Data Science and Deep Learning (2024)

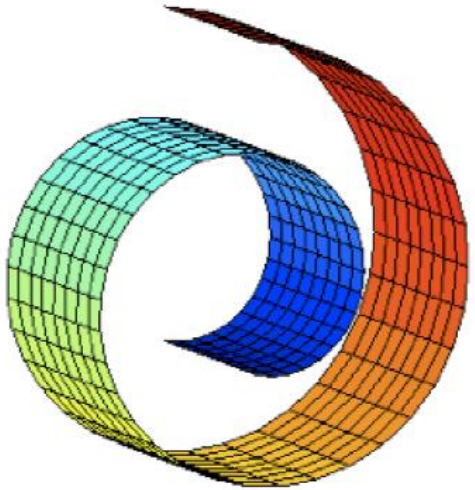
Lecture 5

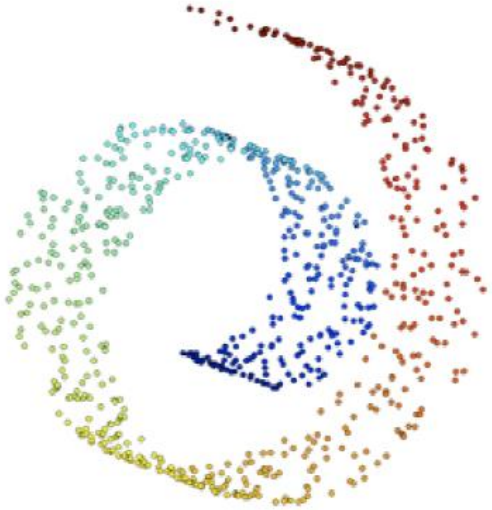
Manifold Learning

Stan Z. Li

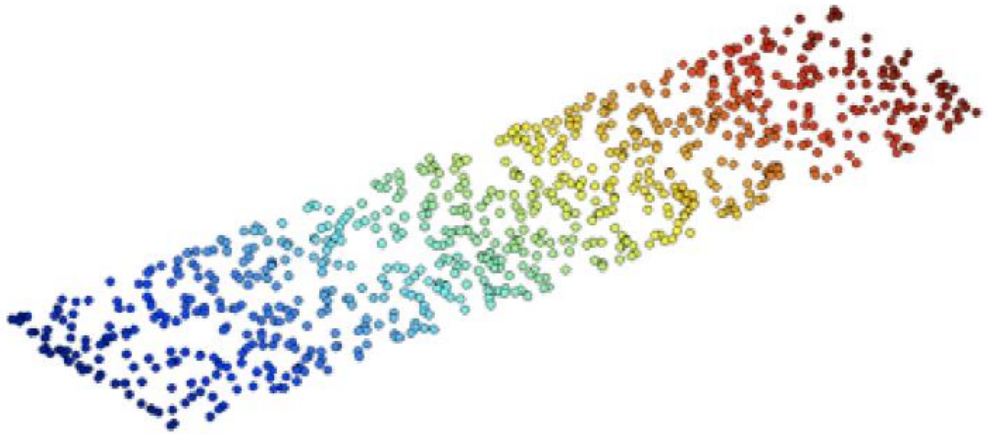
西湖大學
WESTLAKE UNIVERSITY

Unrolling 2D Swiss-roll to 2D Plane





The Best Representation:



Swiss Roll:

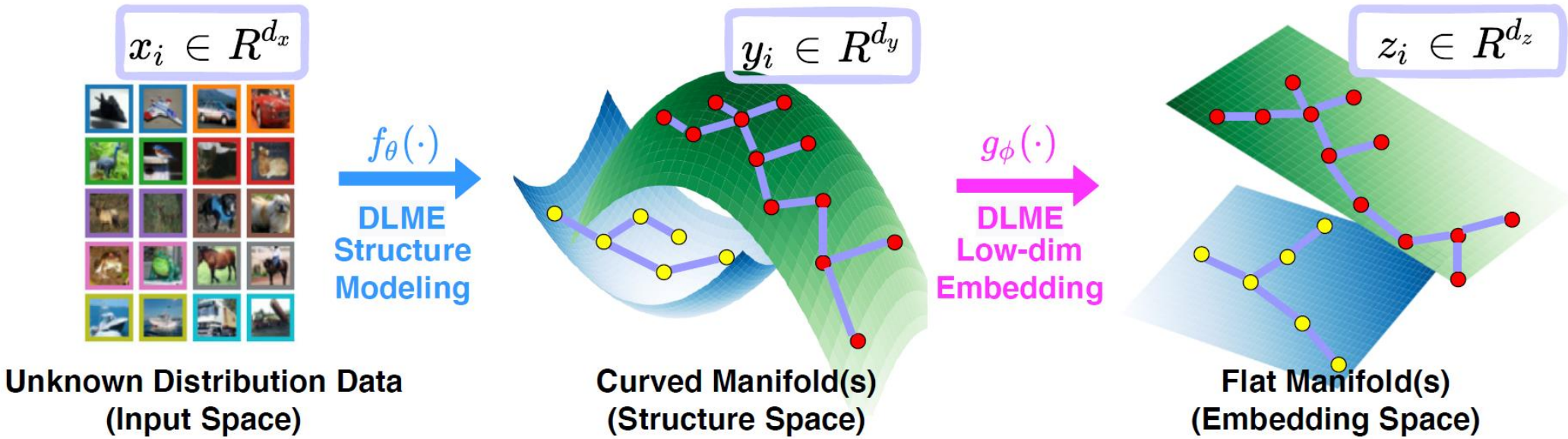
$x=\varphi\cos(\varphi)$, $y=\varphi\sin(\varphi)$, $z=\psi$

$1.5\pi \le \varphi \le 4.5\pi$, $0 \le \psi \le 10$

Manifold: 2D rectangle

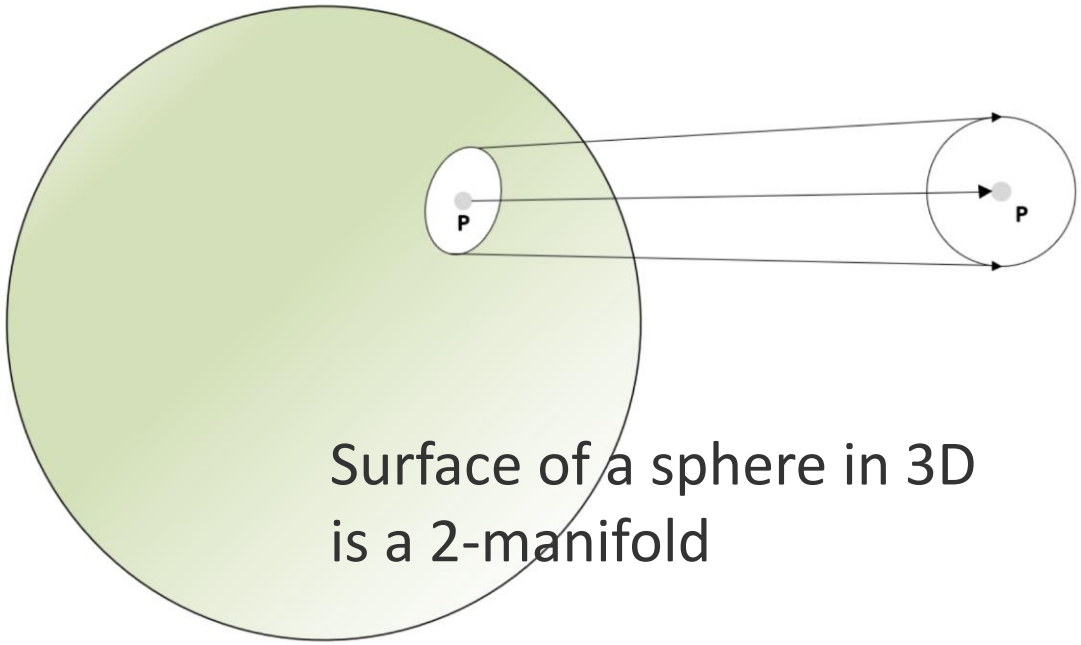
generated by two latent variables φ, ψ

Flattening Curved Surfaces

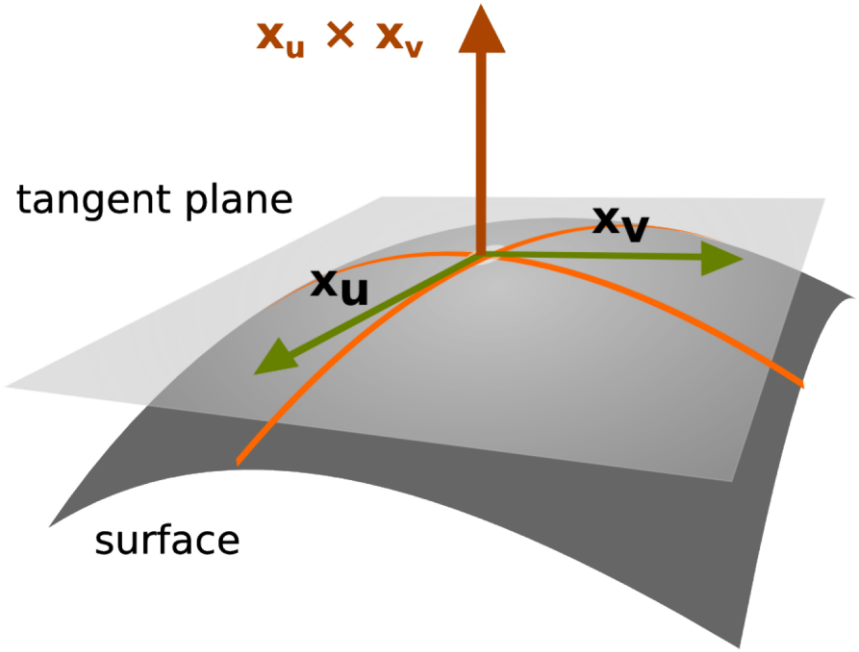


Manifold: Definition

An *n*-manifold is a topological space that is globally curved, but locally homeomorphic （同胚）to an *n*-dimensional Euclidean space

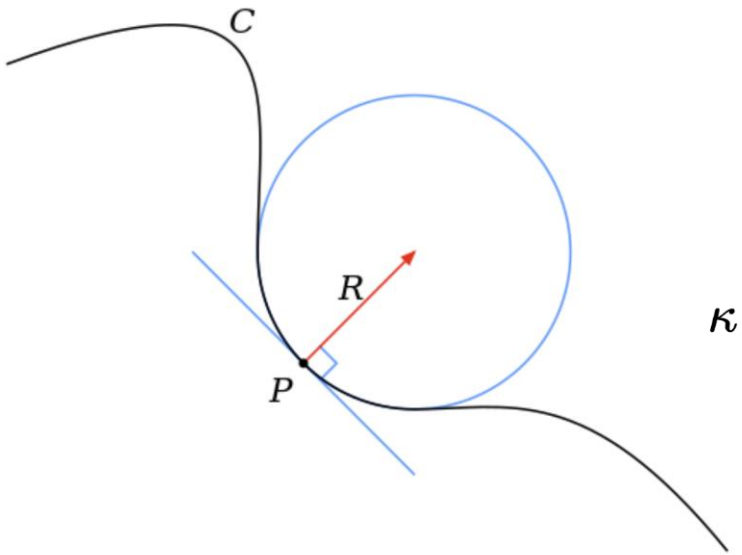


Surface of a sphere in 3D
is a 2-manifold



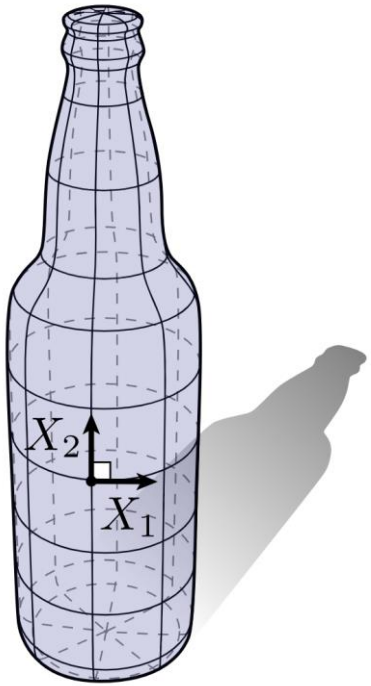
Mastering Machine Learning Algorithms

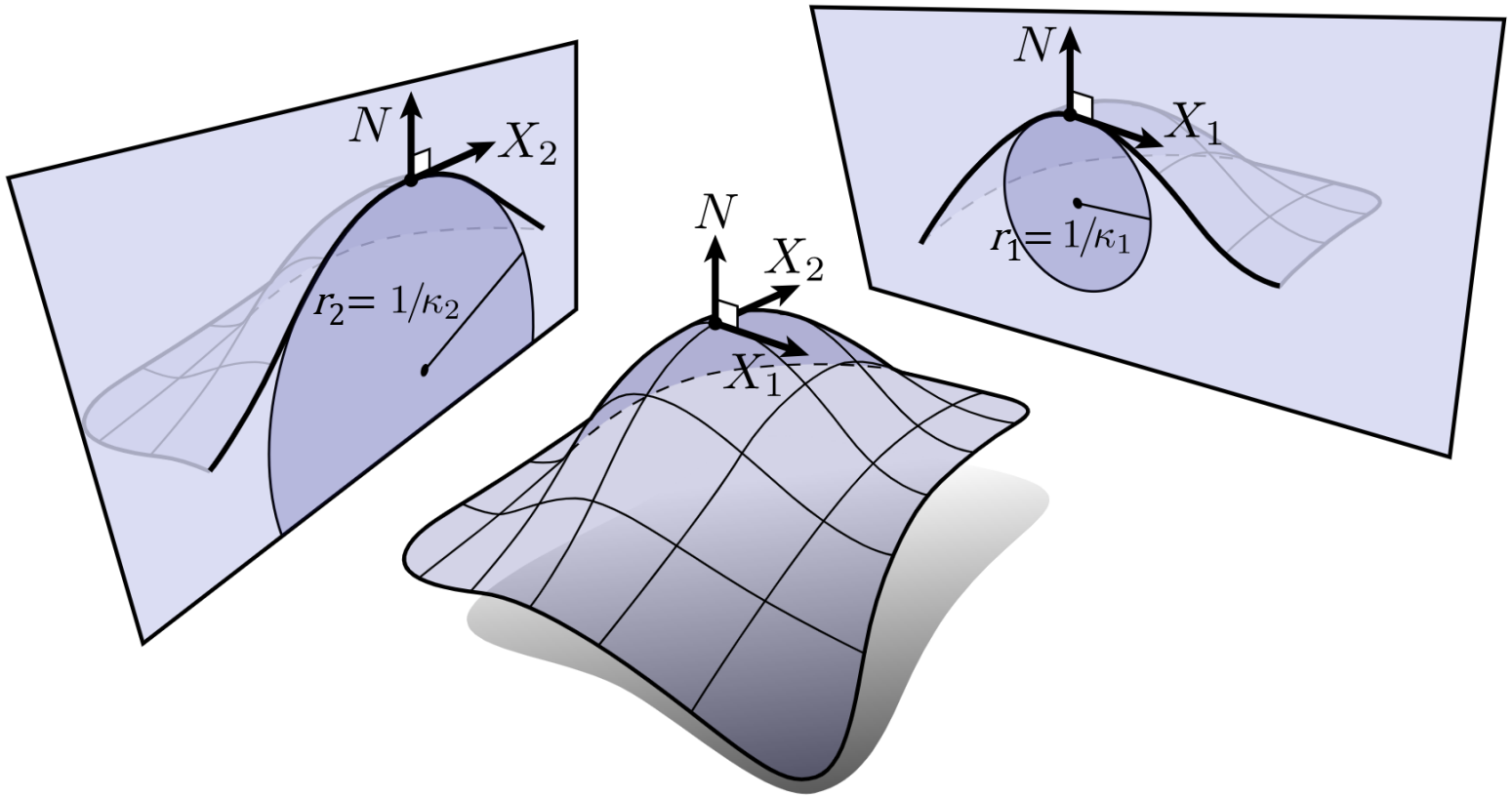
Local Curvature on a Curve



$$\kappa = \frac{1}{R}$$

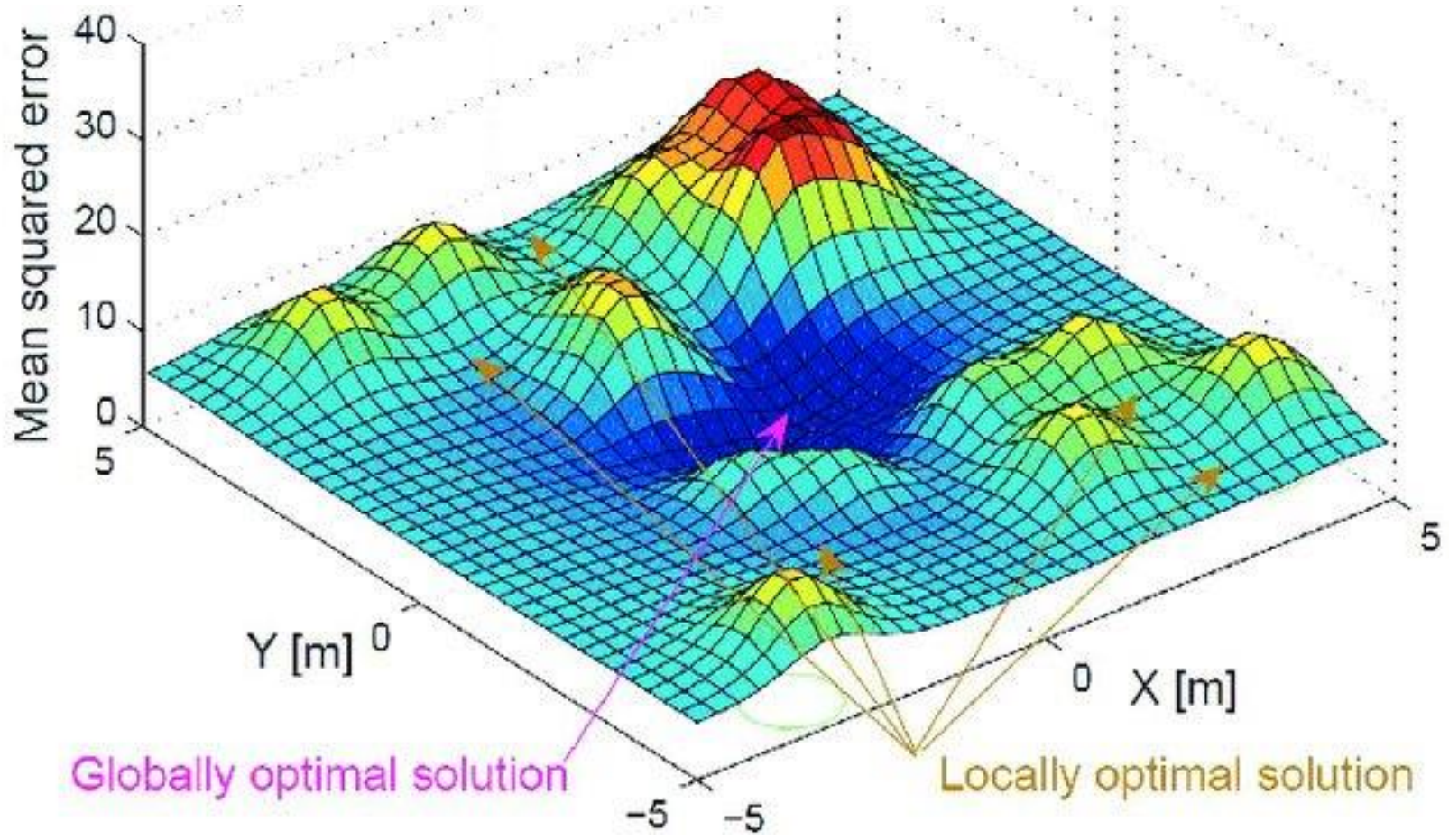
Principal Directions and Curvatures of Surfaces





Ref: [A Quick and Dirty Introduction to the Curvature of Surfaces]

Manifold with Mixed Curvatures



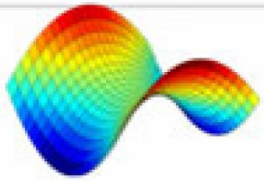
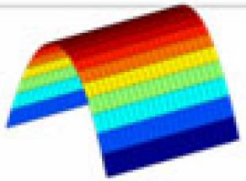
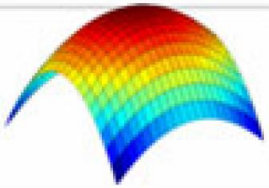
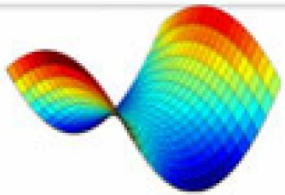
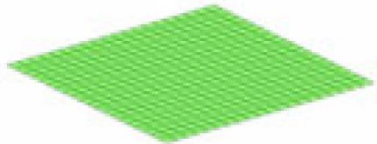
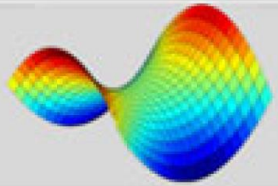
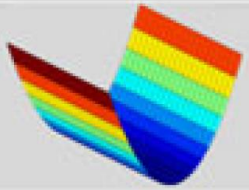
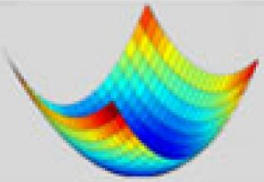
Local Surface Types in 3D

Gaussian Curvature

$$K = \kappa_1 \, \kappa_2$$

Mean Curvature

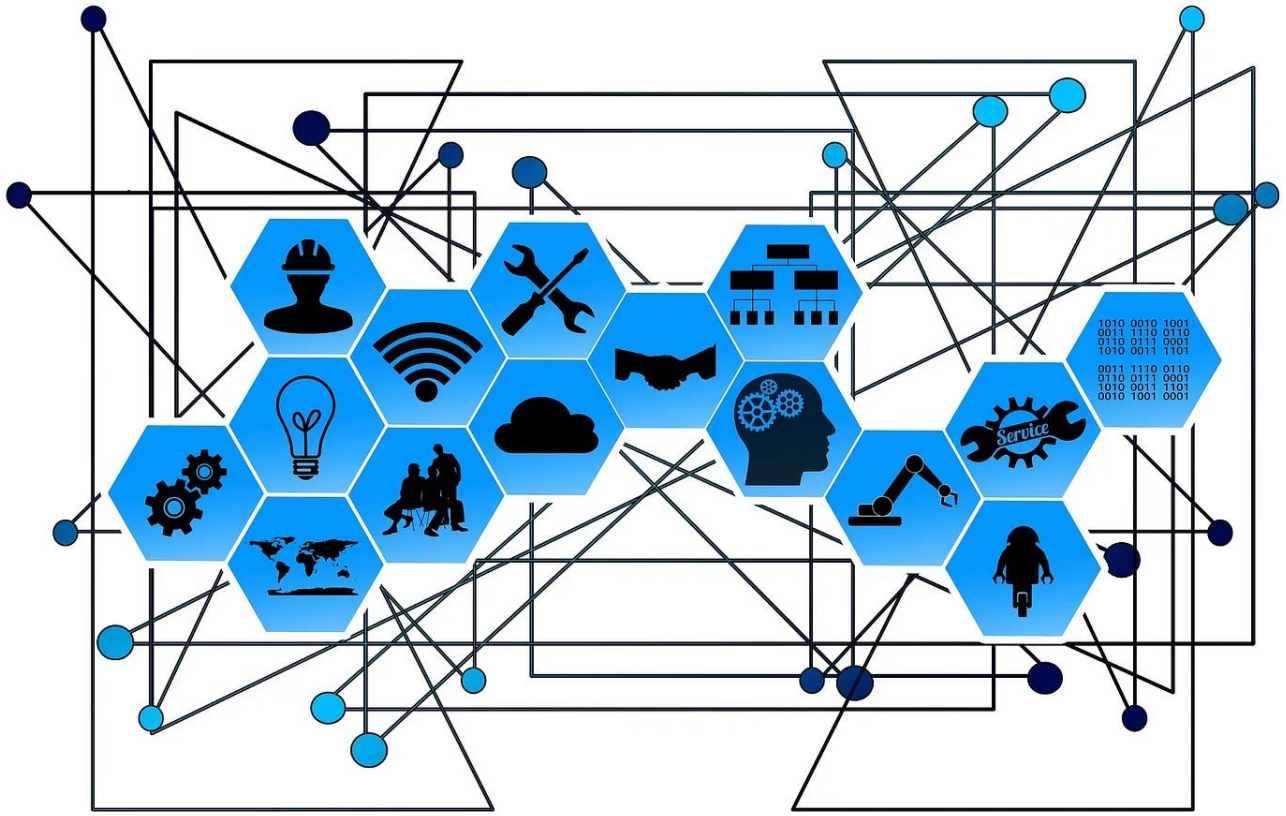
$$H = \frac{1}{2} \, (\kappa_1 + \kappa_2)$$

	$K<0$	$K=0$	$K>0$
$H<0$	*Saddle ridge* 	*Ridge* 	*Peak* 
$H=0$	*Minimal surface* 	*Plane* 	*Not possible*
$H>0$	*Saddle valley* 	*Valley* 	*Pit* 

Importance of Relational Structures

Examples:

- **A and B are friends**
- **Distance between A & B**
- **Similarity between A & B**



These provide information about structures of data

Mapping from Data Space to Embedding Space

Data X

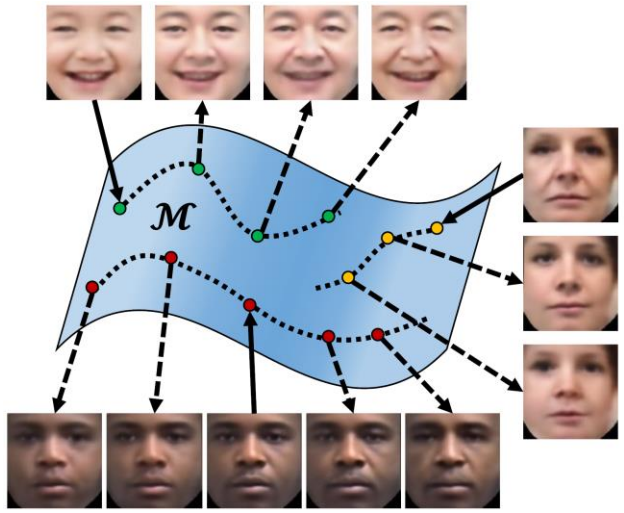
Embedding Y

Similarity

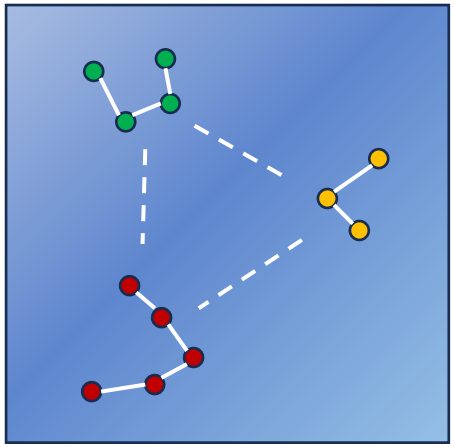
$p_{ij} \in (0, 1)$

Dissimilarity

$\tilde{p}_{ij} = 1 - p_{ij}$



DMT Network



Similarity

$q_{ij} \in (0, 1)$

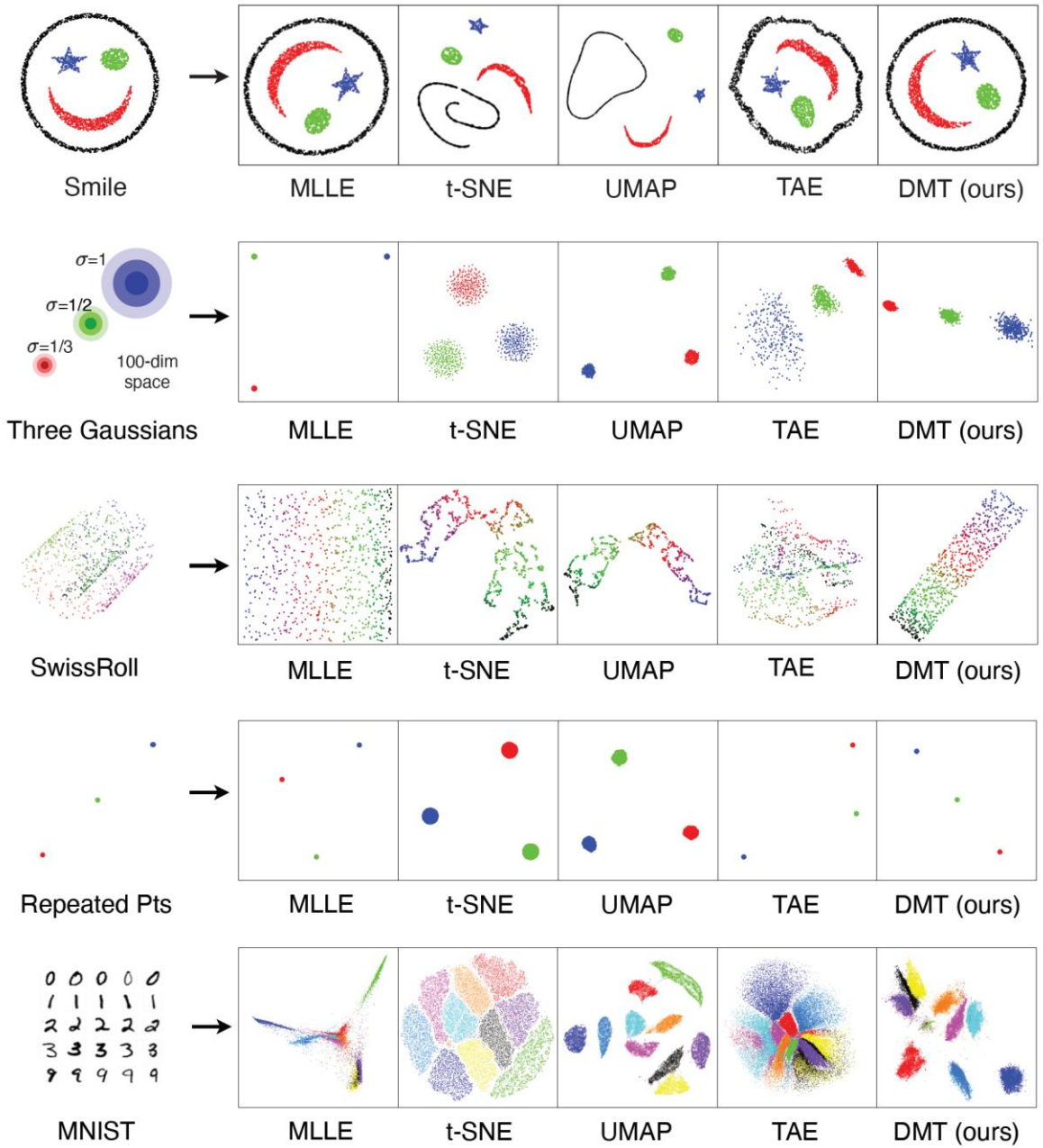
Dissimilarity

$\tilde{q}_{ij} = 1 - q_{ij}$

Local Relation-Preserving Loss for transforming $p_{ij}(X) \rightarrow q_{ij}(Y)$

KL Divergence Loss (t-SNE): $$KL(P\|Q) = \sum_i \sum_j p_{ij} \log \frac{p_{ij}}{q_{ij}}$$

Cross Entropy Loss (UMAP): $$CE(X,Y) = \sum_i \sum_j \left[p_{ij}(X) \log \left(\frac{p_{ij}(X)}{q_{ij}(Y)} \right) + (1 - p_{ij}(X)) \log \left(\frac{1 - p_{ij}(X)}{1 - q_{ij}(Y)} \right) \right]$$


Smile
MLLE
t-SNE
UMAP
TAE
DMT (ours)
σ=1
σ=1/2
σ=1/3
100-dim space
Three Gaussians
MLLE
t-SNE
UMAP
TAE
DMT (ours)
SwissRoll
MLLE
t-SNE
UMAP
TAE
DMT (ours)
Repeated Pts
MLLE
t-SNE
UMAP
TAE
DMT (ours)
MNIST
MLLE
t-SNE
UMAP
TAE
DMT (ours)

Thank You