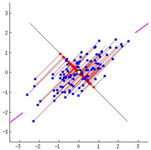
COMP90014

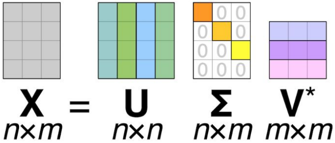
Algorithms for Bioinformatics

Week 9B: Dimensionality Reduction II

Dimensionality Reduction

Linear projections: PCA and SVD





PCA: Finds orthogonal vectors (components) to represent as much variance is as possible. Decomposing the covariance matrix, $C = W\Sigma W^T$. See this animation.

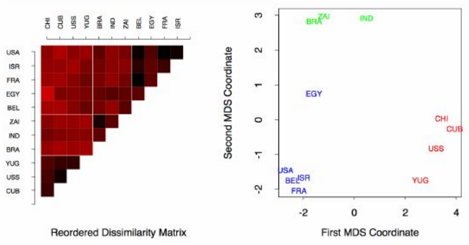
SVD: More efficient
Can interpret PCA as a SVD on the centered covariance matrix

- 🍇 StatQuest: Principal Component Analysis (20 minute video from Josh Starmer)

amoeba via stackexchange; Cmglee via Wikimedia Commons

Dimensionality Reduction

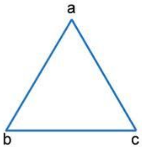
Multi-Dimensional Scaling (MDS)



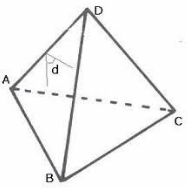
- feature extraction
- produces a lower-dimensional representation that ***preserves pairwise distances or dissimilarities***
- for visualising data
- sometimes called Principal Coordinates Analysis, but it's **not the same as PCA**!

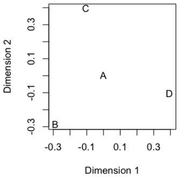
MDS

$$D(x_i,x_j) = \begin{array}{cc} & \begin{array}{ccc} a & b & c \end{array} \\ \begin{array}{c} a \\ b \\ c \end{array} & \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \end{array}$$



$$D(x_i,x_j) = \begin{array}{cc} & \begin{array}{cccc} a & b & c & d \end{array} \\ \begin{array}{c} a \\ b \\ c \\ d \end{array} & \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix} \end{array}$$





- start with a pairwise distance matrix or dissimilarity matrix
- we can represent three points that are equally-spaced in 3D **exactly in 2D**
- we can represent four points that are equally-spaced in 3D **exactly in 3D** ...
- **... but not in 2D**
- in general, we need $N-1$ dimensions to exactly represent pairwise distances between N samples

Types of MDS

Metric (distance-based) MDS

- Minimise ***stress***
- Stress is the error in the distances (lack-of-fit measure)
- Try to preserve distance between each vector x_i, x_j

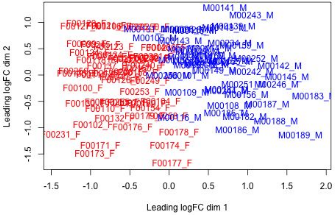
$$\text{Cost} = \sum_{i<j} \left(d_{ij} - \hat{d}_{ij} \right)^2$$

- actual cost/stress used may be more complex

Non-metric MDS

- Try to maintain original ranking of pairwise distances

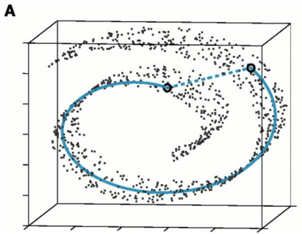
Interpreting low-dimensionality visualisation



- clusters may represent real clusters
- outliers may represent real outliers
- the position of points is ***not useful*** in MDS
- resulting dimensions are not ordered by importance/variance
- can’t reconstruct original data

Dimensionality Reduction

ISOMAP (Isometric Feature Mapping)



ISOMAP

- nonlinear dimensionality reduction
- preserves the global, non-linear geometry of the data by preserving the ***geodesic*** distances

Manifold: a nonlinear low-dimensional surface

- data often lies on or near manifolds

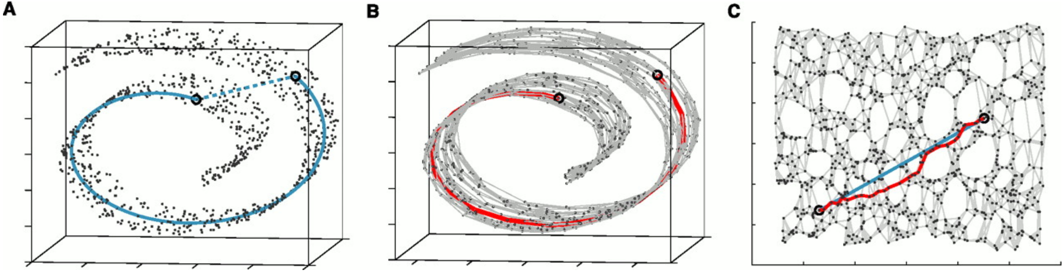
Geodesic: shortest route between two points on the surface of the manifold

- (shortest path on a graph)

Tenenbaum *et al.* 2000. 10.1126/science.290.5500.2319; J. Jeffry Howbert, University of Washington.

ISOMAP

- Goal: use geodesic distance between points (with respect to manifold)
- Estimate manifold using graph. Distance between points given by distance of shortest path
- Embed onto 2D plane so that Euclidean distance approximates graph distance

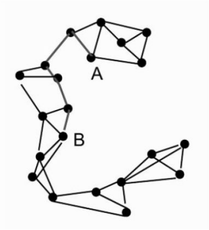


Tenenbaum *et al.* 2000. [10.1126/science.290.5500.2319](https://doi.org/10.1126/science.290.5500.2319).

ISOMAP

Two steps:

1. Calculate the geodesic distance between every pair of points
   - *e.g.* use Euclidean distance for points that are 'close enough'
   - For points that are far apart, calculate geodesic distance by summing up local Euclidean distances
2. **Find Euclidean mapping of the data that preserves the geodesic distance**



ISOMAP

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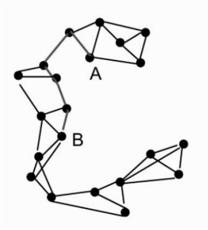


1. construct a graph

if $d(i,j) < \varepsilon$ `// ε-isomap`

    or

  i is one of j's k nearest neighbours   `// k-isomap`

then

  Connect *i* and *j*

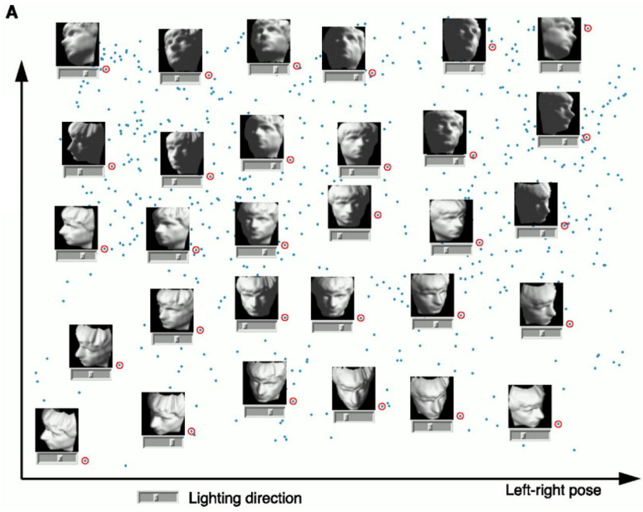
  Set the edge weight as $d(i,j)$ (Euclidean distance)

Compute the geodesic distance between all pairs of points (shortest paths)

Using ISOMAP

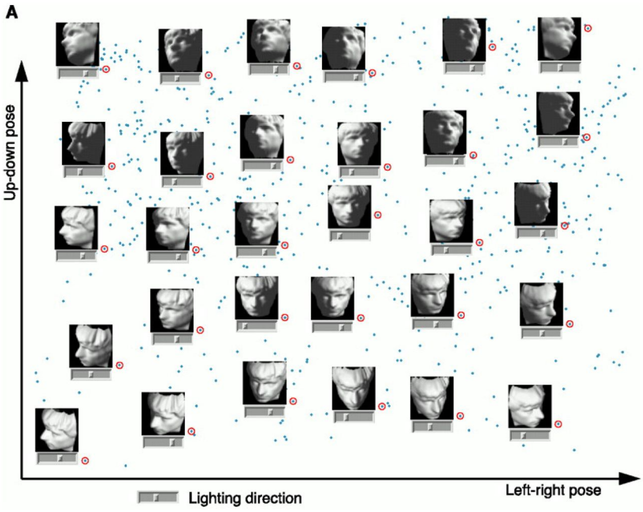
Tenenbaum et al. 2000. https://doi.org/10.1126/science.290.5500.2319

Using ISOMAP



Tenenbaum et al. 2000. https://doi.org/10.1126/science.290.5500.2319

Using ISOMAP



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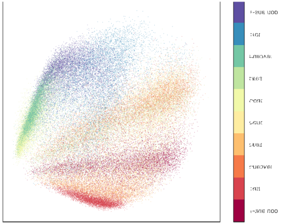
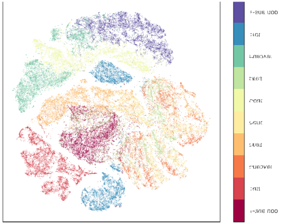
Dimensionality Reduction

Fashion MNIST data set

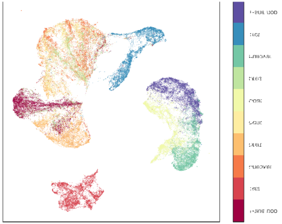
PCA



t-SNE



UMAP



- Based on images of fashion items.
- Each item is categorized
- Dataset: zalandoresearch/fashion-mnist

PCA（主成分分析）：第一个图展示了使用PCA进行降维的结果。PCA试图保持数据的最大方差，并将其映射到新的低维空间。这个图显示了数据在新的维度上的分布，但是类别之间的区分不是非常清晰。

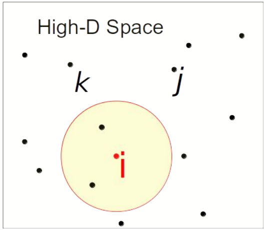
t-SNE（t-分布随机邻域嵌入）：第二个图是使用t-SNE技术的结果，它是一种非线性降维技术，特别擅长保持高维数据的局部结构，并在低维空间中揭示数据的群簇。这个图展示了明显的分离群簇，每个群簇代表不同的时尚物品类别。

UMAP（统一流形逼近和投影）：第三个图使用UMAP，这是一种较新的降维技术，它类似于t-SNE，但通常在计算效率和大规模数据集的可扩展性方面更优。UMAP同样能够很好地在低维空间中区分出不同的类别。

Leland McInnes, SciPy 2018.

t-Distributed Stochastic Neighbour Embedding

t-SNE是一种非线性的降维方法，用于将高维数据映射到二维或三维空间中，以便于可视化。



PCA: tries to preserve **global** structure

PCA旨在保持全局结构，即在降维过程中保留数据中最大的方差。而t-SNE关注于保持数据点之间的局部关系，尤其是在处理非线性结构的数据时非常有效。

t-SNE: tries to preserve **local** structure

- probabilistic version of MDS
- each point in high-dimensionality has a conditional probability of picking each other point as its neighbor
  - probability of picking j given you start at i

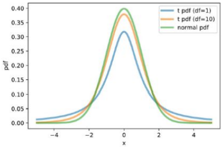
$$p_{j|i} = \frac{\exp\left(\frac{-\|x_i - x_j\|^2}{2\sigma_i^2}\right)}{\sum_{k\neq i} \exp\left(\frac{-\|x_i - k_k\|^2}{2\sigma_i^2}\right)}$$

t-SNE被认为是多维尺度分析（MDS）的概率版本。它通过概率分布来表示高维空间中的点之间的相似性，并在低维空间中保持这些概率分布。
在t-SNE中，每个点在高维空间中都有一个条件概率，这个概率定义了选择另一个点作为其邻居的可能性。
p j i表示在给定起点 i 的情况下选择 j 作为邻居的条件概率。

t-Distributed Stochastic Neighbour Embedding

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

$$q_{ij} = \frac{\left(1 + \|y_i - y_j\|^2\right)^{-1}}{\sum_{k \neq l} \left(1 + \|y_k - y_l\|^2\right)^{-1}}$$

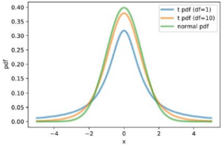


- calculate the Gaussian probabilities ($p_{j|i}$) in high-dimensional space
- compare to a probability in lower-dimensional space

t-Distributed Stochastic Neighbour Embedding

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

$$q_{ij} = \frac{\left(1 + ||y_i - y_j||^2\right)^{-1}}{\sum_{k \neq l} \left(1 + ||y_k - y_l||^2\right)^{-1}}$$



- calculate the Gaussian probabilities ($p_{j|i}$) in high-dimensional space
- compare to a probability in lower-dimensional space

Evaluate a mapping:

- in lower-dimensional space, calculate probabilities using Student's t-distribution (q)
- probability goes to zero more slowly than a Gaussian
- this relaxes distances in lower-dimensional space

t-SNE cost function

Kullback-Liebler divergence: $C = \mathrm{KL}\left(P \,||\, Q\right) = \sum_i \sum_j p_{ij} \log \frac{p_{ij}}{q_{ij}}$

- measures the difference between the high-dimensional probability distributions and the low-dimensional probability distributions
- t-SNE algorithm performs gradient descent on the cost function

t-SNE vs. ISOMAP

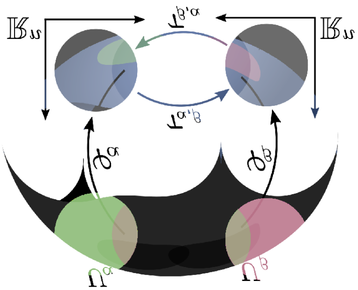
t-SNE ISOMAP

Example on MNIST dataset

- a classic machine learning dataset of images of handwritten digits
- MNIST dataset: yann.lecun.com/exdb/mnist
- t-SNE publication and code: lvdmaaten.github.io/tsne

Dimensionality Reduction

UMAP



Uniform Manifold Approximation and Projection (UMAP):

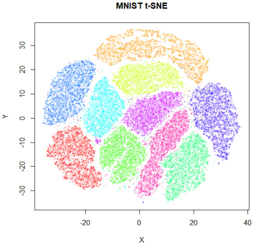
- inspired by t-SNE, based on manifolds and topology rather than probability distributions.
- publications and code at lmcinnes/umap
- UMAP talk at SciPy: youtube.com
- UMAP talk at PyData: youtube.com

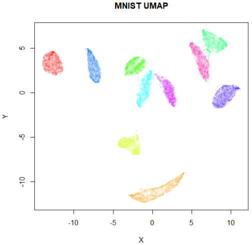
Leland McInnes, SciPy 2018.

UMAP

UMAP的第一步是构建一个加权k邻居图。这意味着算法会测量数据点之间的距离，并且基于最近的k个邻居创建一个图，图中的边缘是根据距离加权的。

UMAP的第二步是计算这个图在低维空间的布局。这涉及到在较低维度的空间中找到数据点的一个新表示，同时尽可能地保持高维空间中的局部和全局结构。





James Melville, jlmelville/uwot.

- In the first phase a weighted *k*-neighbour graph is constructed.
- In the second phase a low dimensional layout of this graph is computed

这是一种在图绘制中常用的算法，用于美观地排列图的节点和边

Force directed graph layout

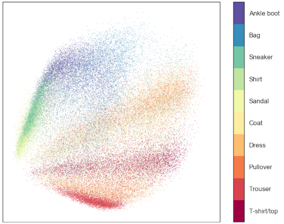
- Edge weights mean that nearby points attract each other
- Weight normalization acts as a global force pushing points apart

- Algorithm: iteratively apply attractive and repulsive forces at each edge or node

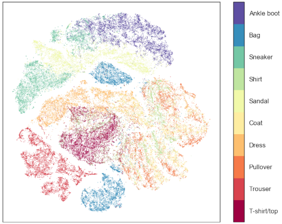
边缘权重意味着相邻的点会相互吸引。
权重归一化作为一种全局力量，有助于将点分开。
算法迭代地应用吸引力和排斥力在每个边缘或节点上。

Fashion MNIST data set

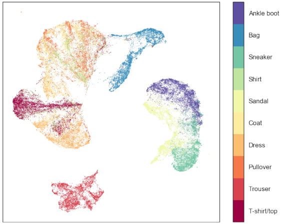
PCA



t-SNE



UMAP



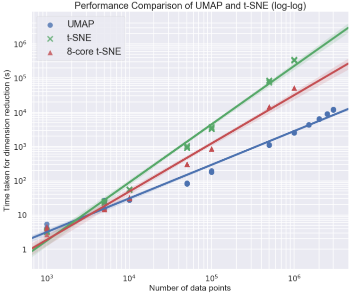
- Based on images of fashion items.
- Each item is categorized
- Dataset: zalandoresearch/fashion-mnist

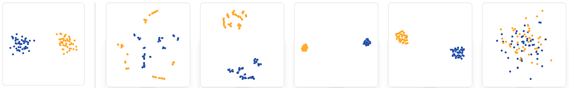
Leland McInnes, SciPy 2018.

UMAP的缺点包括：

图中的距离不是真实的距离。
降维后的维度没有可解释的意义。
超参数需要谨慎调整，并且对结果影响很大。

UMAP





Original

Perplexity: 2
Step: 5,000

Perplexity: 5
Step: 5,000

Perplexity: 30
Step: 5,000

Perplexity: 50
Step: 5,000

Perplexity: 100
Step: 5,000

比t-SNE快一个数量级。
是确定性算法。

Advantages

- an order of magnitude faster than t-SNE
- deterministic
  (t-SNE and MDS are stochastic)

Disadvantages

- distances in the plot are not real distances
- dimensions have no interpretable meaning
- hyperparameters need to be tuned carefully and have a huge impact on the result

McInnes & Healy, 2018. 10.48550/arXiv.1802.03426; Wattenberg *et al.* 2016. via Distill.

Dimensionality Reduction

1. Dimensionality Reduction
2. Multi-dimensional scaling (MDS)
3. ISOMAP
4. t-SNE
5. UMAP

Thank you!

Today: Dimensionality Reduction II

Next time: Unsupervised Learning