# Lecture 8: Multidimensional scaling 

Advanced Applied Multivariate Analysis
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## Multidimensional scaling

Goal of Multidimensional scaling (MDS): Given pairwise dissimilarities, reconstruct a map that preserves distances.

- From any dissimilarity (no need to be a metric)
- Reconstructed map has coordinates $\mathbf{x}_{i}=\left(x_{i 1}, x_{i 2}\right)$ and the natural distance $\left(\left\|\mathbf{x}_{i}-\mathbf{x}_{j}\right\|_{2}\right)$


Reordered Dissimilarity Matrix


## Multidimensional scaling

- MDS is a family of different algorithms, each designed to arrive at optimal low-dimensional configuration ( $p=2$ or 3 )
- MDS methods include
(1) Classical MDS
(2) Metric MDS
(3) Non-metric MDS


## Perception of Color in human vision

- To study the perceptions of color in human vision (Ekman, 1954, Izenman 13.2.1)
- 14 colors differing only in their hue (i.e., wavelengths from $434 \mu \mathrm{~m}$ to $674 \mu \mathrm{~m}$ )
- 31 people to rate on a five-point scale from 0 (no similarity at all) to 4 (identical) for each of $\binom{14}{2}$ pairs of colors.
- Average of 31 ratings for each pair (representing similarity) is then scaled and subtracted from 1 to represent dissimilarities


## Perception of Color in human vision

The resulting $14 \times 14$ dissimilarity matrix is symmetric, and contains zeros in the diagonal. MDS seeks a 2D configuration to represent these colors.

```
    434
445 0.14
465 0.58 0.50
472 0.58 0.56 0.19
490}00.820.78 0.53 0.4
504 0.94 0.91 0.83 0.75 0.39
537}00.930.93 0.90 0.90 0.69 0.38
555 0.96 0.93 0.92 0.91 0.74 0.55 0.27
584 0.98}0.9.980.98 0.98 0.93 0.86 0.78 0.67
600 0.93 0.96 0.99 0.99 0.98 0.92 0.86 0.81 0.42
610}00.910.93 0.98 1.00 0.98 0.98 0.95 0.96 0.63 0.26
628 0.88 0.89 0.99 0.99 0.99 0.98 0.98 0.97 0.73 0.50 0.24
651}00.870.870.95 0.98 0.98 0.98 0.98 0.98 0.80 0.59 0.38 0.15
674 0.84 0.86 0.97 0.96 1.00 0.99 1.00 0.98 0.77 0.72 0.45 0.32 0.24
```


## Perception of Color in human vision

MDS reproduces the well-known two-dimensional color circle.

Non-metric MDS


Metric MDS



## Distance, dissimilarity and similarity

Distance, dissimilarity and similarity (or proximity) are defined for any pair of objects in any space. In mathematics, a distance function (that gives a distance between two objects) is also called metric, satisfying
(1) $d(x, y) \geq 0$,
(2) $d(x, y)=0$ if and only if $x=y$,
(3) $d(x, y)=d(y, x)$,
(4) $d(x, z) \leq d(x, y)+d(y, z)$.

Given a set of dissimilarities, one can ask whether these values are distances and, moreover, whether they can even be interpreted as Euclidean distances

## Euclidean and non-Euclidean distance

Given a dissimilarity (distance) matrix $D=\left(d_{i j}\right)$, MDS seeks to find $\mathbf{x}_{1}, \ldots, \mathbf{x}_{n} \in \mathbb{R}^{p}$ so that

$$
d_{i j} \approx\left\|\mathbf{x}_{i}-\mathbf{x}_{j}\right\|_{2} \text { as close as possible. }
$$

Oftentimes, for some large $p$, there exists a configuration $\mathbf{x}_{1}, \ldots, \mathbf{x}_{n}$ with exact distance match $d_{i j} \equiv\left\|\mathbf{x}_{i}-\mathbf{x}_{j}\right\|_{2}$. In such a case the distance $d$ involved is called a Euclidean distance.
There are, however, cases where the dissimilarity is distance, but there exists no configuration in any $p$ with perfect match

$$
d_{i j} \neq\left\|\mathbf{x}_{i}-\mathbf{x}_{j}\right\|_{2}, \text { for some } i, j
$$

Such a distance is called non-Euclidean distance.

## non-Euclidean distance

- Radian distance function on a circle is a metric.
- Cannot be embedded in $\mathbb{R}$. (Not for any $\mathbb{R}^{p}$, not shown here)

(b)

| Point | a | b | c | d |
| :---: | :---: | :---: | :---: | :---: |
| a | 0.0000 | 3.1416 | 0.7854 | 1.5708 |
| b | 3.1416 | 0.0000 | 2.3562 | 1.5708 |
| c | 0.7854 | 2.3562 | 0.0000 | 2.3562 |
| d | 1.5708 | 1.5708 | 2.3562 | 0.0000 |

- Nevertheless, MDS seeks to find an optimal configuration $\mathbf{x}_{i}$ that gives $d_{i j} \approx\left\|\mathbf{x}_{i}-\mathbf{x}_{j}\right\|_{2}$ as close as possible.


## classical Multidimensional Scaling-theory

Suppose for now we have Euclidean distance matrix $D=\left(d_{i j}\right)$.
The objective of classical Multidimensional Scaling (cMDS) is to find $X=\left[x_{1}, \ldots, x_{n}\right]$ so that $\left\|x_{i}-x_{j}\right\|=d_{i j}$. Such a solution is not unique, because if $X$ is the solution, then $X^{*}=X+c, c \in \mathbb{R}^{q}$ also satisfies $\left\|x_{i}^{*}-x_{j}^{*}\right\|=\left\|\left(x_{i}+c\right)-\left(x_{j}+c\right)\right\|=\left\|x_{i}-x_{j}\right\|=d_{i j}$. Any location $c$ can be used, but the assumption of centered configuration, i.e.,

$$
\begin{equation*}
\sum_{i=1}^{n} x_{i k}=0, \text { for all } k \tag{1}
\end{equation*}
$$

serves well for the purpose of dimension reduction.

## classical Multidimensional Scaling-theory

In short, the cMDS finds the centered configuration
$\mathbf{x}_{1}, \ldots, \mathbf{x}_{n} \in \mathbb{R}^{q}$ for some $q \geq n-1$ so that their pairwise distances are the same as those corresponding distances in $D$.

We may find the $n \times n$ Gram matrix $B=X^{\prime} X$, rather than $X$. The Gram matrix is the inner product matrix since $X$ is assumed to be centered. We have

$$
\begin{equation*}
d_{i j}^{2}=b_{i i}+b_{j j}-2 b_{i j} \tag{2}
\end{equation*}
$$

from $\left\|x_{i}-x_{j}\right\|^{2}=x_{i}^{\prime} x_{i}+x_{j}^{\prime} x_{j}-2 x_{i}^{\prime} x_{j}$.

## classical Multidimensional Scaling-theory

The constraints (1) leads to

$$
\sum_{i=1}^{n} b_{i j}=\sum_{i=1}^{n} \sum_{k=1}^{q} x_{i k} x_{j k}=\sum_{k=1}^{q} x_{j k} \sum_{i=1}^{n} x_{i k}=0
$$

for $j=1, \ldots, n$.
With a notation $T=\operatorname{trace}(B)=\sum_{i=1}^{n} b_{i i}$, we have

$$
\begin{equation*}
\sum_{i=1}^{n} d_{i j}^{2}=T+n b_{j j}, \sum_{j=1}^{n} d_{i j}^{2}=T+n b_{i i}, \sum_{j=1}^{n} \sum_{i=1}^{n} d_{i j}^{2}=2 n T \tag{3}
\end{equation*}
$$

## classical Multidimensional Scaling-theory

Combining (2) and (3), the solution is unique:

$$
b_{i j}=-1 / 2\left(d_{i j}^{2}-d_{. j}^{2}-d_{i .}^{2}+d_{. .}^{2}\right)
$$

or

$$
B=-1 / 2 C D_{2} C
$$

A solution $X$ is then given by the eigen-decomposition of $B$. That is, for $B=V \wedge V^{\prime}$,

$$
\begin{equation*}
X=\Lambda^{1 / 2} V^{\prime} \tag{4}
\end{equation*}
$$

## classical Multidimensional Scaling-theory

The space which $X$ lies is the eigenspace where the first coordinate contains the largest variation, and is identified with $\mathbb{R}^{q}$.

If we wish to reduce the dimension to $p \leq q$, then the first $p$ rows of $X_{(p)}$ best preserves the distances $d_{i j}$ among all other linear dimension reduction of $X$ (to $p$ ). Then

$$
X_{(p)}=\Lambda_{p}^{1 / 2} V_{p}^{\prime}
$$

where $\Lambda_{p}$ is the first $p \times p$ sub matrix of $\Lambda, V_{p}$ is collected through the first $p$ columns of $V$.

## classical Multidimensional Scaling

- cMDS gives configurations $X_{(p)}$ in $\mathbb{R}^{p}$ for any dimension $p=1,2, \ldots, q$.
- Configuration is centered.
- The coordinates are given by the principal order of largest-to-smallest variances.
- Dimension reduction from $X=X_{(q)}$ to $X_{(p)}(p<q)$ is same as PCA.
- Leads exact solution for Euclidean distances
- Can be used for non-Euclidean distances, in fact, for any dissimilarities.


## cMDS examples

- Consider two worked examples: one with Euclidean geometry (tetrahedron-edge length 1), the other from the circular geometry, shown below.

- And the airline distances example (Izenman 13.1.1)


## cMDS examples: tetrahedron

Pairwise distance matrix for tetrahedron (with distance 1)

$$
D=\left(\begin{array}{llll}
0 & 1 & 1 & 1 \\
1 & 0 & 1 & 1 \\
1 & 1 & 0 & 1 \\
1 & 1 & 1 & 0
\end{array}\right)
$$

leading to the gram matrix $B_{(4 \times 4)}$ with eigenvalues (.5,.5,.5, 0). Using dimension $p=3$, we have perfectly retrieved the tetrahedron.


## cMDS examples: circular distances

Pairwise distance matrix

| Point | a | b | c | d |
| :---: | :---: | :---: | :---: | :---: |
| a | 0.0000 | 3.1416 | 0.7854 | 1.5708 |
| b | 3.1416 | 0.0000 | 2.3562 | 1.5708 |
| c | 0.7854 | 2.3562 | 0.0000 | 2.3562 |
| d | 1.5708 | 1.5708 | 2.3562 | 0.0000 |

leading to the gram matrix $B_{(4 \times 4)}$ with eigenvalues

$$
\operatorname{diag}(\Lambda)=(5.6117,-1.2039,-0.0000,2.2234)
$$

In retrieving the coordinate matrix $X$, we cannot take a squareroot of $\Lambda$ since it gives complex numbers.
Remedy: Keep only positive eigenvalues and corresponding coordinates. In this case, take coordinates 1 and 4. This is the price we pay in approximating non-Euclidean geometry by Euclidean geometry.

## cMDS examples: circular distances

Using dimension $p=2$ (cannot use $p>2$ ), configuration $X_{(2)}$ is


Compare the original distance matrix $D$ and approximated distance matrix $\hat{D}=\left\|x_{i}-x_{j}\right\|_{2}$ :

$$
\left(\begin{array}{cccc}
0 & 3.1416 & 0.7854 & 1.5708 \\
3.1416 & 0 & 2.3562 & 1.5708 \\
0.7854 & 2.3562 & 0 & 2.3562 \\
1.5708 & 1.5708 & 2.3562 & 0
\end{array}\right), \quad \hat{D}=\left(\begin{array}{cccc}
0 & 3.1489 & 1.4218 & 1.9784 \\
3.1489 & 0 & 2.5482 & 1.8557 \\
1.4218 & 2.5482 & 0 & 2.3563 \\
1.9784 & 1.8557 & 2.3563 & 0
\end{array}\right)
$$

## cMDS examples: Airline distances

TABLE 13.2. Airline distances ( km ) between 18 cities. Source: Atlas of the World, Revised 6th Edition, National Geographic Society, 1995, p. 131.

|  | Beijing | Cape Town | Hong Kong | Honolulu | London | Melbourne |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Cape Town | 12947 |  |  |  |  |  |
| Hong Kong | 1972 | 11867 |  |  |  |  |
| Honolulu | 8171 | 18562 | 8945 |  |  |  |
| London | 8160 | 9635 | 9646 | 11653 |  |  |
| Melbourne | 9093 | 10338 | 7392 | 8862 | 16902 |  |
| Mexico | 12478 | 13703 | 14155 | 6098 | 8947 | 13557 |
| Montreal | 10490 | 12744 | 12462 | 7915 | 5240 | 16730 |
| Moscow | 5809 | 10101 | 7158 | 11342 | 2506 | 14418 |
| New Delhi | 3788 | 9284 | 3770 | 11930 | 6724 | 10192 |
| New York | 11012 | 12551 | 12984 | 7996 | 5586 | 16671 |
| Paris | 8236 | 9307 | 9650 | 11988 | 341 | 16793 |
| Rio de Janeiro | 17325 | 6075 | 17710 | 13343 | 9254 | 13227 |
| Rome | 8144 | 8417 | 9300 | 12936 | 1434 | 15987 |
| San Francisco | 9524 | 16487 | 11121 | 3857 | 8640 | 12644 |
| Singapore | 4465 | 9671 | 2575 | 10824 | 10860 | 6050 |
| Stockholm | 6725 | 10334 | 8243 | 11059 | 1436 | 15593 |
| Tokyo | 2104 | 14737 | 2893 | 6208 | 9585 | 8159 |
|  | Mexico | Montreal | Moscow | New Delhi | New York | Paris |
| Montreal | 3728 |  |  |  |  |  |
| Moscow | 10740 | 7077 |  |  |  |  |
| New Delhi | 14679 | 11286 | 4349 |  |  |  |
| New York | 3362 | 533 | 7530 | $11779$ |  |  |
| Paris | 9213 | 5522 | 2492 | 6601 | 5851 |  |

## cMDS examples: Airline distances

TABLE 13.6. Eigenvalues of $\mathbf{B}$ and the eigenvectors corresponding to the first three largest eigenvalues (in red) for the airline distances example.

|  | Eigenvalues | Eigenvectors |  |  |
| ---: | ---: | ---: | ---: | ---: |
| 1 | 471582511 | 0.245 | -0.072 | 0.183 |
| 2 | 316824787 | 0.003 | 0.502 | -0.347 |
| 3 | 253943687 | 0.323 | -0.017 | 0.103 |
| 4 | -98466163 | 0.044 | -0.487 | -0.080 |
| 5 | -74912121 | -0.145 | 0.144 | 0.205 |
| 6 | -47505097 | 0.366 | -0.128 | -0.569 |
| 7 | 31736348 | -0.281 | -0.275 | -0.174 |
| 8 | -7508328 | -0.272 | -0.115 | 0.094 |
| 9 | 4338497 | -0.010 | 0.134 | 0.202 |
| 10 | 1747583 | 0.209 | 0.195 | 0.110 |
| 11 | -1498641 | -0.292 | -0.117 | 0.061 |
| 12 | 145113 | -0.141 | 0.163 | 0.196 |
| 13 | -102966 | -0.364 | 0.172 | -0.473 |
| 14 | 60477 | -0.104 | 0.220 | 0.163 |
| 15 | -6334 | -0.140 | -0.356 | -0.009 |
| 16 | -1362 | 0.375 | 0.139 | -0.054 |
| 17 | 100 | -0.074 | 0.112 | 0.215 |
| 18 | 0 | 0.260 | -0.214 | 0.173 |

- Airline distance is non-Euclidean
- Take the first 3 largest eigenvalues (inspection of scree plot)


## cMDS examples: Airline distances



FIGURE 13.1. Two-dimensional map of 18 world cities using the classical scaling algorithm on airline distances between those cities. The colors

## cMDS examples: Airline distances



FIGURE 13.2. Three-dimensional map of 18 world cities using the classical scaling algorithm on airline distances between those cities. The colors reflect the different continents: Asia (purple), North America (red), South America (yellow), Europe (blue), Africa (brown), and Australasia (green).

## Distance Scaling

classical MDS
seeks to find an optimal configuration $\mathbf{x}_{i}$ that gives $d_{i j} \approx \hat{d}_{i j}=\left\|\mathbf{x}_{i}-\mathbf{x}_{j}\right\|_{2}$ as close as possible.

Distance Scaling

- Relaxing $d_{i j} \approx \hat{d}_{i j}$ from cMDS by allowing

$$
\hat{d}_{i j} \approx f\left(d_{i j}\right), \text { for some monotone function } f
$$

- Called metric MDS if dissimilarities $d_{i j}$ are quantitative
- Called non-metric MDS if dissimilarities $d_{i j}$ are qualitative (e.g. ordinal).
- Unlike cMDS, distance scaling is an optimization process minimizing stress function, and is solved by iterative algorithms.


## Metric MDS

## The (usual) metric MDS

Given a (low) dimension $p$ and a monotone function $f$, metric MDS seeks to find an optimal configuration $\mathbf{X} \subset \mathbb{R}^{p}$ that gives $f\left(d_{i j}\right) \approx \hat{d}_{i j}=\left\|\mathbf{x}_{i}-\mathbf{x}_{j}\right\|_{2}$ as close as possible.

- The function $f$ can be taken to be a parametric monotonic function, such as $f\left(d_{i j}\right)=\alpha+\beta d_{i j}$.
- 'As close as possible' is now explicitly stated by square loss

$$
\text { stress }=\mathcal{L}\left(\hat{d}_{i j}\right)=\left(\sum_{i<j}\left(\hat{d}_{i j}-f\left(d_{i j}\right)\right)^{2} / \sum d_{i j}^{2}\right)^{\frac{1}{2}}
$$

and the metric MDS minimizes $\mathcal{L}\left(\hat{d}_{i j}\right)$ over all $\hat{d}_{i j}$ and $\alpha, \beta$.

- The usual metric MDS is the special case $f\left(d_{i j}\right)=d_{i j}$; The usual metric MDS solution (from optimization) $\neq$ that of classical MDS.


## Metric MDS

## Sammon mapping

- Sammon mapping is a generalization of the usual metric MDS.
- Sammon's stress (to be minimized) is

$$
\text { Sammon's stress }\left(\hat{d}_{i j}\right)=\frac{1}{\sum_{\ell<k} d_{\ell k}} \sum_{i<j} \frac{\left(\hat{d}_{i j}-d_{i j}\right)^{2}}{d_{i j}}
$$

- This weighting system normalizes the squared-errors in pairwise distances by using the distance in the original space. As a result, Sammon mapping preserves the small $d_{i j}$, giving them a greater degree of importance in the fitting procedure than for larger values of $d_{i j}$
- Optimal solution is found by numerical computation (initial value by cMDS).


## cMDS vs. Sammon Mapping

1925-1929 Cohort: Classical Scaling


1925-1929 Cohort: Sammon Mapping


- Izenman Figure 13.9 (lower panel)
- Results of cMDS and Sammon mapping for $p=2$ : Sammon mapping better preserves inter-distances for smaller dissimilarities, while proportionally squeezes the inter-distances for larger dissimilarities.


## Non-metric MDS

In many applications of MDS, dissimilarities are known only by their rank order, and the spacing between successively ranked dissimilarities is of no interest or is unavailable

## Non-metric MDS

Given a (low) dimension $p$, non-metric MDS seeks to find an optimal configuration $\mathbf{X} \subset \mathbb{R}^{p}$ that gives $f\left(d_{i j}\right) \approx \hat{d}_{i j}=\left\|\mathbf{x}_{i}-\mathbf{x}_{j}\right\|_{2}$ as close as possible.

- Unlike metric MDS, here $f$ is much general and is only implicitly defined.
- $f\left(d_{i j}\right)=d_{i j}^{*}$ are called disparities, which only preserve the order of $d_{i j}$, i.e.,

$$
\begin{align*}
d_{i j}<d_{k \ell} & \Leftrightarrow f\left(d_{i j}\right) \leq f\left(d_{k \ell}\right)  \tag{5}\\
& \Leftrightarrow d_{i j}^{*} \leq d_{k \ell}^{*}
\end{align*}
$$

## Kruskal's non-metric MDS

- Kruskal's non-metric MDS minimizes the stress-1

$$
\operatorname{stress}-1\left(\hat{d}_{i j}, d^{*} i j\right)=\left(\sum_{i<j} \frac{\left(\hat{d}_{i j}-d_{i j}^{*}\right)^{2}}{\sum \hat{d}_{i j}^{2}}\right)^{\frac{1}{2}}
$$

- Note that the original dissimilarities are only used in checking (5). In fact only the order $d_{i j}<d_{k \ell}<\ldots<d_{m f}$ among dissimilarities is needed.
- the function $f$ works as if it were a regression curve (approximated dissimilarities $\hat{d}_{i j}$ as $y$, disparities $d_{i j}^{*}$ as $\hat{y}$, and the order of dissimilarities as explanatory)



FIGURE 13.10. Shepard diagnam for the artificial example. Left panel:
Isotonic regression. Right panel: Monotone spline. Horizontal axis is rank order. For the red points, the vertical axis is the dissimilarity $d_{i j}$, wherens for the fitted blue points, the vertical axis is the disparity $\hat{d}_{i j}$.

## Example: Letter recognition

Wolford and Hollingsworth (1974) were interested in the confusions made when a person attempts to identify letters of the alphabet viewed for some milliseconds only. A confusion matrix was constructed that shows the frequency with which each stimulus letter was mistakenly called something else. A section of this matrix is shown in the table below.

| Letter | C | D | G | H | M | N | Q | W |
| :---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| C | - |  |  |  |  |  |  |  |
| D | 5 | - |  |  |  |  |  |  |
| G | 12 | 2 | - |  |  |  |  |  |
| H | 2 | 4 | 3 | - |  |  |  |  |
| M | 2 | 3 | 2 | 19 | - |  |  |  |
| N | 2 | 4 | 1 | 18 | 16 | - |  |  |
| Q | 9 | 20 | 9 | 1 | 2 | 8 | - |  |
| W | 1 | 5 | 2 | 5 | 18 | 13 | 4 | - |

Is this a dissimilarity matrix?

## Example: Letter recognition

- How to deduce dissimilarities from a similarity matrix? From similarities $\delta_{i j}$, choose a maximum similarity $c \geq \max \delta_{i j}$, so that $d_{i j}=c-\delta_{i j}$, if $i \neq j$, 0 if $i=j$.
- Which method is more appropriate?

Because we have deduced dissimilarities from similarities, the absolute dissimilarities $d_{i j}$ depend on the value of personally chosen $c$. This is the case where the non-metric MDS makes most sense.
However, we will also see that metric scalings (cMDS and Sammon mapping) do the job as well.

- How many dimension?

By inspection of eigenvalues from the cMDS solution.

## Letter recognition

- First choose $c=21=\max \delta_{i j}+1$.
- Compare MDS with $p=2$, from cMDS, Sammon mapping, and non-metric scaling (stress1):



## Letter recognition:

- First choose $c=21=\max \delta_{i j}+1$.
- Compare MDS with $p=3$, from cMDS, Sammon mapping, and non-metric scaling (stress1):

w

w



## Letter recognition:

- Do you see any clusters?
- With $c=21=\max \delta_{i j}+1$, the eigenvalues of the Gram-matrix $B$ in the calculation of cMDS are:
508.5707
236.0530
124.8229
56.0627
39.7347
-0.0000
-35. 5449
-97. 1992
- The choice of $p=2$ or $p=3$ seems reasonable.


## Letter recognition

- Second choice of $c=210=\max \delta_{i j}+190$.
- Compare MDS with $p=2$, from cMDS, Sammon mapping, and non-metric scaling (stress1):


non-metric MDS



## Letter recognition:

- Second choice of $c=210=\max \delta_{i j}+190$.
- Compare MDS with $p=3$, from cMDS, Sammon mapping, and non-metric scaling (stress1):



## Letter recognition:

- With $c=210$, the eigenvalues of the Gram-matrix $B$ in the calculation of cMDS are:

$$
1.0 \mathrm{e}+04 *
$$

2.7210
2.2978
2.1084
1.9623
1.9133
1.7696
1.6842
0.0000

- May need more than $p>3$ dimensions.


## Letter recognition: Summary

- The structure of the data appropriate for non-metric MDS.
- Kruskal's non-metric scaling:
(1) Appropriate for non-metric dissimilarities (only when their orders are preserved)
(2) Optimization: susceptible to local minima (leading to different configurations);
(3) Time-consuming
- cMDS fast, overall good.
- Sammon mapping fails when $c=210$.


## Letter recognition: Summary

- Clusters $(C, G),(D, Q),(H, M, N, W)$ are confirmed by a cluster analysis for either choice of $c$.

Use agglomerative hierarchical clustering with average linkage:



## MDS in $R$

```
library(MASS)
# compute dissimilarity matrix from a dataset
d <- dist(swiss)
# d is (n x n-1) lower triangle matrix
cmdscale(d, k =2) # classical MDS
sammon(d,k=1) # Sammon Mapping
isoMDS(d,k=2) # Kruskal's Non-metric MDS
```


## Application: Stringing

In K. Chen, K. Chen, H.G. Mueller and J.L. Wang (2011).
Stringing high dimensional data for functional analysis. JASA 106, 275-284.

Basic idea: Multivariate data to functional data

- Compute $p \times p$ dissimilarity matrix for $p$ variables.
- Use MDS to retrieve 1-dimensional configuration consisting of the $p$ points.
- String variables by the order of variables given by MDS configuration.

Many thanks to K. Chen for sharing the next few slides.

## Idea of Stringing



## Why Stringing?

- Methods and results from low dimensional data can not be directly applied to large $p$ problems.
- Large $p$ is not a problem for FDA, we have $\sqrt{n}$ consistency for covariance, leading eigenvalues and eigenfunctions.
- Smooth structure: $G(s, t)=\sum_{k=1}^{\infty} \lambda_{k} \phi_{k}(s) \phi_{k}(t)$, with $\sum_{k=1}^{\infty} \lambda_{k}<\infty$.
- Neighbors defined over a continuum: Smoothing techniques for noisy, irregular or missing data.


## How to Perform Stringing

- Define a distance between $p$ predictors and estimate the $p \times p$ distance matrix $D$.
- Assign a location $s_{j} \in[0,1]$ to each predictor variable $X_{j}$ to minimize stress function

$$
S_{\mathbf{D}}\left(s_{1}, \ldots, s_{p}\right)=\sum_{j<k}\left(\left|s_{j}-s_{k}\right|-D_{j k}\right)^{2}
$$

- Computational similar but conceptually different form MDS.

1. Preserve the dissimilarity between $p$ variables not $n$ samples.
2. The goal is not dimension reduction. The coordinate $s_{i}$ is an auxiliary location to define random functions.

## Application in High-Dimensional Regression

Two key assumptions essential for current Lasso type methodology:

- Sparsity: Only very few predictors matter
- Uncorrelatedness: Correlations between predictors are small

What if predictors are highly correlated and effects are not sparse?
Stringing:

$$
\begin{gathered}
E(Y \mid X)=g^{-1}(X \beta) \\
\Rightarrow E(Y \mid Z)=g^{-1}\left(\mu_{Y}+\int Z(s) \beta(s) d s\right)
\end{gathered}
$$

## Simulation Settings

$$
Y=X \beta+\varepsilon
$$

- $\operatorname{cov}\left(X_{i}, X_{j}\right)=\sigma(i, j)=\mathscr{U}(0,1)$, chosen as i.i.d. uniform random numbers, projected to non-negative definite matrix space
- Varying sparsity of regression coefficients, generated as $\beta_{j} \sim \mathscr{U}(0,1), j=1, \ldots, p$, where the fraction of nonzero coefficients is controlled at $100 \%, 50 \%, 10 \%$.
- Varying $p, n$, test sets of size 50 and 200 simulations


## Functional Regression Versus LASSO



## Stringing Gene Expressions


$\xrightarrow{\text { Stringing }}$


