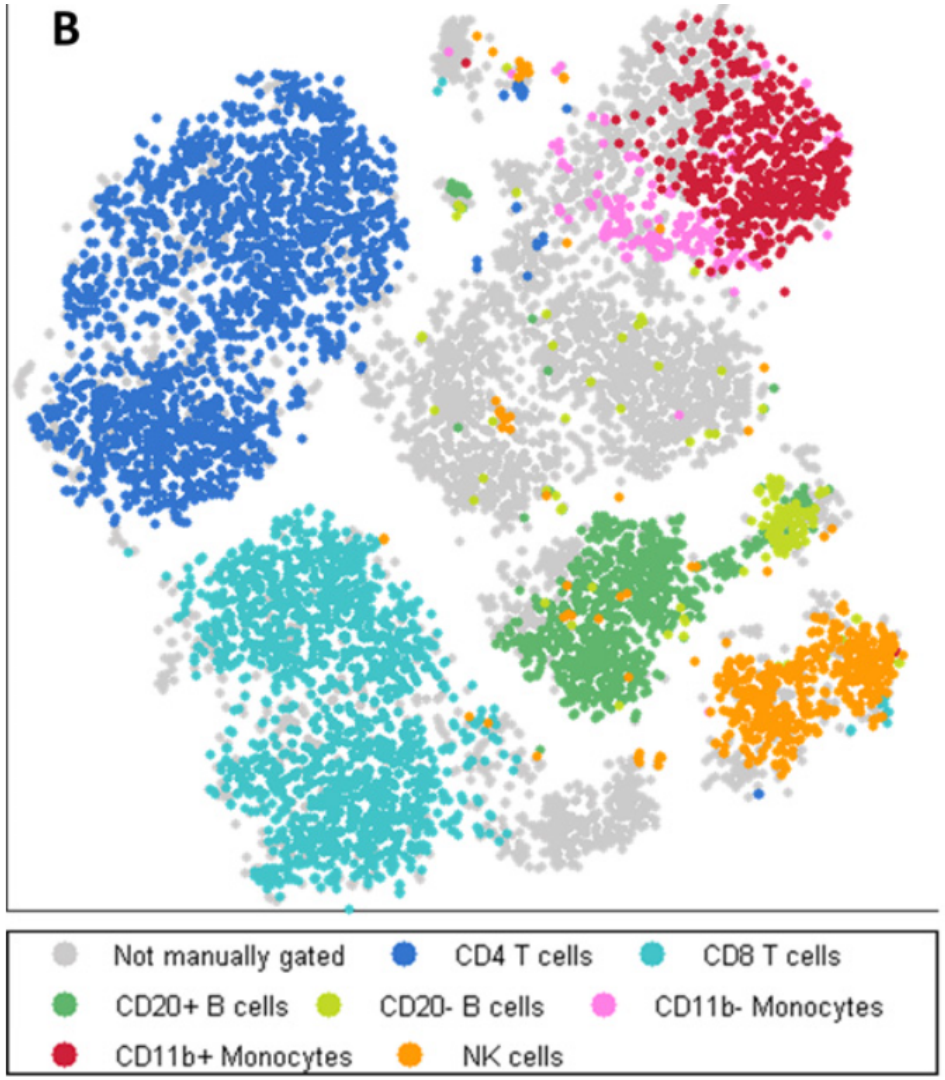
http://jasneet.me/assets/files/wiki_tsne_report.pdf

t-SNE on Product Features



http://blog.kaggle.com/2015/06/09/otto-product-classification-winners-interview-2nd-place-alexander-guschin/

t-SNE on Leukemia Heterogeneity



http://www.ncbi.nlm.nih.gov/pmc/articles/PMC4076922/

End of Part 4: Key Concepts

- We discussed linear latent-factor models:

$$f(W,Z) = \sum_{i=1}^{n}\sum_{j=1}^{d}(w_j^T z_i - x_{ij})^2$$

$$= \sum_{i=1}^{n} \|W^T z_i - x_i\|^2$$

$$= \|ZW - X\|_F^2$$

- Represent 'X' as linear combination of latent factors 'W'.
  - Latent features 'Z' gives a lower-dimensional version of 'X'.
  - When k=1, finds direction that minimizes orthogonal distance.
- Applications:
  - Outlier detection, dimensionality reduction, data compression, features for linear models, visualization, factor discovery, filling in missing entries.

End of Part 4: Key Concepts

- We discussed linear latent-factor models:

$$f(W,Z) = \sum_{i=1}^{n} \sum_{j=1}^{d} (w_j^T z_i - x_{ij})^2$$

- Principal component analysis (PCA):
  - Uses orthogonal factors and fits them sequentially.
- Non-negative matrix factorization:
  - Uses non-negative factors giving sparsity.
  - Can be minimized with projected gradient.
- Many variations are possible:
  - Different regularizers (sparse coding) or loss functions (robust/binary PCA).
  - Missing values (recommender systems) or change of basis (kernel PCA).

End of Part 4: Key Concepts

- We discussed multi-dimensional scaling (MDS):
  - Non-parametric method for high-dimensional data visualization.
  - Tries to match distance/similarity in high-/low-dimensions.
    - "Gradient descent on scatterplot points".
- Main challenge in MDS methods is "crowding" effect:
  - Methods focus on large distances and lose local structure.
- Common solutions:
  - Sammon mapping: use weighted cost function.
  - ISOMAP: approximate geodesic distance using via shortest paths in graph.
  - T-SNE: give up on large distances and focus on small distances.

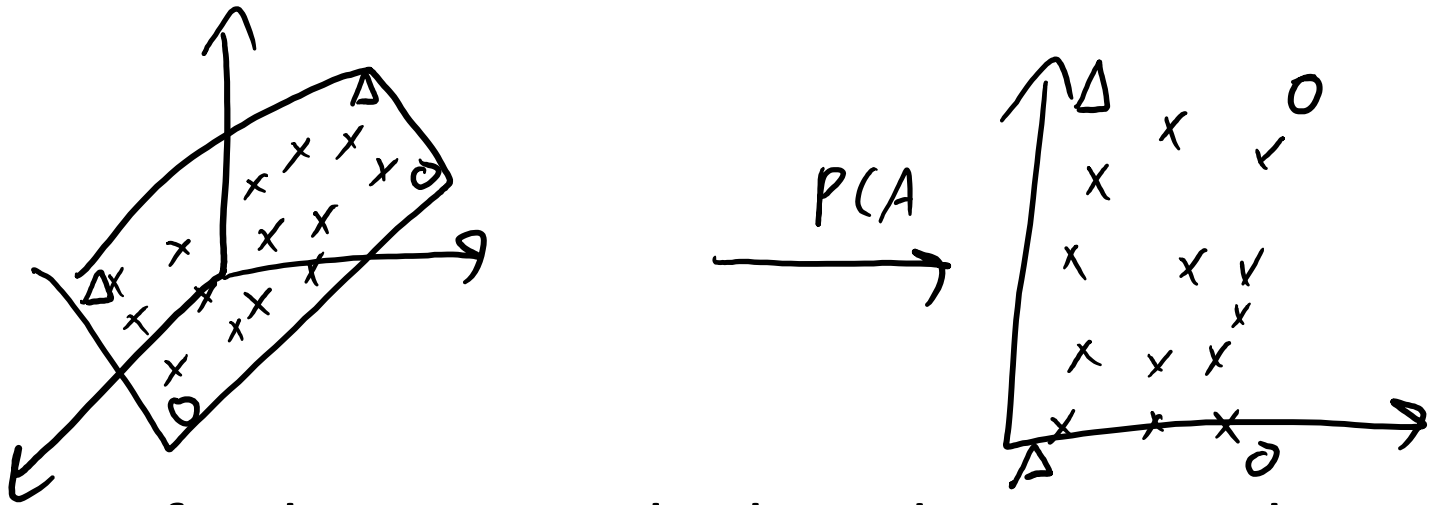
Summary

- MDS with different distances/losses/weights usually gives better results.
- Manifold learning focuses on low-dimensional curved structures.
- ISOMAP is most common approach:
  - Approximates geodesic distance by shortest path in weighted graph.
- t-SNE is promising new data MDS method.

- Next time: why is it called “neural”?

Does t-SNE always outperform PCA?

- Consider 3D data living on a 2D hyper-plane:



- PCA can perfectly capture the low-dimensional structure.
- T-SNE can capture the local structure, but can "twist" the plane.
  - It doesn't try to get long distances correct.