Geometric Models

School of Electronic and Computer Engineering
Peking University

Wang Wenmin

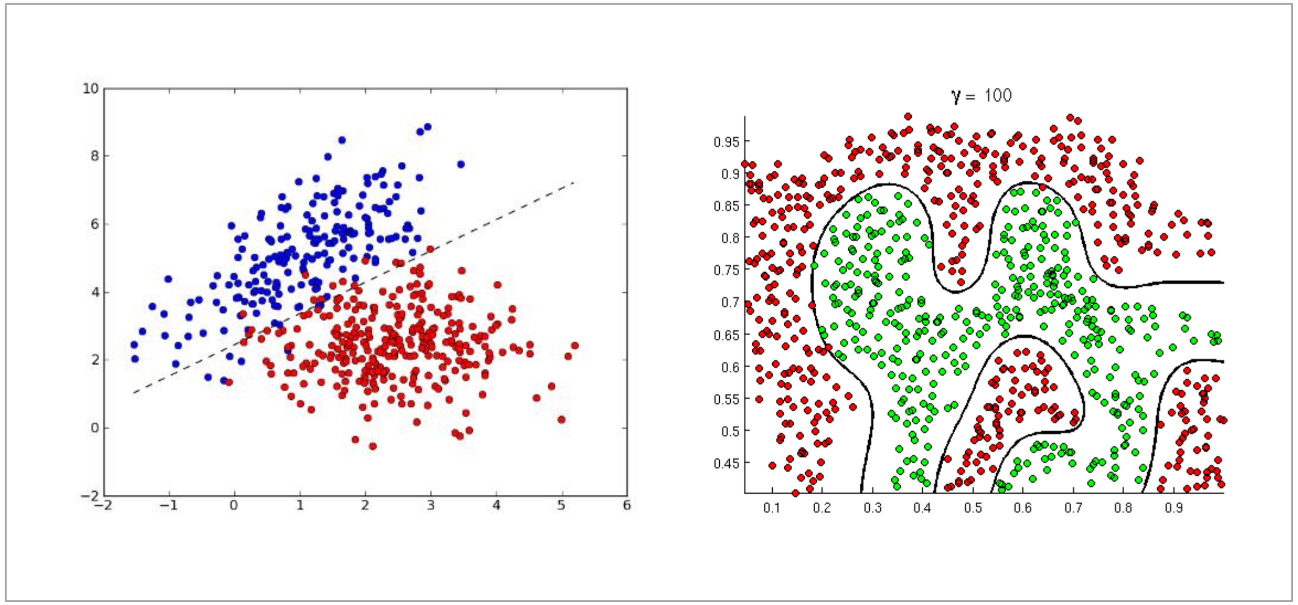
Contents:

What are Geometric Models 什么是几何模型

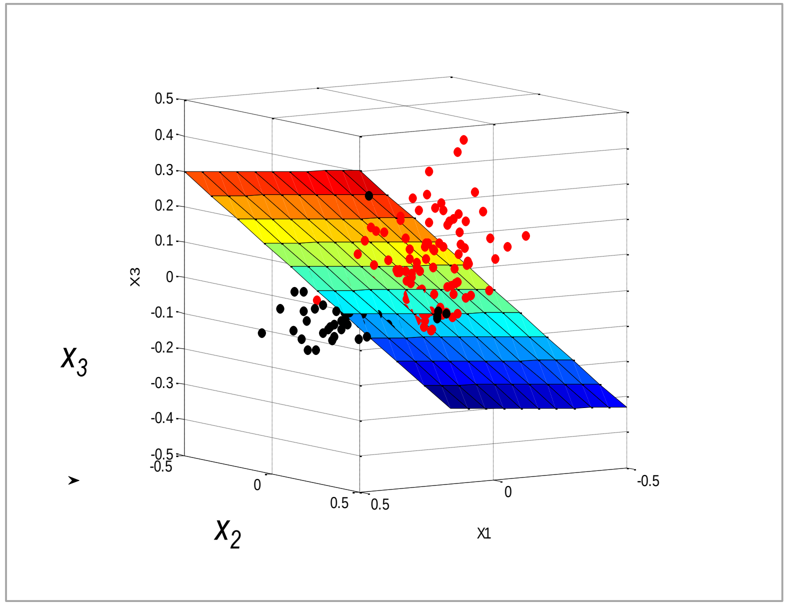
- A geometric model is constructed directly in instance space. The space can be thought as the geometric concepts, such as,
  几何模型直接在**实例空间**构建。空间可以被认为是几何的概念，例如:
  - Euclidean geometry: e.g., lines, planes, and Euclidean distances.
    欧式几何：如线、面、以及欧式距离。
  - Riemannian geometry: e.g., manifold, and Riemannian distances.
    黎曼几何：如流形、黎曼距离。
- The geometric model keeping to two or three dimensions is easy to visualize.
  二维或三维的几何模型**易于可视化**。
- Geometric concepts that potentially apply to high-dimensional spaces are usually prefixed with ‘hyper’: e.g., hyper-plane.
  可能适用于高维空间的几何概念通常冠以hyper (超)，例如：hyper-plane (超平面)。

Line and Plane 线与面

- Using such geometric models as line or plane to construct some algorithms for machine learning.
  使用线或平面这样的几何模型来构建一些机器学习算法。



A line in two dimension
二维中的线

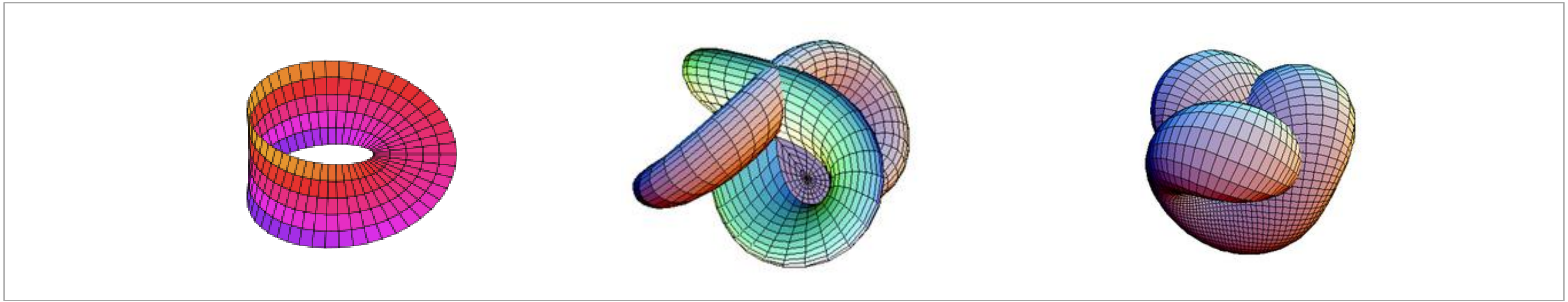


A plane in three dimensions
三维中的平面

Manifold 流形

What is Manifold 什么是流形

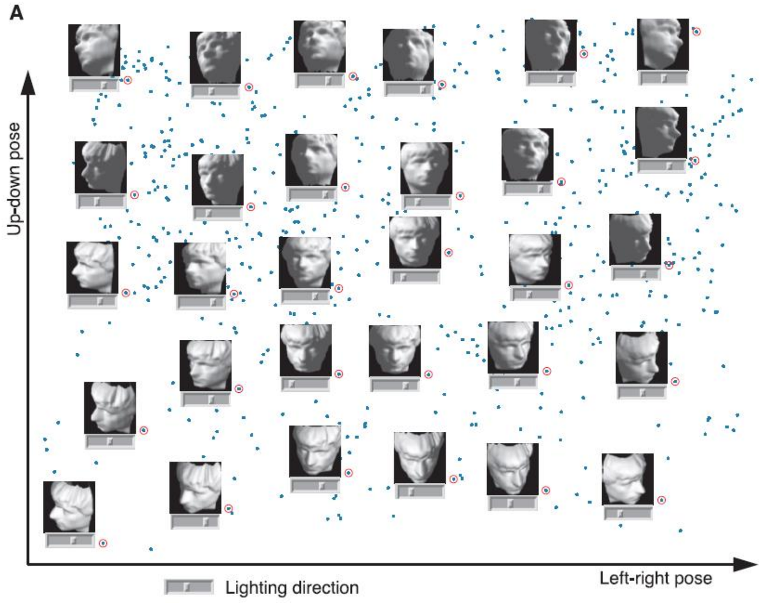
- A topological space that resembles Euclidean space near each point.
  一种拓扑空间，其每个点附近存在近似的**欧几里得空间**。
- More precisely, each point of an *n*-dimensional manifold has a neighborhood that is homeomorphic to the Euclidean space of dimension *n*.
  更精确地说，一个*n*维流形的每个点都有一个相邻点，它与维度为*n*的欧几里得空间同胚。

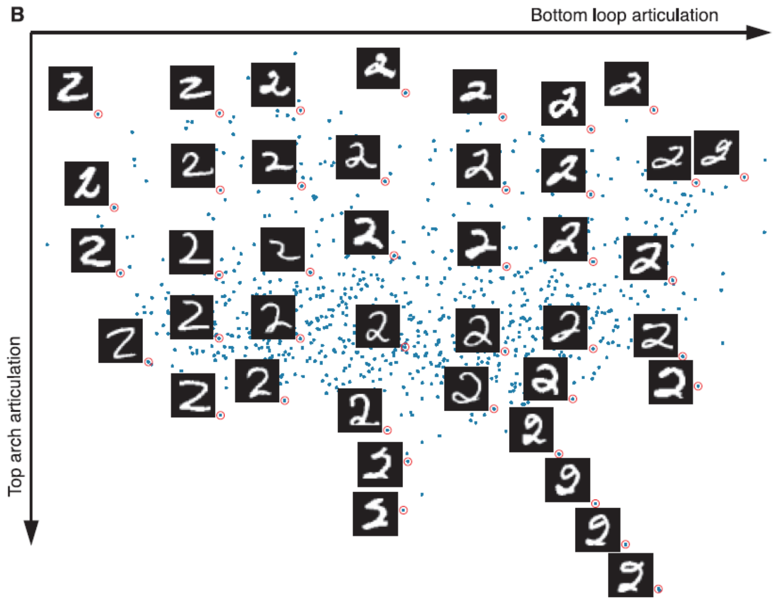


Manifold 流形

Why need Manifold 为什么需要流形

Source: Science, 290, 2000





(A) A sequence of 4096-dimensional vectors, representing the brightness values of 64x64 pixel images of a face rendered with different *poses* and *lighting directions*.

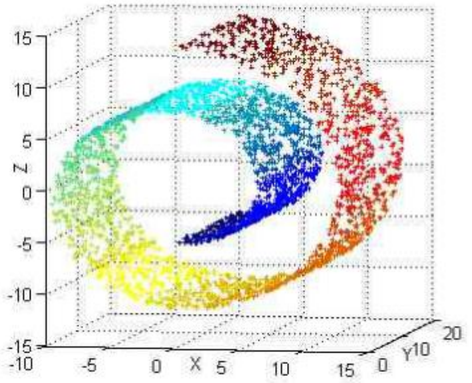
一个4096维的向量序列，表示64×64像素人脸图像的亮度值，呈现不同姿势和光照角度。

(B) N = 1000 handwritten “2”. The two most significant dimensions articulate the major features of the “2”: bottom loop articulation (x axis) and top arch articulations (y axis).

N = 1000的手写体“2”。两个最重要的维度刻画了“2”的主要特征： “2”的底部变化(x轴)和顶部变化 (y轴)。

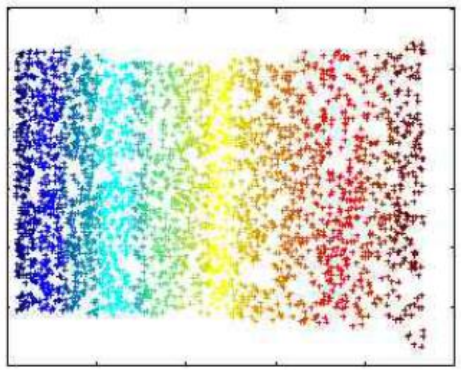
Manifold 流形

- Low-dimensional Structure of Data 数据的低维结构
  - Intrinsic low-dimensional properties can be found in high-dimensional input data.
    高维输入数据中可以发现其**固有的低维特性**。
- Low-dimensional Manifold Assumption 低维流形假设
  - High-dimensional input data is lying on a low-dimensional manifold.
    高维输入数据依附于一个**低维流形**。



Data points in a spiraling band (Swiss roll)
螺旋带（瑞士卷）上的数据点

Mapping



Unrolled manifold
拉平后的流形

Typical Algorithms of Manifold Learning 典型的流形学习的算法

- **Isomap** (Isometric mapping 等距映射)
  - Tenenbaum et al, "A Global Geometric Framework for Nonlinear Dimension Reduction" —种非线性降维的全局几何框架, *Science*, 290, 2000.
- **LLE** (Locally Linear Embeddings 局部线性嵌入)
  - Roweis et al, "Nonlinear Dimensionality Reduction by Locally Linear Embeddings" 凭借局部线性嵌入的非线性降维, *Science*, 290, 2000.
- **LE** (Laplacian Eigenmaps 拉普拉斯特征映射)
  - Belkin et al, "Laplacian Eigenmaps for Dimensionality Reduction and Data Representation" 用于降维和数据表达的特征映射, *NIPS* 2001.

Typical Algorithms of Manifold Learning 典型的流形学习的算法

- LTSA (Local Tangent Space Alignment 局部切空间对齐)
  - Zhang et al, “Principal Manifolds and Nonlinear Dimensionality Reduction via Local Tangent Space Alignment” 主要流形与采用局部切空间对齐的非线性降维, *SIAM Journal on Scientific Computing*, 26(1), 2005.
- Inductive Manifold Learning 归纳流形学习
  - Kim et al, “Inductive Manifold Learning Using Structured Support Vector Machine” 采用结构化支撑向量机的归纳流形学习, *Pattern Recognition*, 27(1), 2014.

Case Study 1: Isomap (Isometric mapping) 等距映射

- Isomap algorithm preserves geodesic distances but not the Euclidean distance.
  Isomap算法保留数据之间的测地线距离而不是欧几里得距离。
- A high-level description of the algorithm: 算法的简要描述

Source: Science, 290, 2000

确定每个点的相邻点。

Determine neighbors of each point.

构建一个邻接图。

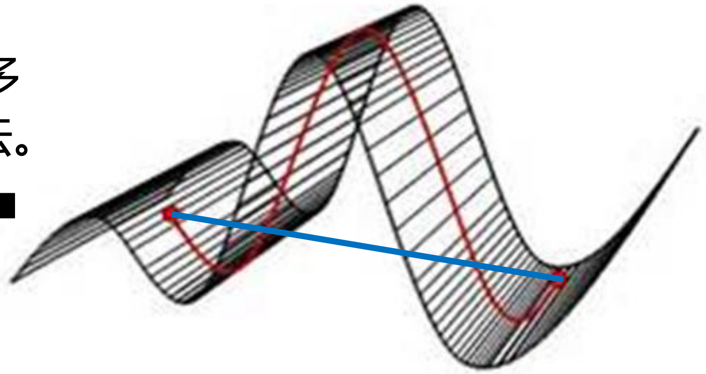
Construct a neighborhood graph.

计算两点之间的最短距离。

Compute shortest path between two nodes.

计算低维嵌入，采用多元尺度分析(MDS)方法。

Compute lower-dimensional embedding using Multi-dimensional Scaling (MDS).



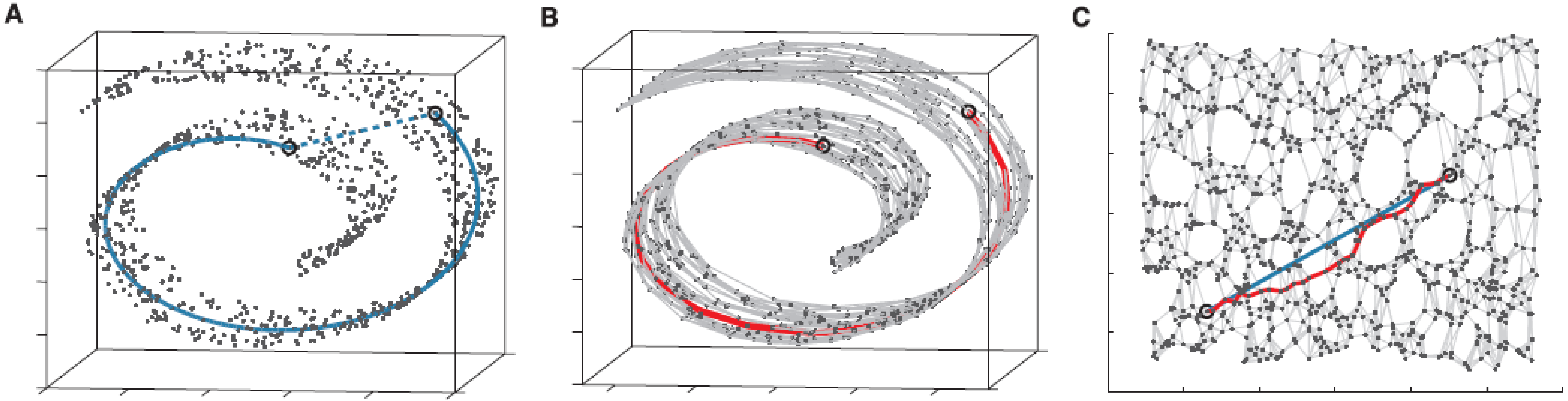
Geodesic distances
测地线距离

Euclidean distance
欧氏距离

Case Study 1: Isomap (Isometric mapping) 等距映射

- Using the “Swiss roll” data set to illustrate how Isomap exploits geodesic paths for nonlinear dimensionality reduction.

  采用“瑞士卷”数据集来说明Isomap如何利用测地线路径进行非线性降维。

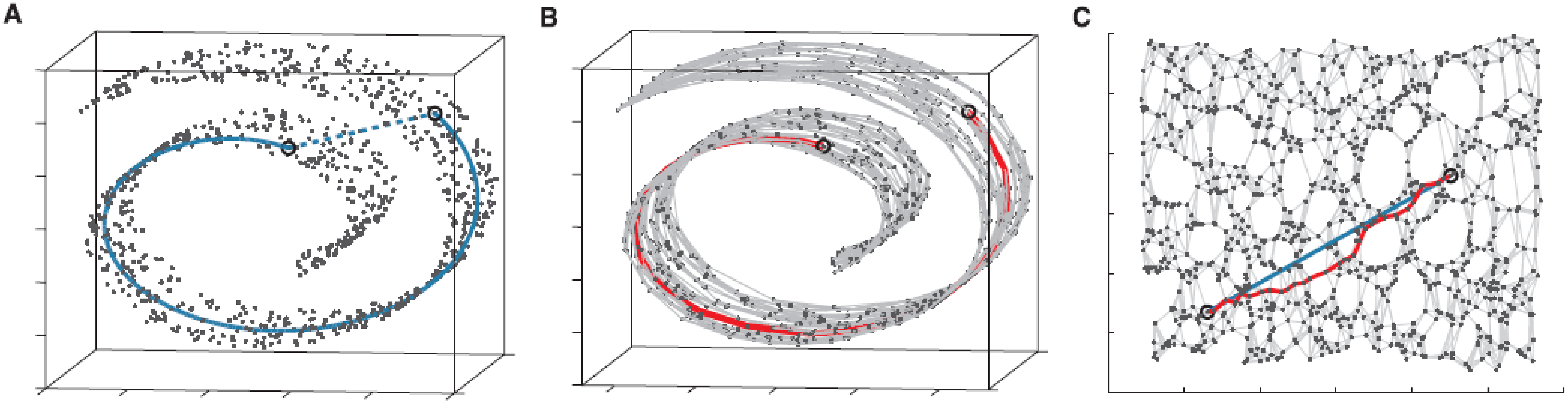


A. For two arbitrary points on a nonlinear manifold, their Euclidean distance is not equal to their geodesic distance.
图A：在非线性流形上任意两点间，其欧氏距离不等于其测地线距离。

Case Study 1: Isomap (Isometric mapping) 等距映射

- Using the “Swiss roll” data set to illustrate how Isomap exploits geodesic paths for nonlinear dimensionality reduction.

  采用“瑞士卷”数据集来说明Isomap如何利用测地线路径进行非线性降维。

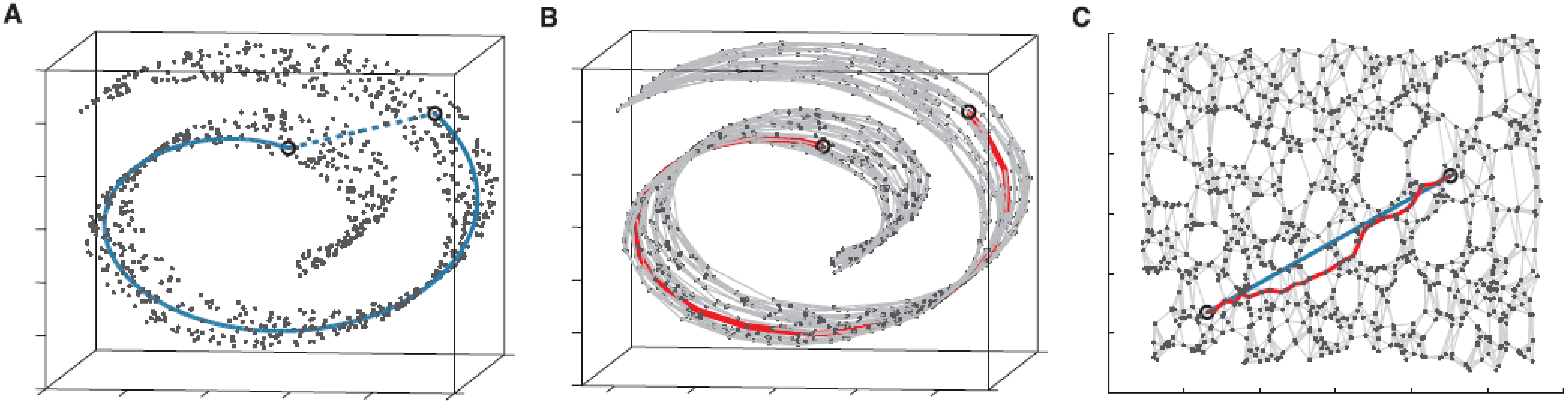


B. The neighborhood graph constructed by Isomap allows an approximation to the true geodesic path.
图B：由Isomap构建的邻接图，得到一条近似于真正的测地线路径。

Case Study 1: Isomap (Isometric mapping) 等距映射

- Using the “Swiss roll” data set to illustrate how Isomap exploits geodesic paths for nonlinear dimensionality reduction.

  采用“瑞士卷”数据集来说明Isomap如何利用测地线路径进行非线性降维。



C. The two-dimensional embedding by Isomap best preserves the shortest path distances in the neighborhood graph.
图C：由Isomap生成的二维嵌入，很好地保持了邻接图中最短路径的距离。

Case Study 2: LLE (Locally Linear Embedding) 局部线性嵌入

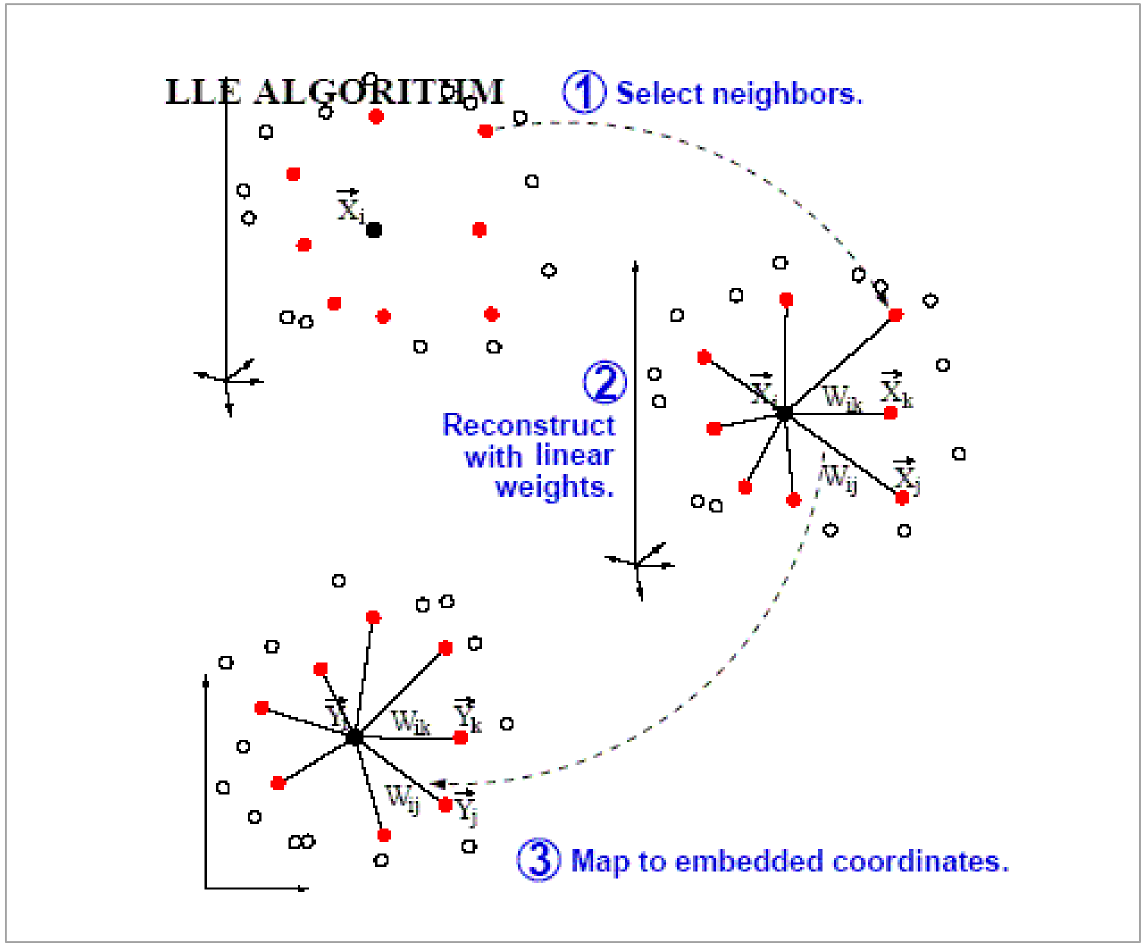
Source: Science, 290, 2000

- LLE embeds data points in a low-dimensional space by finding the optimal linear reconstruction in a small neighborhood.

  LLE通过在小邻域中找到最佳线性重构，将数据点嵌入在低维空间中。

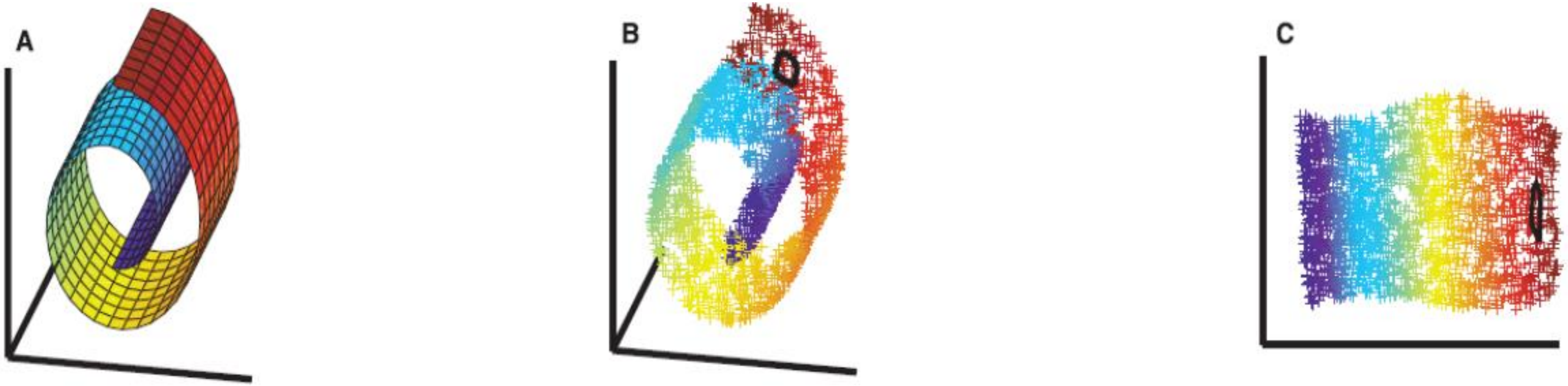
- It computes the reconstruction weights for each point, and then minimizes the embedding cost by solving an eigenvalue problem.

  它计算每个点的重建权重，然后通过求解特征值问题对嵌入成本进行最小化。



Case Study 2: LLE (Locally Linear Embedding) 局部线性嵌入

- Using the “Swiss roll” data set to illustrate how LLE exploits neighborhood for nonlinear dimensionality reduction. 采用“瑞士卷”数据集来说明LLE如何利用邻域来处理非线性降维。



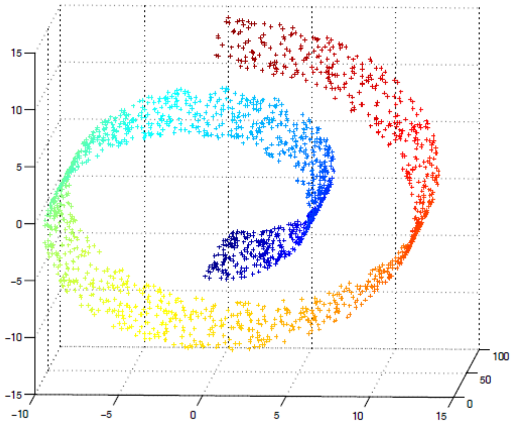
(A) The color coding illustrates the neighborhood preserving mapping discovered by LLE.
颜色编码说明由LLE获得的邻域保留映射。

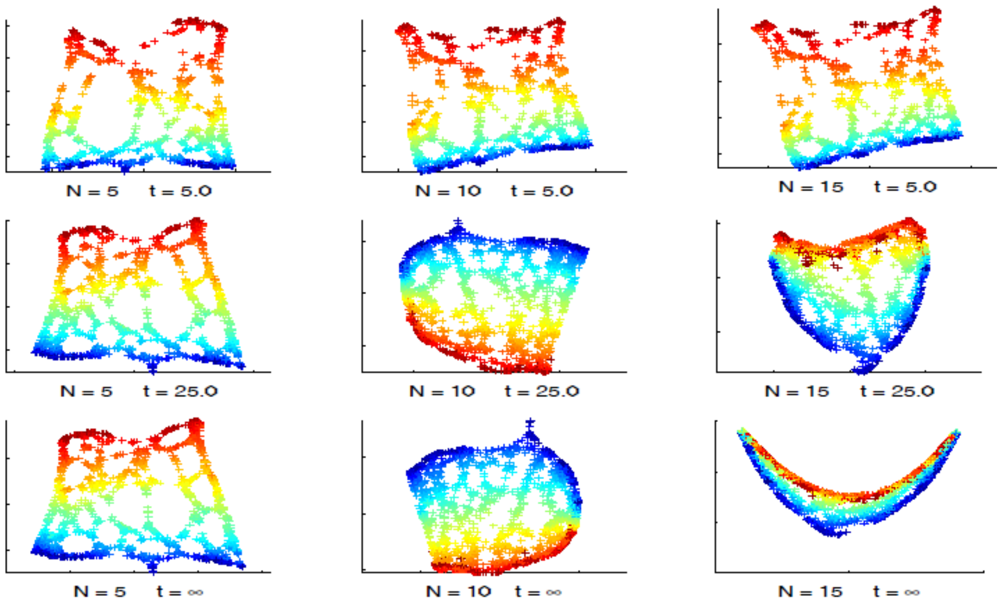
(B) Black outlines show the neighborhood of a single point on the “Swiss roll” .
黑色轮廓显示出在“瑞士卷”上单个点的邻域。

(C) Black outlines show the neighborhood of a single point on the unrolled roll”.
黑色轮廓显示出在拉平的“瑞士卷”上单个点的邻域。

Case Study 3: LE (Laplacian Eigenmaps) 拉普拉斯特征映射

- LE restates the nonlinear mapping problem as an embedding of vertices in a graph, and uses the graph Laplacian to derive a smooth mapping.
  LE重申将非线性映射问题作为一种图的顶点嵌入，并且采用图拉普拉斯来生成一个平滑的映射。

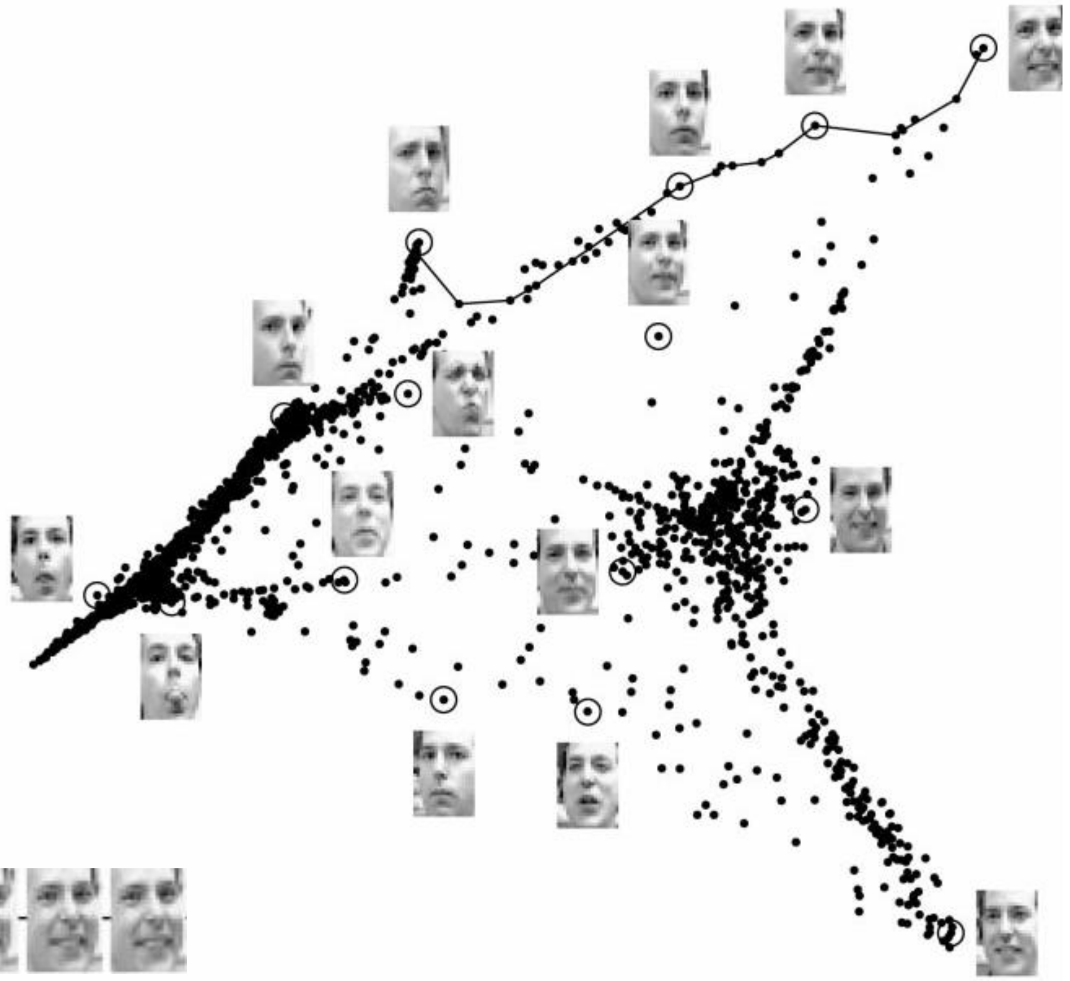




N denotes number of nearest neighbors, and *t* denotes kernel parameters.
*N*表示最近邻接点的数量，而*t*表示核参数。

Typical Applications of Manifold Learning 典型的流形学习应用

- Image processing 图像处理
- Gene expression profiles 基因表达图谱
- Handwriting recognition 手写体识别
- Face recognition 人脸识别



Source: Science, 290, 2000

The right and bottom images show the two-dimensional embeddings of faces discovered by LLE algorithm.

右侧和下面的图像展示由LLE算法获得的人脸二维线性嵌入。

Thank you for your attention!

AI