

Statistical Machine Learning

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Slide credits and other course material can be found at:

http://www.stats.ox.ac.uk/~palamara/SML_BDI.html

Summary: PCA

PCA

Find an orthogonal basis $\{v_1, v_2, \dots, v_p\}$ for the data space such that:

- The first principal component (PC) v_1 is the **direction of greatest variance** of data.
- The j -th PC v_j is the **direction orthogonal to v_1, v_2, \dots, v_{j-1} of greatest variance**, for $j = 2, \dots, p$.

- **Eigendecomposition of the sample covariance matrix**

$$S = \frac{1}{n-1} \sum_{i=1}^n x_i x_i^\top.$$

$$S = V \Lambda V^\top.$$

- Λ is a diagonal matrix with eigenvalues (variances along each principal component) $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_p \geq 0$
- V is a $p \times p$ orthogonal matrix whose columns are the p eigenvectors of S , i.e. the principal components v_1, \dots, v_p
- Dimensionality reduction by projecting $x_i \in \mathbb{R}^p$ onto first k principal components:

$$z_i = [v_1^\top x_i, \dots, v_k^\top x_i]^\top \in \mathbb{R}^k.$$

Summary: PCA

$$S = \frac{1}{n-1} \sum_{i=1}^n x_i x_i^\top = \frac{1}{n-1} \mathbf{X}^\top \mathbf{X}.$$

- S is a **real and symmetric** matrix, so there exist p eigenvectors v_1, \dots, v_p that are pairwise orthogonal and p associated eigenvalues $\lambda_1, \dots, \lambda_p$ which satisfy the eigenvalue equation $Sv_i = \lambda_i v_i$. In particular, V is an orthogonal matrix:

$$VV^\top = V^\top V = I_p.$$

- S is a **positive-semidefinite** matrix, so the eigenvalues are non-negative:

$$\lambda_i \geq 0, \forall i.$$

Why is S symmetric? Why is S positive-semidefinite?

Reminder: A symmetric $p \times p$ matrix R is said to be positive-semidefinite if

$$\forall a \in \mathbb{R}^p, a^\top R a \geq 0.$$

Singular Value Decomposition (SVD)

SVD

Any real-valued $n \times p$ matrix \mathbf{X} can be written as $\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^\top$ where

- \mathbf{U} is an $n \times n$ orthogonal matrix: $\mathbf{U}\mathbf{U}^\top = \mathbf{U}^\top\mathbf{U} = \mathbf{I}_n$
 - \mathbf{D} is a $n \times p$ matrix with decreasing **non-negative** elements on the diagonal (the singular values) and zero off-diagonal elements.
 - \mathbf{V} is a $p \times p$ orthogonal matrix: $\mathbf{V}\mathbf{V}^\top = \mathbf{V}^\top\mathbf{V} = \mathbf{I}_p$
-
- SVD **always** exists, even for non-square matrices.
 - Fast and numerically stable algorithms for SVD are available in most packages. The relevant R command is `svd`.

SVD and PCA

- Let $\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^\top$ be the SVD of the $n \times p$ data matrix \mathbf{X} .
- Note that

$$(n-1)S = \mathbf{X}^\top \mathbf{X} = (\mathbf{U}\mathbf{D}\mathbf{V}^\top)^\top (\mathbf{U}\mathbf{D}\mathbf{V}^\top) = \mathbf{V}\mathbf{D}^\top \mathbf{U}^\top \mathbf{U}\mathbf{D}\mathbf{V}^\top = \mathbf{V}\mathbf{D}^\top \mathbf{D}\mathbf{V}^\top,$$

using orthogonality ($\mathbf{U}^\top \mathbf{U} = \mathbf{I}_n$) of \mathbf{U} .

- The eigenvalues of S are thus the diagonal entries of $\Lambda = \frac{1}{n-1} \mathbf{D}^\top \mathbf{D}$.
- We also have (using orthogonality $\mathbf{V}^\top \mathbf{V} = \mathbf{I}_p$)

$$\mathbf{X}\mathbf{X}^\top = (\mathbf{U}\mathbf{D}\mathbf{V}^\top)(\mathbf{U}\mathbf{D}\mathbf{V}^\top)^\top = \mathbf{U}\mathbf{D}\mathbf{V}^\top \mathbf{V}\mathbf{D}^\top \mathbf{U}^\top = \mathbf{U}\mathbf{D}\mathbf{D}^\top \mathbf{U}^\top,$$

Gram matrix

$\mathbf{B} = \mathbf{X}\mathbf{X}^\top$, $\mathbf{B}_{ij} = x_i^\top x_j$ is called the Gram matrix of dataset \mathbf{X} .

\mathbf{B} and $(n-1)S = \mathbf{X}^\top \mathbf{X}$ have the same nonzero eigenvalues, equal to the non-zero squared singular values of \mathbf{X} .

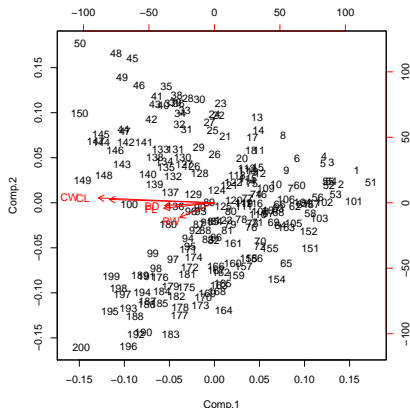
Projection:

$$\mathbf{Z} = \mathbf{X}\mathbf{V} = \mathbf{U}\mathbf{D}\mathbf{V}^\top \mathbf{V} = \mathbf{U}\mathbf{D}.$$

Can be obtain by eigendecomposition of \mathbf{B} , less computation if $p > n$.

Biplots

```
> biplot(Crabs.pca, scale=1)
```



- PCA plots show the data items (rows of \mathbf{X}) in the space spanned by PCs.
- **Biplots** allow us to visualize the **original variables** $X^{(1)}, \dots, X^{(p)}$ (corresponding to columns of \mathbf{X}) in the same plot.

Biplots

Recall that $X = [X^{(1)}, \dots, X^{(p)}]^\top$ and $\mathbf{X} = UDV^\top$ is the SVD of the data matrix.

- The 'full' PC projection of x_i is the i -th row of UD :

$$z_i = V^\top x_i = D^\top U_i^\top, \text{ equivalently: } \mathbf{XV} = UD.$$

- The j -th unit vector $\mathbf{e}_j \in \mathbb{R}^p$ points in the direction of the original variable $X^{(j)}$. Its PC projection η_j is:

$$\eta_j = V^\top \mathbf{e}_j = V_j^\top \quad (\text{the } j\text{-th row of } V)$$

- The projection of \mathbf{e}_j indicates the weighting each PC gives to the original variable $X^{(j)}$.
- Dot products between these projections give entries of the data matrix:

$$x_{ij} = \sum_{k=1}^{\min\{n,p\}} U_{ik} D_{kk} V_{jk} = \langle D^\top U_i^\top, V_j^\top \rangle = \langle z_i, \eta_j \rangle.$$

- Biplots focus on the first two PCs and the quality depends on the **proportion of variance explained** by the first two PCs.

Iris Data

50 samples from each of the 3 species of iris:
setosa, *versicolor*, and *virginica*

Each measuring the length and widths of
both sepal and petals

Collected by E. Anderson (1935) and
analysed by R.A. Fisher (1936)

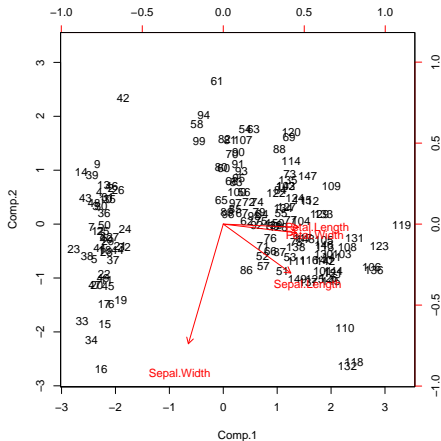


Iris Data

```
> data(iris)
> iris[sample(150,20),]
      Sepal.Length Sepal.Width Petal.Length Petal.Width   Species
54          5.5         2.3         4.0         1.3 versicolor
33          5.2         4.1         1.5         0.1   setosa
30          4.7         3.2         1.6         0.2   setosa
73          6.3         2.5         4.9         1.5 versicolor
107         4.9         2.5         4.5         1.7  virginica
4           4.6         3.1         1.5         0.2   setosa
90          5.5         2.5         4.0         1.3 versicolor
83          5.8         2.7         3.9         1.2 versicolor
50          5.0         3.3         1.4         0.2   setosa
92          6.1         3.0         4.6         1.4 versicolor
128         6.1         3.0         4.9         1.8  virginica
57          6.3         3.3         4.7         1.6 versicolor
9           4.4         2.9         1.4         0.2   setosa
2           4.9         3.0         1.4         0.2   setosa
86          6.0         3.4         4.5         1.6 versicolor
66          6.7         3.1         4.4         1.4 versicolor
85          5.4         3.0         4.5         1.5 versicolor
147         6.3         2.5         5.0         1.9  virginica
8           5.0         3.4         1.5         0.2   setosa
41          5.0         3.5         1.3         0.3   setosa
```

Iris data biplot

```
> iris.pca<-princomp(iris[,-5],cor=TRUE)
> biplot(iris.pca,scale=0)
```



Biplots

- There are other projections we can consider for biplots (assuming $p < n$ to simplify notation):

$$x_{ij} = \sum_{k=1}^p U_{ik} D_{kk} V_{jk} = \langle D_{1:p,1:p}^\top U_{i,1:p}^\top, V_j^\top \rangle = \langle D_{1:p,1:p}^{1-\alpha} U_{i,1:p}^\top, D_{1:p,1:p}^\alpha V_j^\top \rangle.$$

where $0 \leq \alpha \leq 1$, i.e., we change representation to

$$\tilde{z}_i = D_{1:p,1:p}^{1-\alpha} U_{i,1:p}^\top, \quad \tilde{\eta}_j = D_{1:p,1:p}^\alpha V_j^\top$$

- case $\alpha = 1$:
 - Sample covariance of the projected points is:

$$\widehat{\text{Cov}}(\tilde{Z}) = \frac{1}{n-1} U_{1:n,1:p}^\top U_{1:n,1:p} = \frac{1}{n-1} I_p.$$

Projected points are uncorrelated and dimensions are equi-variance.

- Sample covariance between $X^{(i)}$ and $X^{(j)}$ is:

$$\hat{\mathbb{E}}(X^{(i)} X^{(j)}) = \frac{1}{n-1} (VD^\top DV^\top)_{i,j} = \frac{1}{n-1} \langle D_{1:p,1:p} V_i^\top, D_{1:p,1:p} V_j^\top \rangle$$

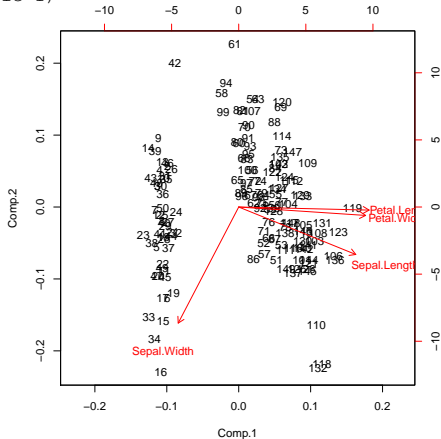
The angle between the projected variables maps to their correlation.

Iris Data biplot - scaled

```

> ?biplot
...
scale: The variables are scaled by lambda ^ scale and the observations
are scaled by lambda ^ (1-scale) where lambda are the singular values
as computed by princomp. (default=1)
...
> biplot(iris.pca,scale=1)

```



US Arrests Data

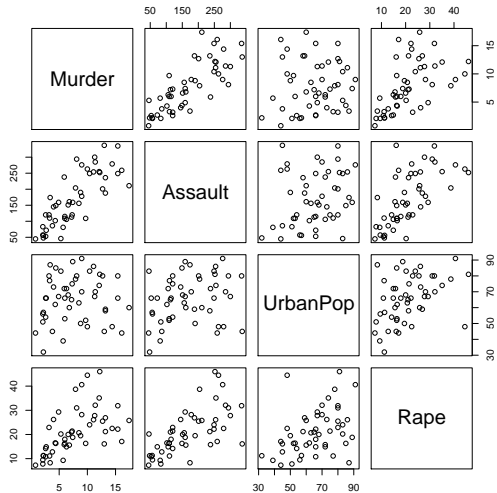
This data set contains statistics, in arrests per 100,000 residents for assault, murder, and rape in each of the 50 US states in 1973. Also given is the percent of the population living in urban areas.

```
pairs(USArrests)
usarrests.pca <- princomp(USArrests, cor=T)
plot(usarrests.pca)

pairs(predict(usarrests.pca))
biplot(usarrests.pca)
```

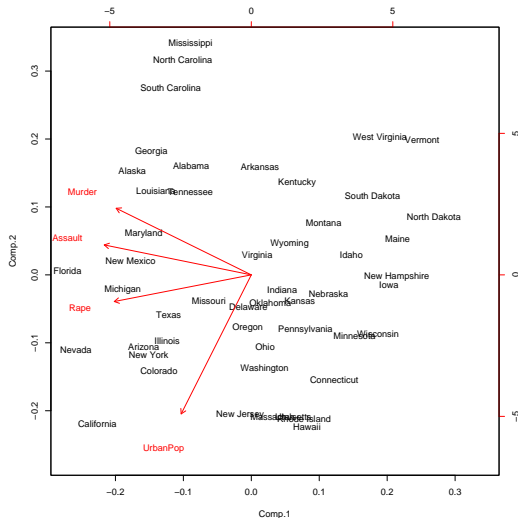
US Arrests Data Pairs Plot

```
> pairs(USArrests)
```



US Arrests Data Biplot

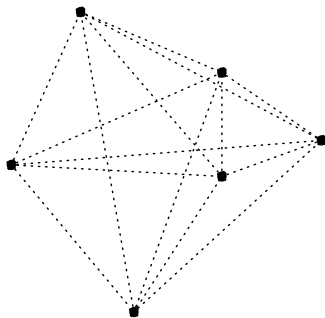
```
> biplot(usarrests.pca, scale=1)
```



Multidimensional Scaling

Suppose there are n points \mathbf{X} in \mathbb{R}^p , but we are only given the $n \times n$ matrix \mathbf{D} of inter-point distances.

Can we reconstruct \mathbf{X} ?



Multidimensional Scaling

Rigid transformations (translations, rotations and reflections) do not change inter-point distances so cannot recover \mathbf{X} exactly. However \mathbf{X} can be recovered up to these transformations!

- Let $d_{ij} = \|x_i - x_j\|_2$ be the distance between points x_i and x_j .

$$\begin{aligned}d_{ij}^2 &= \|x_i - x_j\|_2^2 \\ &= (x_i - x_j)^\top (x_i - x_j) \\ &= x_i^\top x_i + x_j^\top x_j - 2x_i^\top x_j\end{aligned}$$

- Let $\mathbf{B} = \mathbf{X}\mathbf{X}^\top$ be the $n \times n$ matrix of dot-products, $b_{ij} = x_i^\top x_j$. The above shows that \mathbf{D} can be computed from \mathbf{B} .
- Some algebraic exercise shows that \mathbf{B} can be recovered from \mathbf{D} if we assume $\sum_{i=1}^n x_i = 0$.

Multidimensional Scaling

- If we knew \mathbf{X} , then SVD gives $\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^\top$. As \mathbf{X} has rank at most $r = \min(n, p)$, we have at most r non-zero singular values in \mathbf{D} and we can assume $\mathbf{U} \in \mathbb{R}^{n \times r}$, $\mathbf{D} \in \mathbb{R}^{r \times r}$ and $\mathbf{V}^\top \in \mathbb{R}^{r \times p}$.
- The eigendecomposition of \mathbf{B} is then:

$$\mathbf{B} = \mathbf{X}\mathbf{X}^\top = \mathbf{U}\mathbf{D}^2\mathbf{U}^\top = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\top.$$

- This eigendecomposition can be obtained from \mathbf{B} without knowing \mathbf{X} !
- Let $\tilde{x}_i^\top = U_i \mathbf{\Lambda}^{\frac{1}{2}} \in \mathbb{R}^r$. If $r < p$, pad \tilde{x}_i with 0s so that it has length p . Then,

$$\tilde{x}_i^\top \tilde{x}_j = U_i \mathbf{\Lambda} U_j^\top = b_{ij} = x_i^\top x_j$$

and we have found a set of vectors with dot-products given by \mathbf{B} , as desired.

- The vectors \tilde{x}_i differs from x_i only via the orthogonal matrix \mathbf{V}^\top (recall that $x_i^\top = U_i \mathbf{D} \mathbf{V}^\top = \tilde{x}_i^\top \mathbf{V}^\top$) so are equivalent up to rotation and reflections.

US City Flight Distances

We present a table of flying mileages between 10 American cities, distances calculated from our 2-dimensional world. Using D as the starting point, metric MDS finds a configuration with the same distance matrix.

| ATLA | CHIG | DENV | HOUS | LA | MIAM | NY | SF | SEAT | DC |
|------|------|------|------|------|------|------|------|------|------|
| 0 | 587 | 1212 | 701 | 1936 | 604 | 748 | 2139 | 2182 | 543 |
| 587 | 0 | 920 | 940 | 1745 | 1188 | 713 | 1858 | 1737 | 597 |
| 1212 | 920 | 0 | 879 | 831 | 1726 | 1631 | 949 | 1021 | 1494 |
| 701 | 940 | 879 | 0 | 1374 | 968 | 1420 | 1645 | 1891 | 1220 |
| 1936 | 1745 | 831 | 1374 | 0 | 2339 | 2451 | 347 | 959 | 2300 |
| 604 | 1188 | 1726 | 968 | 2339 | 0 | 1092 | 2594 | 2734 | 923 |
| 748 | 713 | 1631 | 1420 | 2451 | 1092 | 0 | 2571 | 2408 | 205 |
| 2139 | 1858 | 949 | 1645 | 347 | 2594 | 2571 | 0 | 678 | 2442 |
| 2182 | 1737 | 1021 | 1891 | 959 | 2734 | 2408 | 678 | 0 | 2329 |
| 543 | 597 | 1494 | 1220 | 2300 | 923 | 205 | 2442 | 2329 | 0 |

US City Flight Distances

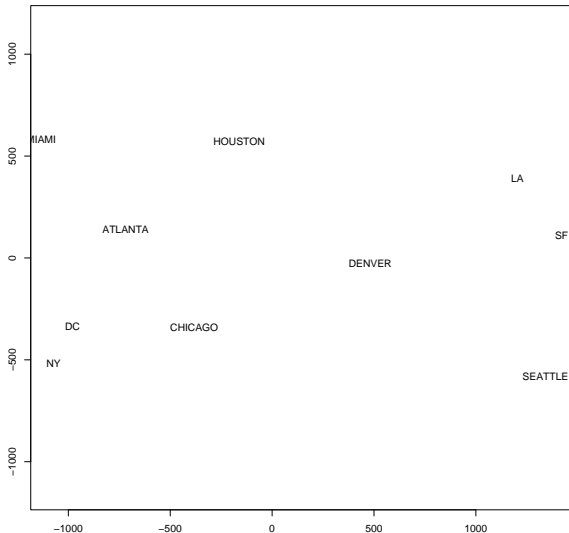
```
library(MASS)

us <- read.csv("http://www.stats.ox.ac.uk/~palamara/teaching/SML19/uscities.csv")

## use classical MDS to find lower dimensional views of the data
## recover X in 2 dimensions

us.classical <- cmdscale(d=us,k=2)
plot(us.classical)
text(us.classical,labels=names(us))
```

US City Flight Distances



Lower-dimensional Reconstructions

In classical MDS derivation, we used all eigenvalues in the eigendecomposition of \mathbf{B} to reconstruct

$$\tilde{x}_i = U_i \Lambda^{\frac{1}{2}}.$$

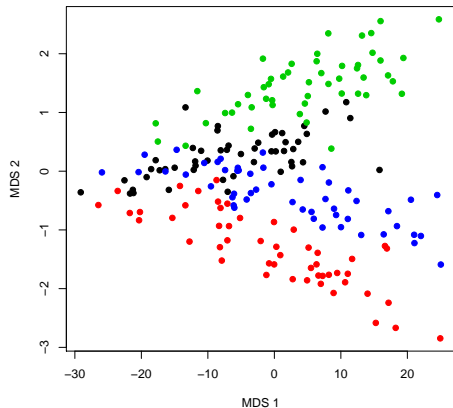
We can use only the largest $k < \min(n, p)$ eigenvalues and eigenvectors in the reconstruction, giving the ‘best’ k -dimensional view of the data.

This is analogous to PCA, where only the largest eigenvalues of $\mathbf{X}^T \mathbf{X}$ are used, and the smallest ones effectively suppressed.

Indeed, PCA and classical MDS are duals and yield effectively the same result.

Crabs Data

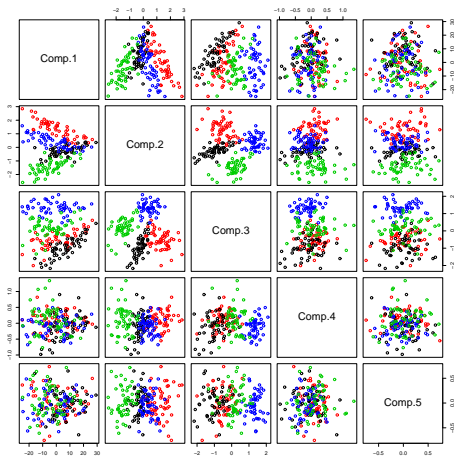
```
library(MASS)
crabs$spsex=paste(crabs$sp, crabs$sex, sep=" ")
varnames<-c('FL', 'RW', 'CL', 'CW', 'BD')
Crabs <- crabs[,varnames]
Crabs.class <- factor(crabs$spsex)
crabsmds <- cmdscale(d= dist(Crabs), k=2)
plot(crabsmds, pch=20, cex=2, col=unclass(Crabs.class))
```



Crabs Data

Compare with previous PCA analysis.

Classical MDS solution corresponds to the first 2 PCs.



Varieties of MDS

Generally, MDS is a class of dimensionality reduction techniques which represents data points $x_1, \dots, x_n \in \mathbb{R}^p$ in a lower-dimensional space $z_1, \dots, z_n \in \mathbb{R}^k$ which tries to preserve inter-point (dis)similarities.

- It requires only the matrix \mathbf{D} of pairwise dissimilarities $d_{ij} = d(x_i, x_j)$. For example, we can use Euclidean distance $d_{ij} = \|x_i - x_j\|_2$, but other dissimilarities are possible.
- MDS finds representations $z_1, \dots, z_n \in \mathbb{R}^k$ such that

$$\|z_i - z_j\|_2 \approx d(x_i, x_j) = d_{ij},$$

and differences in dissimilarities are measured by the appropriate loss $\Delta(d_{ij}, \|z_i - z_j\|_2)$.

- Goal: Find \mathbf{Z} which minimizes the **stress function**

$$S(\mathbf{Z}) = \sum_{i \neq j} \Delta(d_{ij}, \|z_i - z_j\|_2).$$

Varieties of MDS

- Choices of (dis)similarities and stress functions $S(\mathbf{Z})$ lead to different algorithms.
 - **Classical/Torgerson**: preserves inner products instead - **strain function** (`cmdscale`)

$$S(\mathbf{Z}) = \sum_{i \neq j} (b_{ij} - \langle z_i - \bar{z}, z_j - \bar{z} \rangle)^2$$

- **Metric Shephard-Kruskal**: preserves distances w.r.t. squared stress

$$S(\mathbf{Z}) = \sum_{i \neq j} (d_{ij} - \|z_i - z_j\|_2)^2$$

- **Sammon**: preserves shorter distances more (`sammon`)

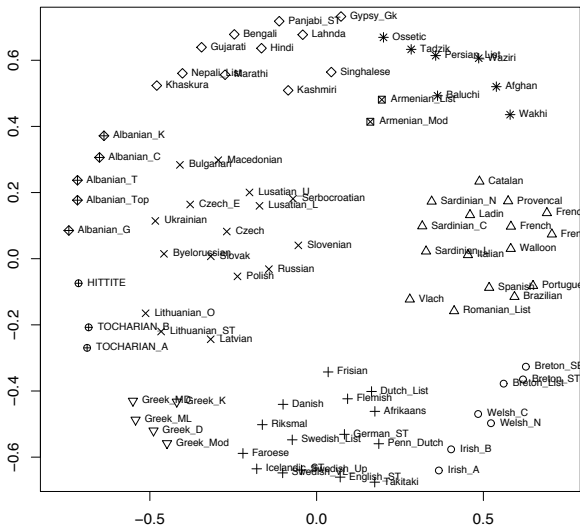
$$S(\mathbf{Z}) = \sum_{i \neq j} \frac{(d_{ij} - \|z_i - z_j\|_2)^2}{d_{ij}}$$

- **Non-Metric Shephard-Kruskal**: ignores actual distance values, only preserves ranks (`isoMDS`)

$$S(\mathbf{Z}) = \min_{g \text{ increasing}} \frac{\sum_{i \neq j} (g(d_{ij}) - \|z_i - z_j\|_2)^2}{\sum_{i \neq j} \|z_i - z_j\|_2^2}$$

Example: Language data

Using MDS with non-metric (Sammon) scaling.

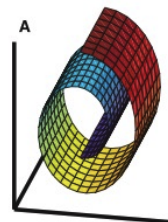


Nonlinear Dimensionality Reduction

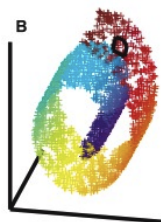
Two aims of different varieties of MDS:

- To visualize the (dis)similarities among items in a dataset, where these (dis)similarities may not have Euclidean geometric interpretations.
- To perform **nonlinear** dimensionality reduction.

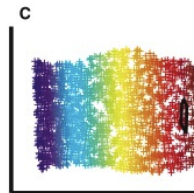
Many high-dimensional datasets exhibit low-dimensional structure (“live on a low-dimensional manifold”).



high-dim distribution



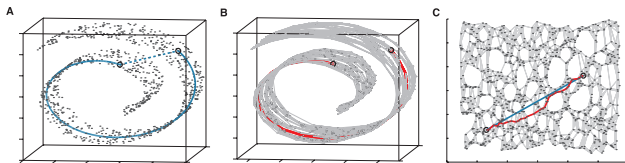
high-dim samples



estimated manifold

Isomap

Isomap is a non-linear dimensional reduction technique based on classical MDS. Differs from other MDSs as it uses estimates of **geodesic distances** between the data points.

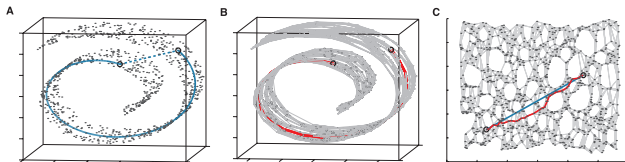


Tenenbaum et al. (2000)

Isomap

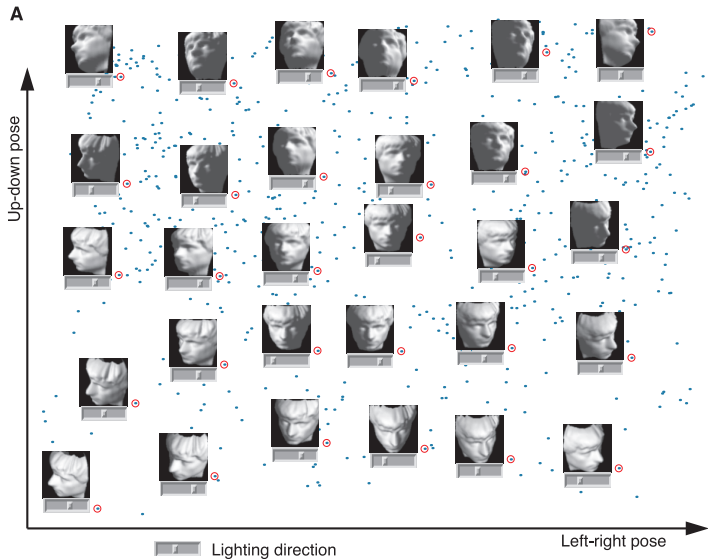
Isomap

- Calculate Euclidean distances \mathbf{D}_{ij} for $i, j = 1, \dots, n$ between all data points.
- Form a graph G with n samples as nodes, and edges between the respective K nearest neighbours (K -Isomap) or between i and j if $\mathbf{D}_{ij} < \epsilon$ (ϵ -Isomap).
- For i, j linked by an edge, set $\mathbf{D}_{ij}^G = \mathbf{D}_{ij}$. Otherwise, set \mathbf{D}_{ij}^G to be the shortest-path distance between i and j in G .
- Run classical MDS using distances \mathbf{D}_{ij}^G .



R function: `isomap{vegan}`.

Faces



Handwritten Characters

