Reducing Complexity in Nonlinear Data

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Overview

Manifold learning for dimensionality reduction

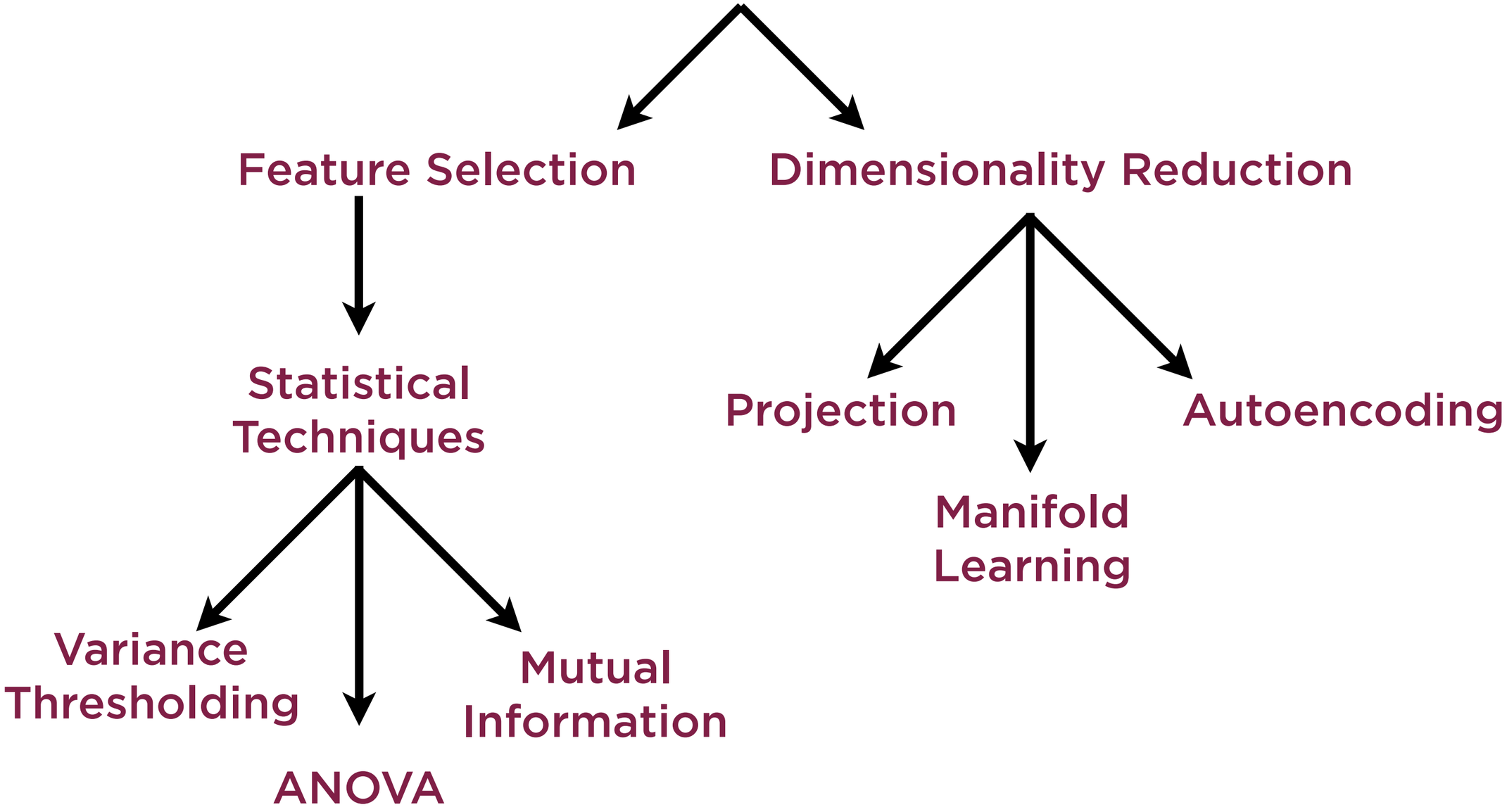
Implementations of manifold learning

Multidimensional scaling, Isomap, Locally Linear Embedding

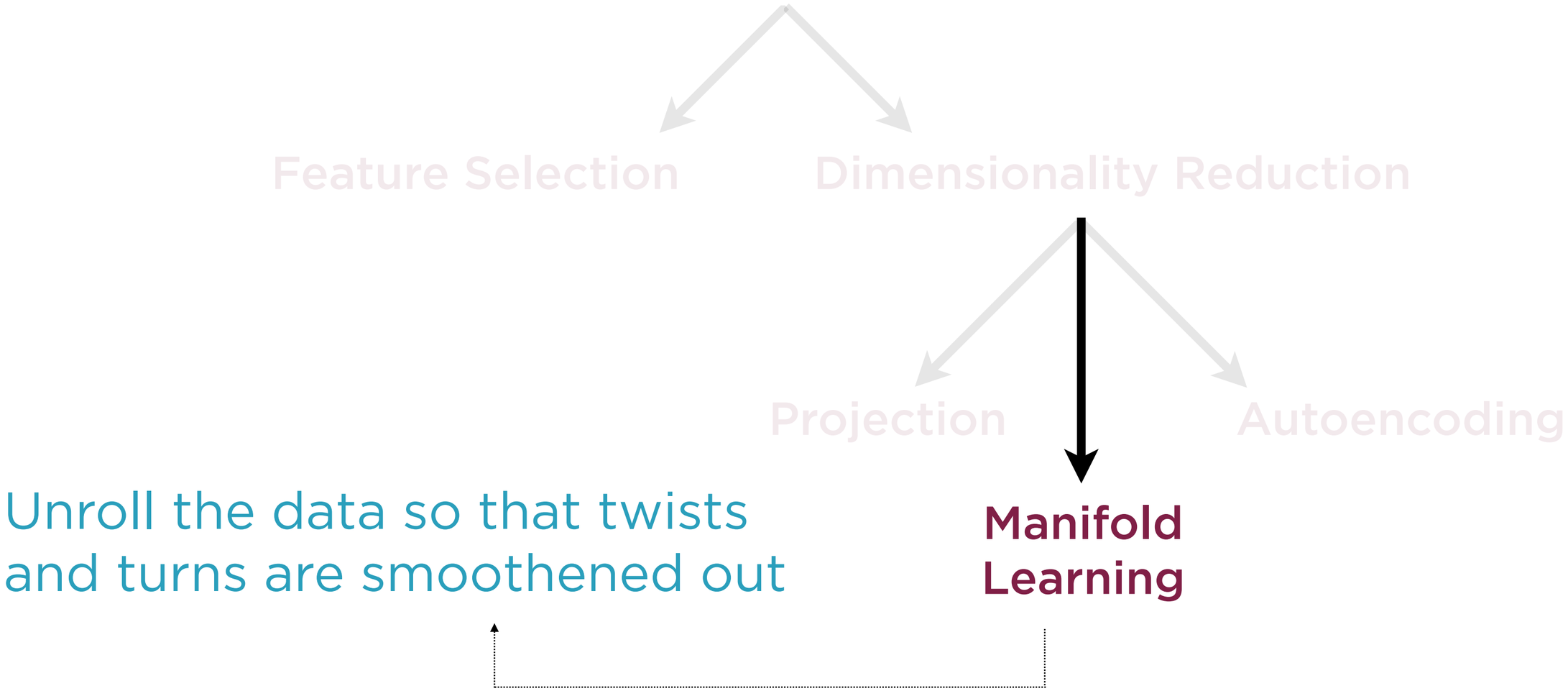
t-Distributed Stochastic Neighbor Embedding (t-SNE)

Kernel PCA

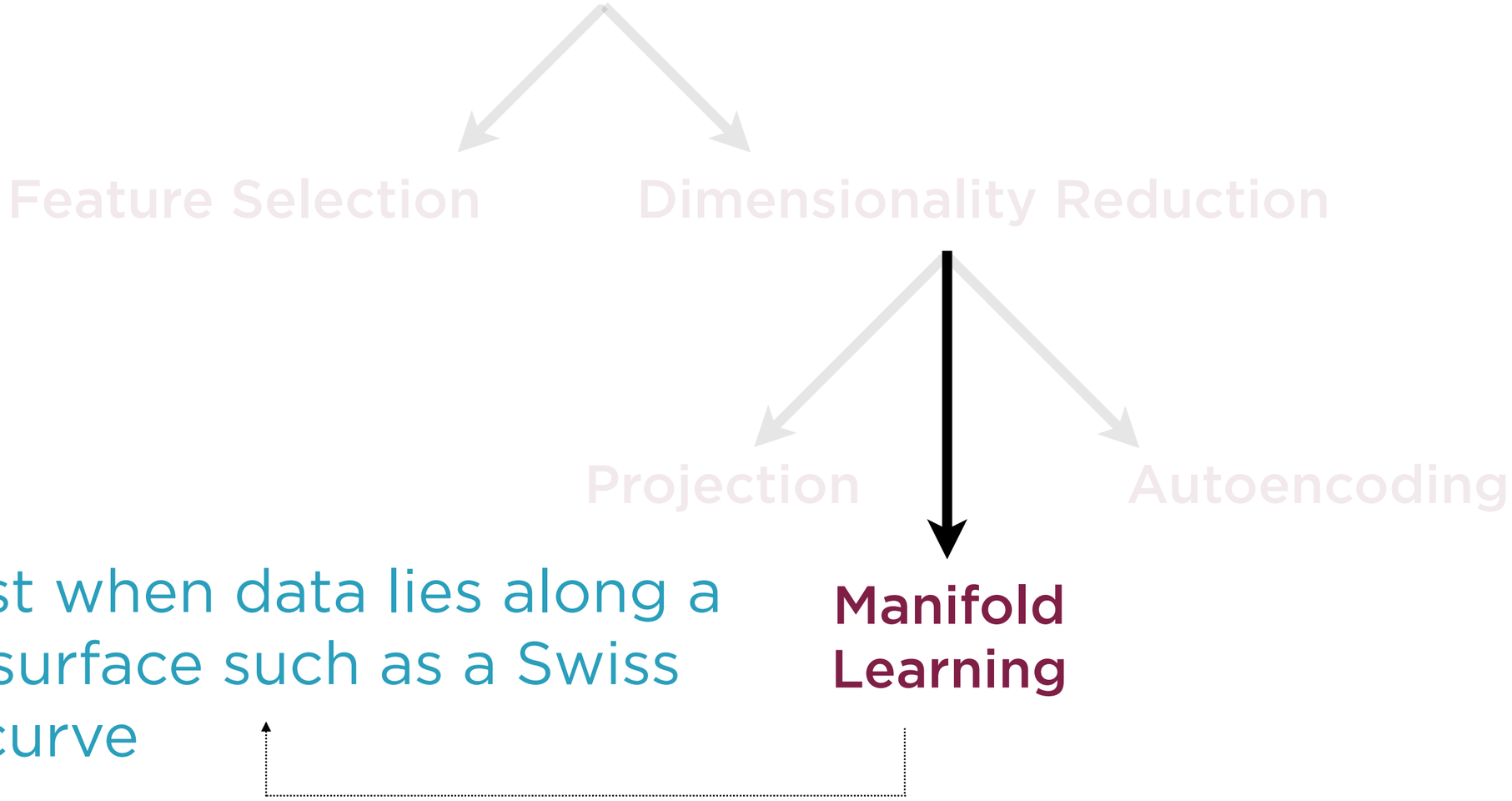
Reducing Complexity



Reducing Complexity

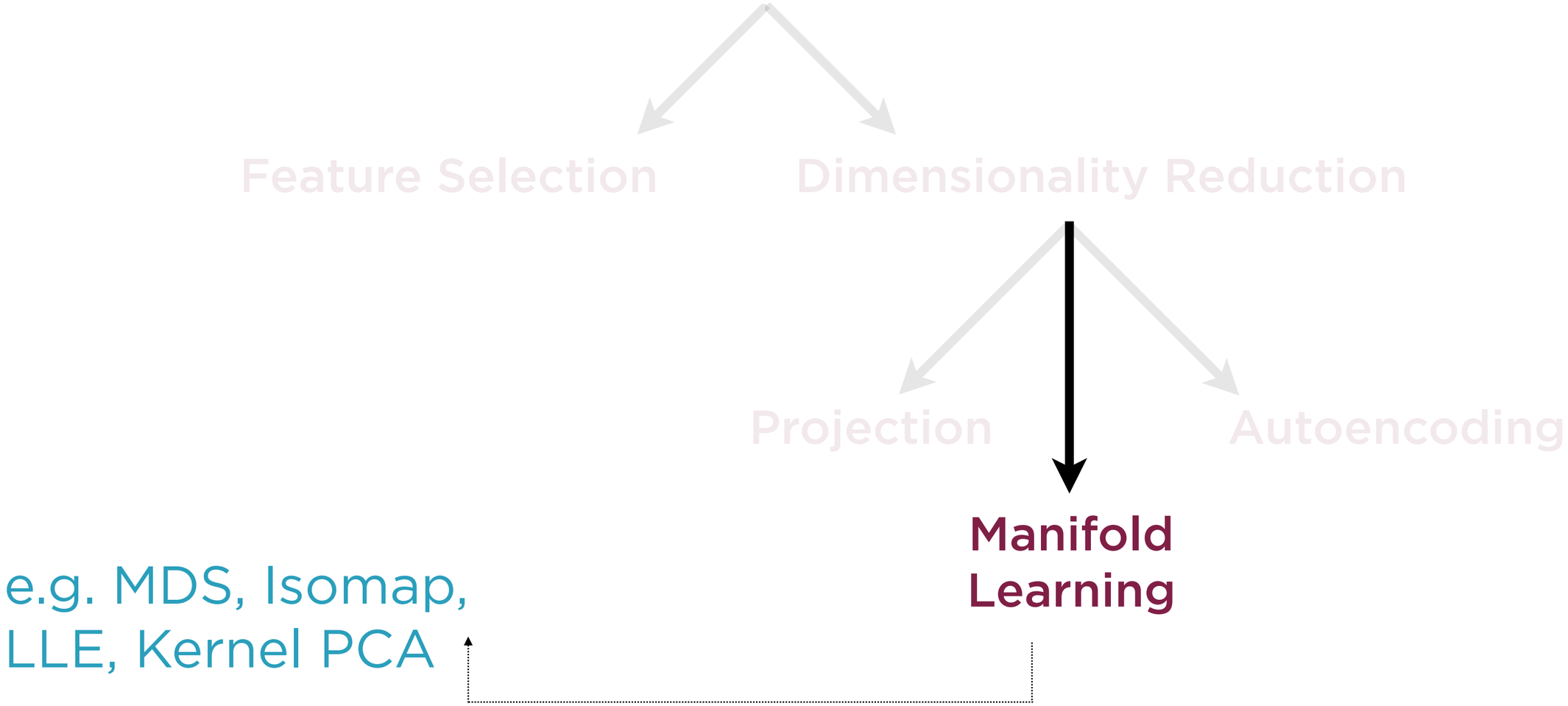


Reducing Complexity



Works best when data lies along a rolled-up surface such as a Swiss Roll or S-curve

Reducing Complexity



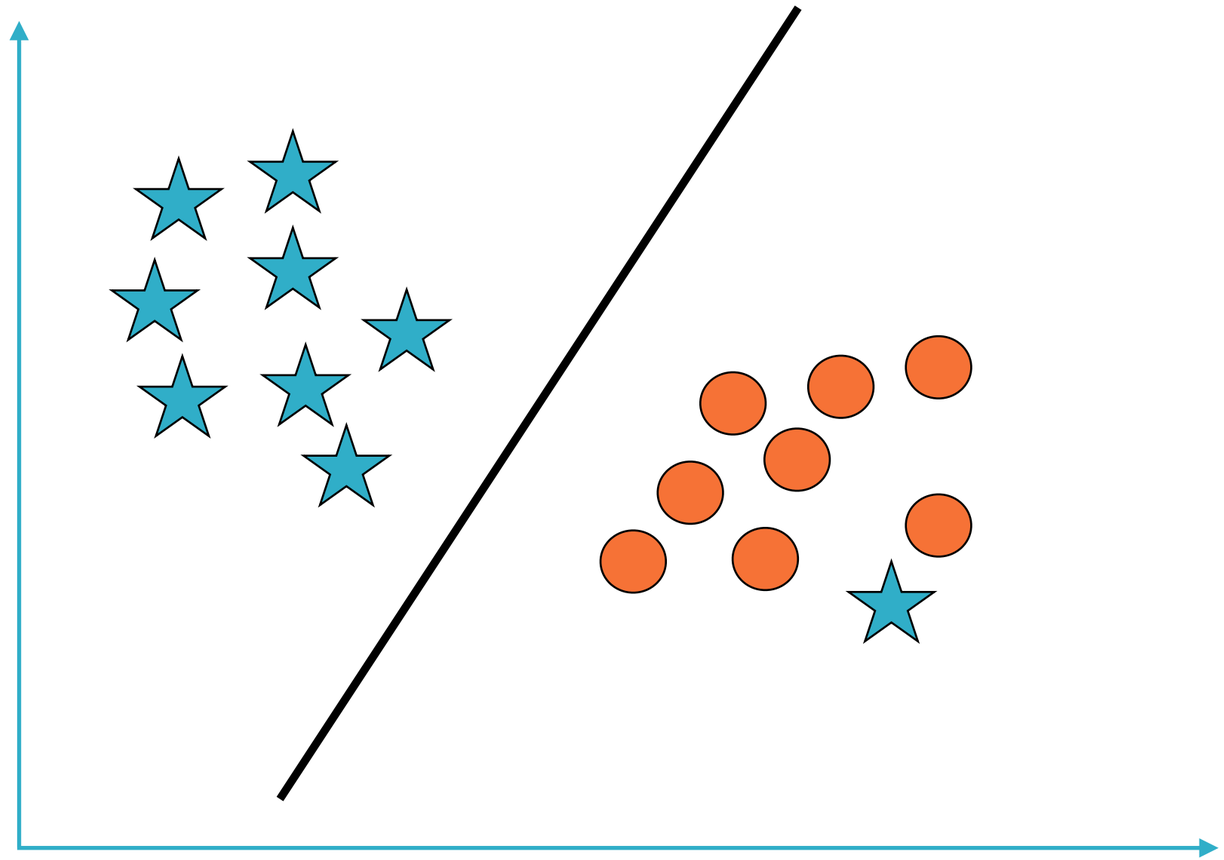
Manifold Learning

Manifold Hypothesis:
Very complicated data is often not that complicated after all

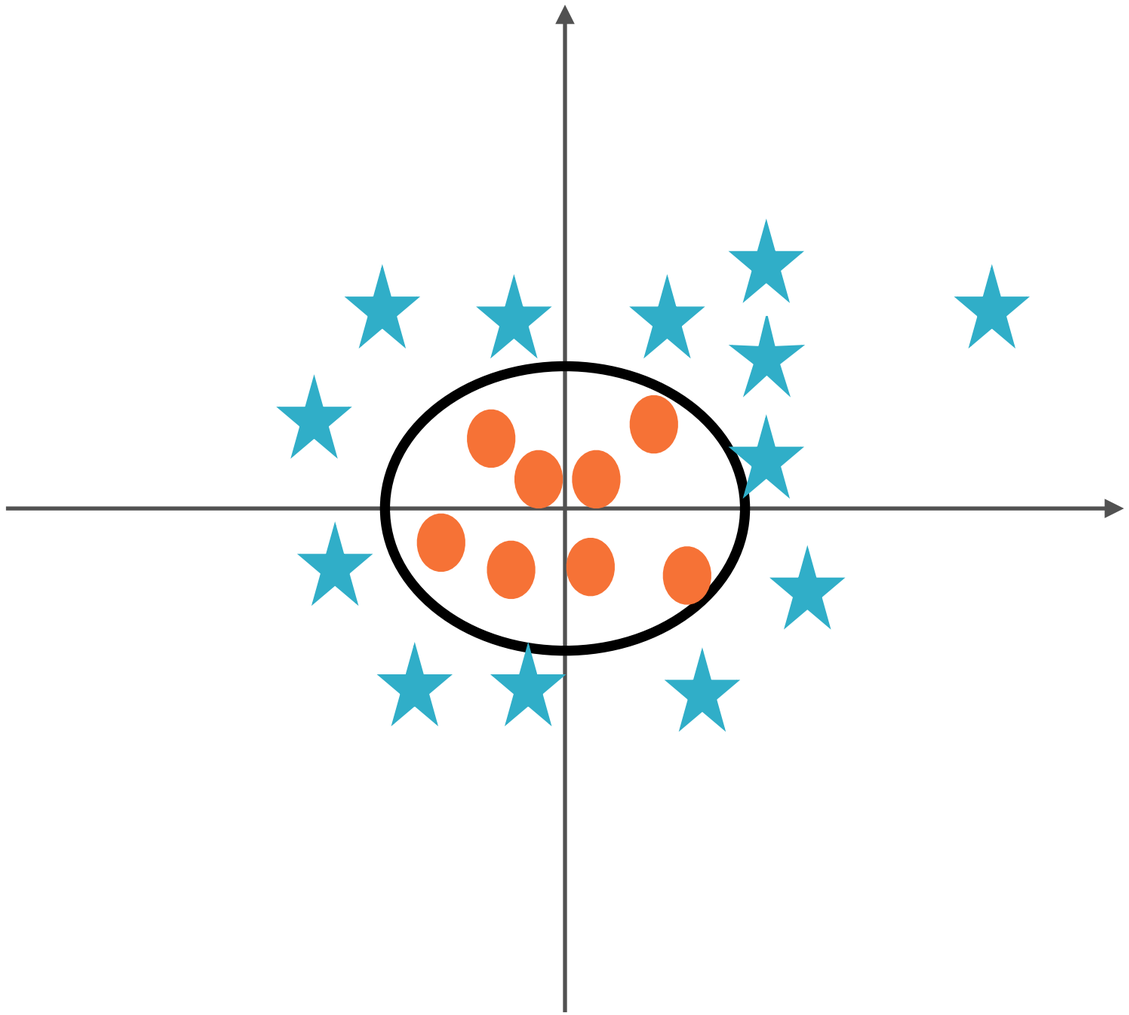
Choosing Manifold Learning

Use Case	Possible Solution
Y not linearly related to X	Manifold learning
Very high dimensionality of X (e.g. pixel counts in image data)	
Many constraints on allowable values of X-variables (sparse features)	
Three-dimensional plots of Y against pairs of X indicate manifold shape	

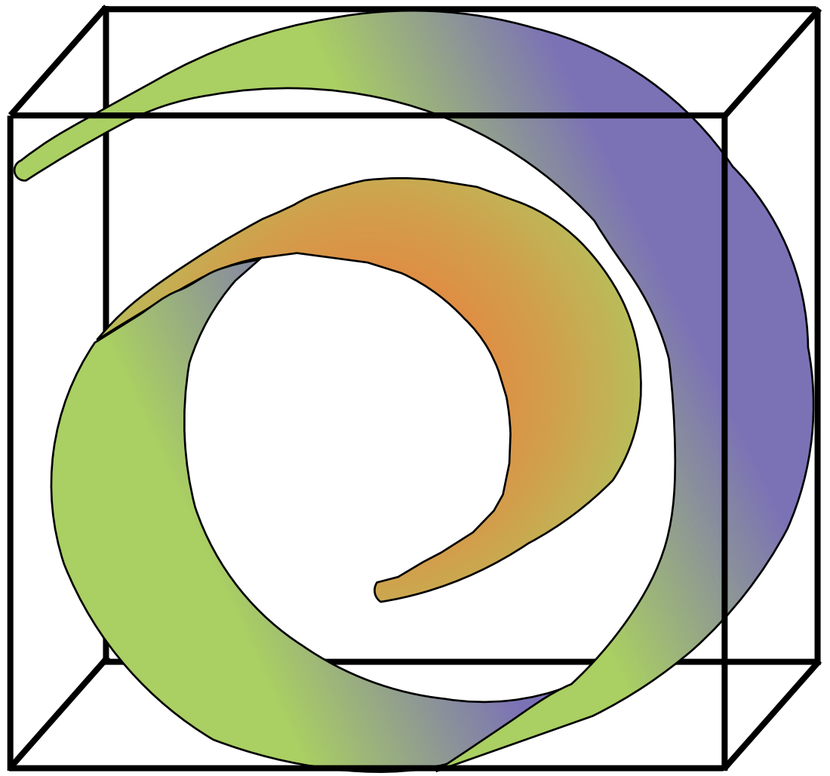
Linear Data



Nonlinear Data



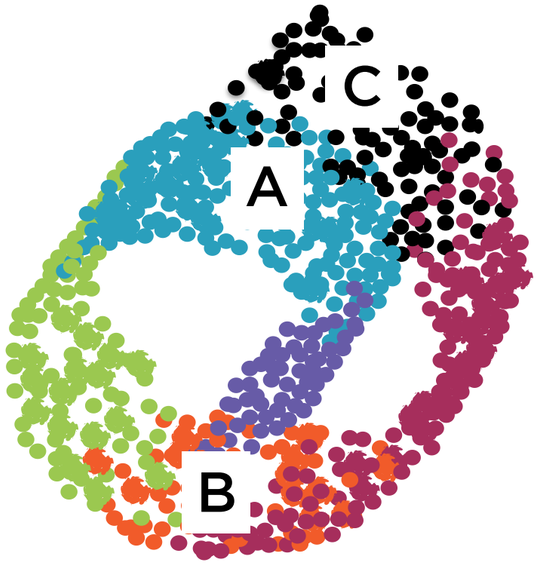
Manifold Data



Manifold Hypothesis

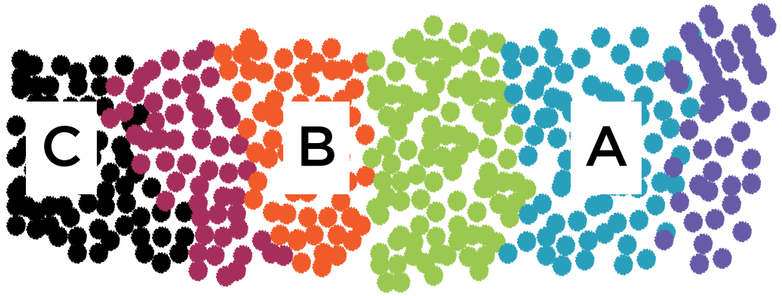
Many high-dimensional datasets can be easily unrolled so that they lie along a much lower dimensional manifold

Manifold Hypothesis



High-dimensional data

Manifold Learning



Low-dimensional embedding

Manifold Learning Techniques

MDS	Isomap	Kernel PCA
LLE	t-SNE	Spectral Embedding

Multidimensional Scaling (MDS)

Aims to preserve pair-wise Euclidean distances between all points while reducing dimensionality. Some intuitive similarities to MSE regression in underlying math.

Isomap

Aims to preserve pair-wise Euclidean distances between neighboring points only (not all points) while reducing dimensionality; works out equivalent to preserving geodesic distance between all points.

Locally Linear Embedding

Expresses each point as centroid (weighted average) of nearest neighbors; then tries to maintain same weights upon conversion to new dimensions.

Spectral Embeddings

Builds a graph where each point serves as a node; then fits a smooth function in lower dimensional space to pass through all nodes. Often implemented using technique called Laplacian Eigenmaps.

t-distributed Stochastic Neighbor Embedding (t-SNE)

Aims to keep similar points together and dissimilar points apart. First fits a Student-t probability distribution to the data, hence the name. Widely used in visualizing clusters.

Kernel PCA

First apply technique called the kernel trick to go to even higher (infinite) number of dimensions, then perform PCA to come down to very low-dimensional space.

Demo

Implement Manifold Learning using a Swiss Roll dataset

Demo

Implement Kernel PCA

Summary

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t-Distributed Stochastic Neighbor Embedding (t-SNE)

Kernel PCA