Manifold Learning

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STAT 4690–Applied Multivariate Analysis

Dimension reduction redux i

- Recall Pearson's approach to PCA: **best approximation of the data by a linear manifold**.
- Let's unpack this definition:
    - We're looking for a linear subspace of $\mathbb{R}^p$ of dimension k.
    - For a fixed k, we want to minimise the error when projecting onto the linear subspace.
    - We can also identify that subspace with $\mathbb{R}^k$ (e.g. for visualisation).

Dimension reduction redux ii

- **Manifold learning** is a nonlinear approach to dimension reduction, where:
  - We assume the data lies on (or close to) a nonlinear manifold of dimension k in $\mathbb{R}^p$.
  - We project the data from the manifold to $\mathbb{R}^k$.
- There are two main classes of methods:
  - Distance preserving (e.g. Isomap);
  - Topology preserving (e.g. Locally linear embedding)

Manifolds–Definition

- Roughly speaking, **manifolds** of dimension k are geometric objects that locally look like $\mathbb{R}^k$.
    - Every point on the manifold has an open neighbourhood that is equivalent to an open ball in $\mathbb{R}^k$.
- Examples in $\mathbb{R}^p$ include any curve, the $(p-1)$-dimensional sphere, or any linear subspace.
- Some manifolds have boundaries (e.g. a cylinder) or corners (e.g. a cube).

Swiss roll i

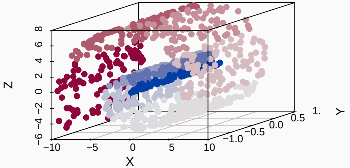
```r
n <- 1000
F1 <- runif(n, 0, 10)
F2 <- runif(n, -1, 1)
```

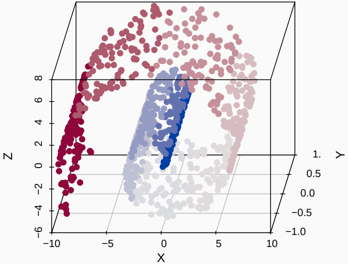
```r
X <- F1 * cos(F1)
Y <- F2
Z <- F1 * sin(F1)
```

Swiss roll ii

```r
library(scatterplot3d)
library(colorspace)
colours <- cut(F1, breaks = seq(0, 10),
               labels = diverging_hcl(10))
par(mfrow = c(1, 2))
scatterplot3d(X, Y, Z, pch = 19, asp = 1,
              color = colours)
scatterplot3d(X, Y, Z, pch = 19, asp = 1,
              color = colours, angle = 80)
```

Swiss roll iii



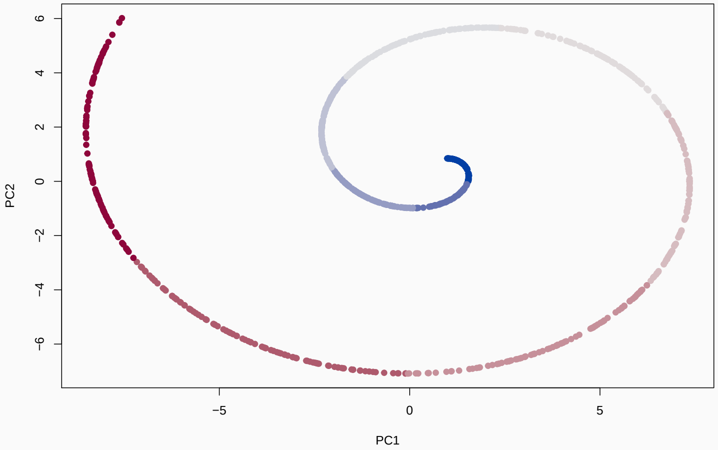


Swiss roll iv

```r
# Let's see if PCA can unroll the Swiss roll
decomp <- prcomp(cbind(X, Y, Z))

plot(decomp$x[,1:2],
     col = as.character(colours), pch = 19)
```

Swiss roll v



MNIST data revisited

- To study the nonlinear dimension reduction methods in this lecture, we will restrict our attention to the digit 2 in the MNIST dataset.
- The reason: we can think of the different shapes of 2 as "smooth deformations" of one another.
    - This would work for other digits too (e.g. 6, 9, 8), but not all (e.g. 4, 7).

Example i

```r
library(dslabs)
library(tidyverse)

mnist <- read_mnist()

data <- mnist$train$images[mnist$train$labels == 2, ]
```

Example ii

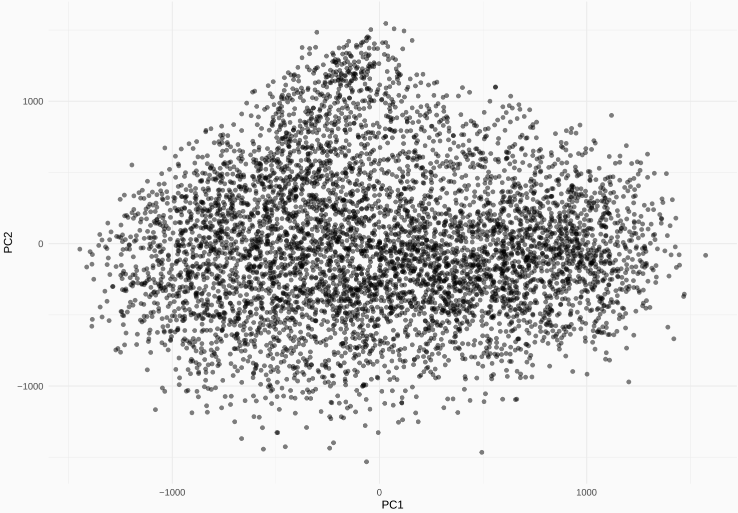
```r
par(mfrow = c(1, 2))
# With crossing
matrix(data[1,], ncol = 28)[ , 28:1] %>%
  image(col = gray.colors(12, rev = TRUE),
        axes = FALSE, asp = 1)
# Without crossing
matrix(data[4,], ncol = 28)[ , 28:1] %>%
  image(col = gray.colors(12, rev = TRUE),
        axes = FALSE, asp = 1)
```

Example iii

Example iv

```r
decomp <- prcomp(data)
decomp$x[,1:2] %>%
  as.data.frame() %>%
  ggplot(aes(PC1, PC2)) +
  geom_point(alpha = 0.5) +
  theme_minimal()
```

Example v



Example vi

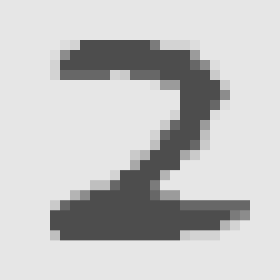
```r
# First PC
par(mfrow = c(1, 2))
index_right <- which.max(decomp$x[,1])
matrix(data[index_right,], ncol = 28)[ , 28:1] %>%
  image(col = gray.colors(12, rev = TRUE),
        axes = FALSE, asp = 1)
index_left <- which.min(decomp$x[,1])
matrix(data[index_left,], ncol = 28)[ , 28:1] %>%
  image(col = gray.colors(12, rev = TRUE),
        axes = FALSE, asp = 1)
```

Example vii

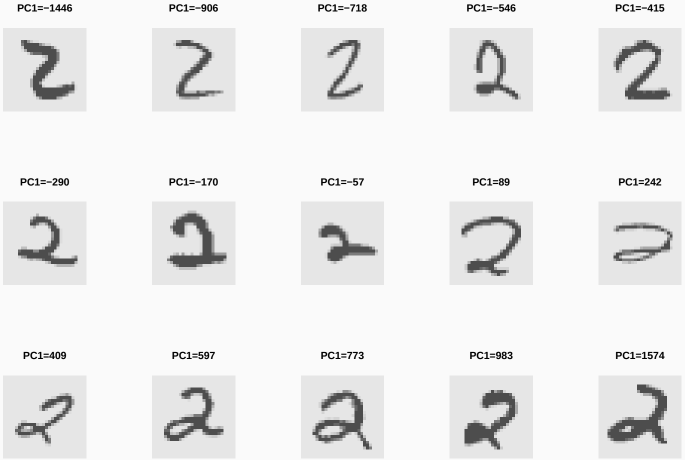
Example viii

```
# Second PC
par(mfrow = c(1, 2))
index_top <- which.max(decomp$x[,2])
matrix(data[index_top,], ncol = 28)[ , 28:1] %>%
  image(col = gray.colors(12, rev = TRUE),
        axes = FALSE, asp = 1)
index_bottom <- which.min(decomp$x[,2])
matrix(data[index_bottom,], ncol = 28)[ , 28:1] %>%
  image(col = gray.colors(12, rev = TRUE),
        axes = FALSE, asp = 1)
```

Example ix



Example x



PC1=−1446
PC1=−906
PC1=−718
PC1=−546
PC1=−415
PC1=−290
PC1=−170
PC1=−57
PC1=89
PC1=242
PC1=409
PC1=597
PC1=773
PC1=983
PC1=1574

Example xi

Isomap

Isomap

- Let's look at the algorithm and study each step separately.

Basic algorithm

1. Create a graph $\mathcal{G}$ from the data, where each data point is a node, and two nodes are connected if they are "neighbours".
2. Each edge gets a weight corresponding to the Euclidean distance between the two data points.
3. Create a distance matrix Δ, where the (i, j)-th element is the length of the shortest path in $\mathcal{G}$ between the data points corresponding to nodes i and j.
4. Perform metric Multidimensional Scaling on Δ to obtain the projection onto a lower dimensional subspace.

Definition of neighbourhood

- Two ways of defining the neighbours of a point $\mathbf{Y}$:
  - For an integer $K \geq 1$, we could look at the K-nearest neighbours, i.e. the K points $\mathbf{Y}_1, \ldots, \mathbf{Y}_K$ that are closest (in Euclidean distance) to $\mathbf{Y}$.
  - For a real number $\epsilon > 0$, we could look at all points $\mathbf{Y}_1, \ldots, \mathbf{Y}_{n(\epsilon)}$ whose distance from $\mathbf{Y}$ is less than ϵ.
- **Note**: The first definition guarantees that every point has neighbours, whereas you could get unconnected points using the second definition.
- You could also use a hybrid of both approaches where you take the K-nearest neighbours, but discard neighbours that are "too far away".

Shortest path distance i

- Once we have our weighted graph $\mathcal{G}$ (i.e. nodes represent data points, edges represent neighbours, weights are Euclidean distances), we can compute the length of any path from $\mathbf{Y}_i$ to $\mathbf{Y}_j$ by summing the weights of all the edges along the path.
- We then define a **distance** function on $\mathcal{G}$ by

$$\Delta_{ij} = \min \{\text{Length of path } \gamma \mid \gamma \text{ is a path from } \mathbf{Y}_i \text{ to } \mathbf{Y}_j\}.$$

Shortest path distance ii

- There are efficient algorithms for computing this distance for any weighted graph:
  - Dijkstra's algorithm;
  - Floyd–Warshall algorithm.
- For more details about these algorithms, take a course on graph theory!

Multidimensional Scaling

Recall the algorithm for MDS.

Algorithm (MDS)
Input: Δ; Output: $\tilde{X}$

1. Create the matrix D containing the square of the entries in Δ.
2. Create S by centering both the rows and the columns and multiplying by $-\frac{1}{2}$.
3. Compute the eigenvalue decomposition $S = U\Lambda U^T$.
4. Let $\tilde{X}$ be the matrix containing the first r columns of $\Lambda^{1/2}U^T$.

Swiss roll i

```
library(dimRed)
```

```
isomap_sr <- embed(cbind(X, Y, Z), "Isomap", knn = 10,
                   ndim = 2)
```

```
## 2019-11-20 10:08:31: Isomap START
```

```
## 2019-11-20 10:08:31: constructing knn graph
```

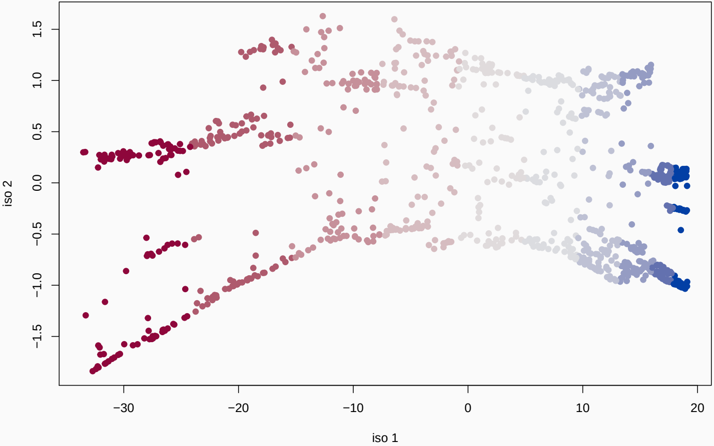
```
## 2019-11-20 10:08:31: calculating geodesic distances
```

Swiss roll ii

```
## 2019-11-20 10:08:31: Classical Scaling
```

```
isomap_sr@data@data %>%
  plot(col = as.character(colours), pch = 19)
```

Swiss roll iii



Example i

```
isomap_res <- embed(data, "Isomap", knn = 10,
                    ndim = 2)
```

```
## 2019-11-20 10:08:32: Isomap START
```

```
## 2019-11-20 10:08:32: constructing knn graph
```

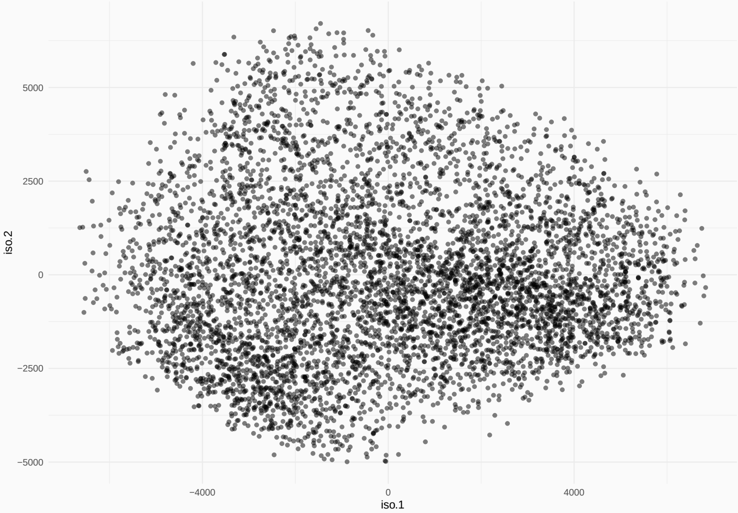
```
## 2019-11-20 10:08:52: calculating geodesic distances
```

```
## 2019-11-20 10:09:05: Classical Scaling
```

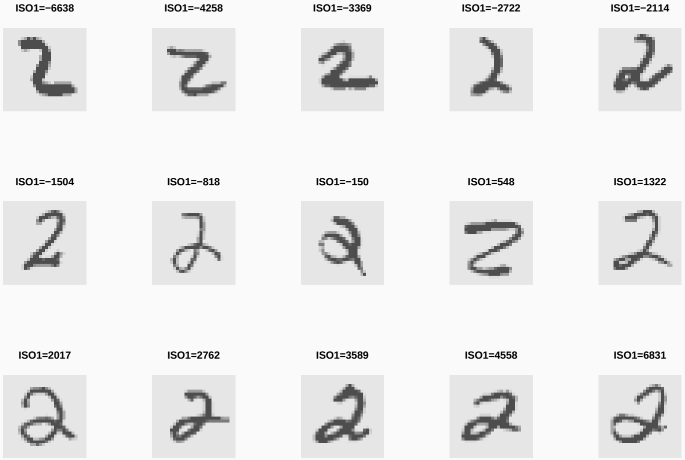
Example ii

```r
isomap_res@data %>%
  as.data.frame() %>%
  ggplot(aes(iso.1, iso.2)) +
  geom_point(alpha = 0.5) +
  theme_minimal()
```

Example iii



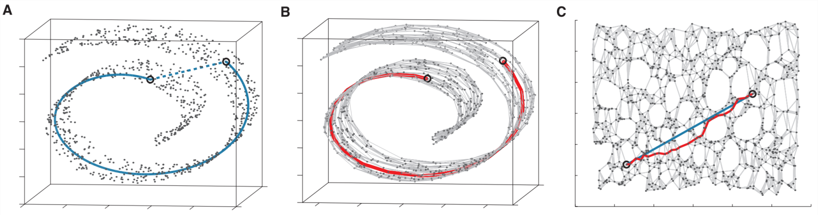
Example iv


ISO1=−6638
ISO1=−4258
ISO1=−3369
ISO1=−2722
ISO1=−2114
ISO1=−1504
ISO1=−818
ISO1=−150
ISO1=548
ISO1=1322
ISO1=2017
ISO1=2762
ISO1=3589
ISO1=4558
ISO1=6831

Intuition i

- The reason why Isomap works is because the shortest path distance approximates the **geodesic** distance on the manifold
    - "Train tracks distance"
- If we embed the weighted graph in $\mathbb{R}^p$, with each nodes at its corresponding data point, and each edge having length equal to the Euclidean distance, we can see the graph as a scaffold of the manifold.
- As we increase the sample size, the scaffold "converges" to the actual manifold.

Intuition ii



Tenenbaum *et al.* Science (2000)

Further examples i

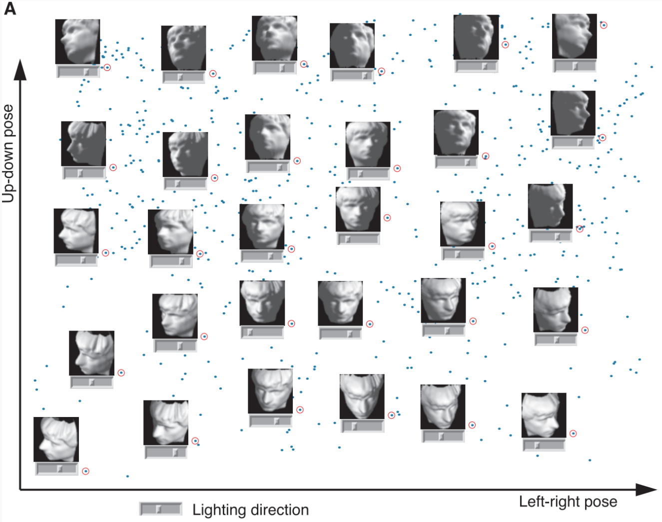


Figure 1

Further examples ii

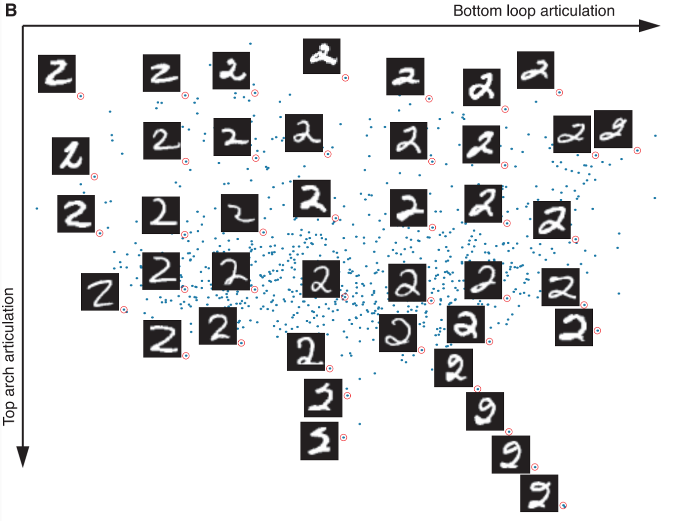


Figure 2

Comments

- Advantages:
  - Simple extension of MDS
  - Preserves distance relationship on the manifold
- Disadvantages:
  - Computing the shortest path distance can be expensive with many data points
  - Doesn't work well with all manifolds (e.g. it fails when the underlying manifold has holes or many folds)