C01

維度縮減

Dimension Reduction

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Visualizing High-dimensional Data: Dimension Reduction Techniques

- Why Reduce Dimensionality?
- Feature Selection vs Extraction
- Dimension Reduction Techniques
  1) Spectral Decomposition (Eigen) 譜(特徵值)分解
  2) Singular Value Decomposition (SVD) 奇異值分解
  3) Principal Component Analysis (PCA) 主成份分析
  4) Biplot 雙標圖
  5) Factor Analysis (FA) 因子分析
  6) Multidimensional Scaling (MDS) 多元尺度法
  7) Isometric Feature Mapping (ISOMAP) 等軸距特徵映射
  8) Linear Discriminant Analysis (LDA) 線性區別分析
  9) Sliced Inverse Regression (SIR) 切片逆迴歸法
  10) Canonical Correlation Analysis (CCA) 典型相關分析
- The high-dimension low sample size data (HDLSS)
- DR Quality Assessment

Dimension Reduction

keep information as much as possible without loss of information.

input data matrix: X

Group	Data	X1	X2	X3	•••	Xp
1	subject01	0.81	-1.29	-0.50		1.13
1	subject02	0.64	2.16	-1.51		0.00
2	subject03	0.13	0.60	1.10		0.11
2	subject04	-0.17	0.31	-0.37		-0.50
3	subject05	-1.01	0.99	0.70		-0.08
3	subject06	0.95	0.75	-0.83		0.60
3	subject07	0.72	1.12	-1.35		-1.22
1	subject08	0.77	1.24	-0.04		1.03
1	subject09	-0.49	0.02	-1.73		1.61
1	subject10	1.93	0.45	-0.01		0.03
3	subject11	-0.15	-1.36	1.05		0.50
3	subject12	-1.16	0.11	-0.57		-0.80
3	subject13	-0.02	2.05	-1.18		0.45
3	subject14	-0.05	0.79	1.33		0.81
2	subject15	-0.21	-0.38	0.72		-0.61
1	subject16	-0.28	0.57	1.02		-0.01
⋮	⋮					
2	subjectN	0.33	0.01	1.19		-0.33

PCA
FA
MDS

transformed data matrix: Z

Data	Z1	Z2	•••	Zk
subject01	-1.55	-0.66		0.60
subject02	0.57	-0.51		-1.03
subject03	1.99	1.44		-0.60
subject04	0.10	0.20		-1.21
subject05	-0.20	-0.64		0.24
subject06	2.85	1.32		-0.61
subject07	-0.34	-0.35		0.15
subject08	0.66	0.44		0.28
subject09	8.44	1.66		2.12
subject10	0.37	-0.17		-1.73
subject11	-1.14	0.01		0.61
subject12	-1.73	-1.13		0.81
subject13	1.53	0.67		0.48
subject14	-0.21	-0.14		-0.29
subject15	-0.03	0.66		0.17
subject16	2.56	-2.25		0.26
⋮				
subjectN	2.04	0.71		0.76

- Visualization
- Clustering
- Classification
- ....

Y

Methods using additional information *y:* LDA, Sufficient Dimension Reduction (SIR, SAVE, pHd, IRE,...)

Why Reduce Dimensionality?

- **Reduces time complexity**:
  less computation
- **Reduces space complexity**:
  Less parameters
- **Saves the cost** of observing the features:
  input is unnecessary.
- **Simpler models are more robust on small datasets**:
  simpler models vary less depending on the particulars of a sample.
- **More interpretable; simpler explanation**
- **Data visualization** (structure, groups, outliers, etc) if plotted in 2 or 3 dimensions. (Dimension reduction visualization is often adopted for presenting grouping structure for methods such as K-means.)

DR: Feature Selection vs Extraction

Feature Selection

- Choosing $k<d$ important features
- Ignoring the remaining $d - k$
- Subset selection algorithms

$z = w^T x$

	a1	a2	a3	⋯	ap
Data	X1	X2	X3	⋯	Xp
subject01	0.81	-1.29	-0.50		1.13
subject02	0.64	2.16	-1.51		0.00
subject03	0.13	0.60	1.10		0.11
subject04	-0.17	0.31	-0.37		-0.50
subject05	-1.01	0.99	0.70		-0.08
subject06	0.95	0.75	-0.83		0.60
subject07	0.72	1.12	-1.35		-1.22
subject08	0.77	1.24	-0.04		1.03
subject09	-0.49	0.02	-1.73		1.61
subject10	1.93	0.45	-0.01		0.03
subject11	-0.15	-1.36	1.05		0.50
subject12	-1.16	0.11	-0.57		-0.80
subject13	-0.02	2.05	-1.18		0.45
subject14	-0.05	0.79	1.33		0.81
subject15	-0.21	-0.38	0.72		-0.61
subject16	-0.28	0.57	1.02		-0.01
⋮					
subjectN	0.33	0.01	1.19		-0.33

Feature Extraction

- **Project** the original x_i , $i = 1,\ldots,d$ dimensions to new $k<d$ dimensions, z_j , $j = 1,\ldots,k$.
- $z = w^T x$
- PCA, FA, MDS, LDA, SIR

Subset Selection

- Finding the best subset of the set of features.
- ***Best***: contains the least number of dimensions that most contribute to accuracy.

Forward Search: Add the best feature at each step

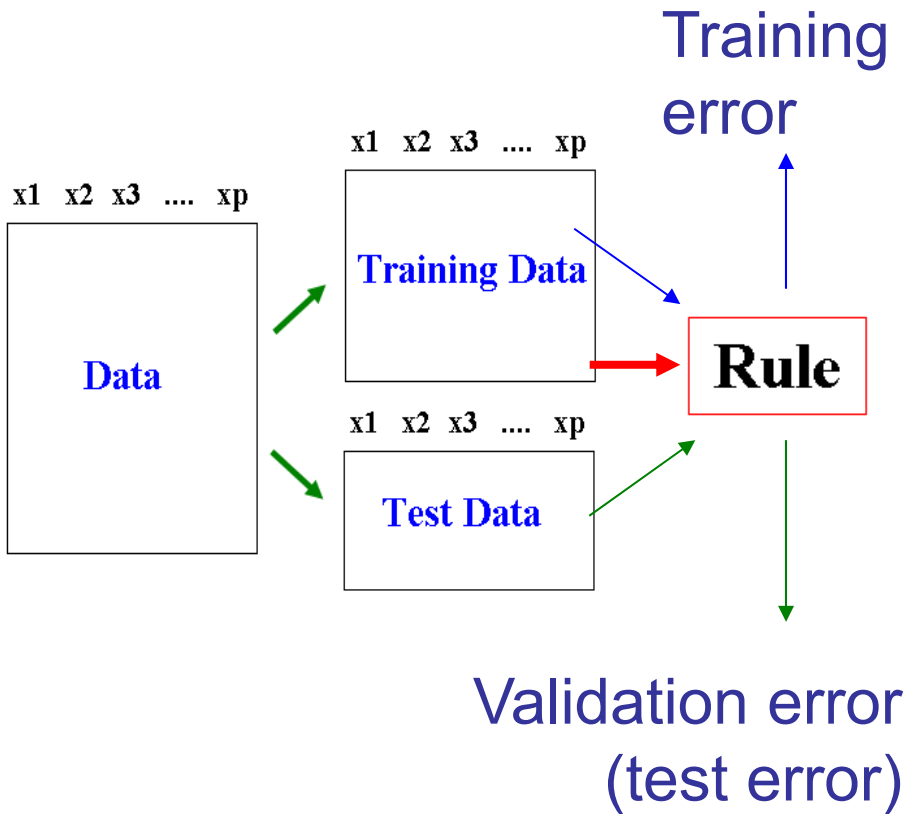
1. Set of features F initially $\emptyset$.
2. At each iteration, find the best new feature
3. $j = \text{argmin}_i E(F \cup x_i)$
4. Add x_i to F if $E(F \cup x_i) < E(F)$
5. Stop: $|E^t - E^{t+1}| < epsilon$

Backward Search:

Start with all features and remove one at a time

1. Set of features F initially ALL.
2. At each iteration, find the best new feature
3. $j = \text{argmin}_i E(F - x_i)$
4. remove x_i from F if $E(F - x_i) < E(F)$
5. Stop: $|E^t - E^{t+1}| < epsilon$

Others: Floating search (Add k, Remove l), . . .



(1) Spectral Decomposition (1/2)

- Definition: Let A be a $m \times m$ real symmetric matrix. Then there exists an orthogonal matrix $\boldsymbol{C}$ such that $\boldsymbol{C^T A C = D}$ or $\boldsymbol{A = C\,D C^T}$, where $\boldsymbol{D}$ is a diagonal matrix of eigenvalues, and the $\boldsymbol{C}$ matrix has the eigenvectors.
  (A. L. Cauchy established the Spectral Decomposition in 1829.)

- Eigen-decomposition : $Ac_i = \lambda_i c_i,\ i = 1,\ldots,m.$

- Let $\boldsymbol{Z = W^T X}$, or $\boldsymbol{Z = W^T (X - m)}$ center the data on the origin. To find a matrix $\boldsymbol{W}$ such that when we have $\boldsymbol{Z = W^T X}$, we will get $\boldsymbol{Cov(Z) = D}$ is any diagonal matrix.

Spectral Decomposition (2/2)

- We would like to get uncorrelated z_i.
- Let $C = [c_i]$ be the normalized eigenvector of S, then

(1) $C^T C = I$ and

(2)
$$\begin{aligned} S &= SCC^T \\ &= S(c_1, c_2, \cdots, c_d)C^T \\ &= (Sc_1, Sc_2, \cdots, Sc_d)C^T \\ &= (\lambda_1 c_1, \lambda_2 c_2, \cdots, \lambda_d c_d)C^T \\ &= \lambda_1 c_1 c_1^T + \lambda_2 c_2 c_2^T + \cdots + \lambda_d c_d c_d^T \\ &= CDC^T \end{aligned}$$

$$S = (CD^{1/2})(CD^{1/2})^T$$

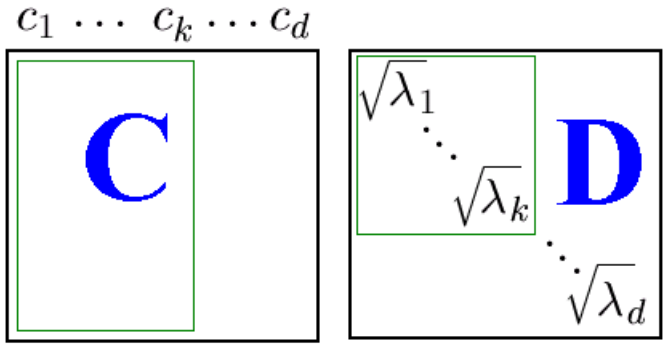
$[d \times d] \quad [d \times d] \quad [d \times d]$

$$\widehat{S} = (CD^{1/2})(CD^{1/2})^T$$

$[d \times d] \quad [d \times k] \quad [k \times k]$

Application:

- Data reduction.
- Image processing and compression.
- K-selection for K-means clustering
- Multivariate outliers detection
- Noise filtering
- Trend detection in the observations.



Spectral Decomposition in R

```
> # Spectral Decomposition
> X <- iris[,1:4]
> (S <- cov(X))
             Sepal.Length Sepal.Width Petal.Length Petal.Width
Sepal.Length    0.6856935  -0.0424340    1.2743154   0.5162707
Sepal.Width    -0.0424340   0.1899794   -0.3296564  -0.1216394
Petal.Length    1.2743154  -0.3296564    3.1162779   1.2956094
Petal.Width     0.5162707  -0.1216394    1.2956094   0.5810063
> (e <- eigen(S))
eigen() decomposition
$values
[1] 4.22824171 0.24267075 0.07820950 0.02383509

$vectors
            [,1]        [,2]        [,3]       [,4]
[1,]  0.36138659  0.65658877 -0.58202985  0.3154872
[2,] -0.08452251  0.73016143  0.59791083 -0.3197231
[3,]  0.85667061 -0.17337266  0.07623608 -0.4798390
[4,]  0.35828920 -0.07548102  0.54583143  0.7536574

> D <- diag(e$values)
> C <- e$vectors
> C%*%D%*%t(C)
           [,1]       [,2]       [,3]       [,4]
[1,]  0.6856935 -0.0424340  1.2743154  0.5162707
[2,] -0.0424340  0.1899794 -0.3296564 -0.1216394
[3,]  1.2743154 -0.3296564  3.1162779  1.2956094
[4,]  0.5162707 -0.1216394  1.2956094  0.5810063
```

```
> # Eigen-decomposition
> S%*%C[,1]
                    [,1]
Sepal.Length  1.5280299
Sepal.Width  -0.3573816
Petal.Length  3.6222104
Petal.Width   1.5149333
> D[1]*C[,1]
[1]  1.5280299 -0.3573816
[3]  3.6222104  1.5149333
```

Some Decompositions in R

```
> eigen(cov(iris[,1:4]))
```

- Eigen-decomposition
  - `eigen {base}`: Spectral Decomposition of a Matrix
- LU decomposition
  - `LU-class {Matrix}`: LU (dense) Matrix Decompositions
  - `lu {Matrix}`: (Generalized) Triangular Decomposition of a Matrix
  - `LU.decompose {optR}`: LU decomposition
- `svd {base}`: **Singular Value Decomposition** of a Matrix
- `qr {base}`: The **QR Decomposition** of a Matrix
  - If A is a $m \times n$ matrix with linearly independent columns, then A can be decomposed as , $A=QR$, where Q is a $m \times n$ matrix whose columns form an orthonormal basis for the column space of A and R is an nonsingular upper triangular matrix.
- `chol {base}`: The **Choleski Decomposition**
  - Cholesky Decomposition: If A is a real, symmetric and positive definite matrix then there exists a unique lower triangular matrix L with positive diagonal element such that $A=LL^T$.

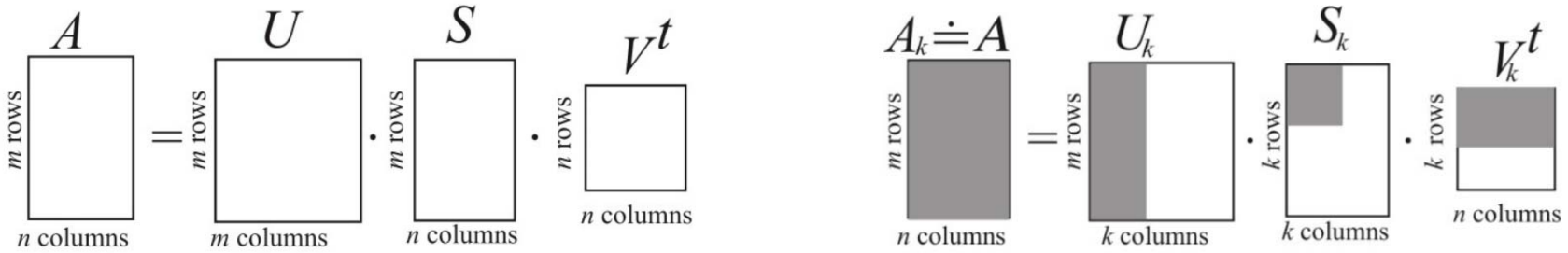
(2) Singular Value Decomposition

奇異值分解

Singular Value Decomposition (SVD) factorizes a general $m \times n$ (assume $m \geq n$) matrix in the form

$$A = USV^t,$$

where U is an $m \times m$ orthogonal matrix, V is an $n \times n$ orthogonal matrix, and S is an $m \times n$ matrix whose only nonzero elements lie along the main diagonal.



- The m columns of $\boldsymbol{U}$ are called the left singular vectors. The n columns of $\boldsymbol{V}$ are called the right singular vectors.
  - The right singular vectors are eigenvectors of $\boldsymbol{A^TA}$.
  - The left singular vectors are eigenvectors of $\boldsymbol{AA^T}$.
  - The non-zero values of $\boldsymbol{S}$ are the square root of the eigenvalues of $\boldsymbol{AA^T}$ and $\boldsymbol{A^TA}$ are called the singular values
- $\boldsymbol{U}$ and $\boldsymbol{V}$ are unitary matrixes, i.e. $\boldsymbol{UU^T=I}$, $\boldsymbol{VV^T=I}$.

SVD Examples

SVD in R

- **svd{base}**: **Singular Value Decomposition** of a Matrix

https://stat.ethz.ch/R-manual/R-devel/library/base/html/svd.html

- **fast.svd{corpcor}**: Fast Singular Value Decomposition

http://svitsrv25.epfl.ch/R-doc/library/corpcor/html/fast.svd.html

- R Package '**svd**': Interfaces to various state-of-art SVD and eigensolvers

https://cran.r-project.org/web/packages/svd/index.html

- R Package '**svdvisual**' : SVD visualization tools

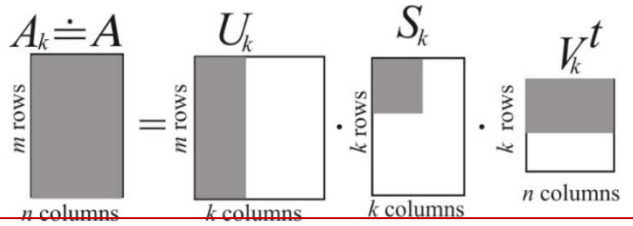
https://cran.r-project.org/web/packages/svdvisual/index.html

R Code Examples

- Data Mining Algorithms In R/Dimensionality Reduction/Singular Value Decomposition
  https://en.wikibooks.org/wiki/Data_Mining_Algorithms_In_R/Dimensionality_Reduction/Singular_Value_Decomposition
- R Code Fragments, Examples of Singular Value Decomposition
  http://www.ats.ucla.edu/stat/r/pages/svd_demos.htm
- Running PCA and SVD in R
  http://genomicsclass.github.io/book/pages/pca_svd.html
- R-bloggers: Using the SVD to find the needle in the haystack
  http://www.r-bloggers.com/using-the-svd-to-find-the-needle-in-the-haystack/
- Image Compression with the SVD in R
  http://www.johnmyleswhite.com/notebook/2009/12/17/image-compression-with-the-svd-in-r/
- The Netflix Prize, Big Data, SVD and R
  http://blog.revolutionanalytics.com/2011/05/the-neflix-prize-big-data-svd-and-r.html
- Singular Value Decomposition in R
  http://www.di.fc.ul.pt/~jpn/r/svd/svd.html

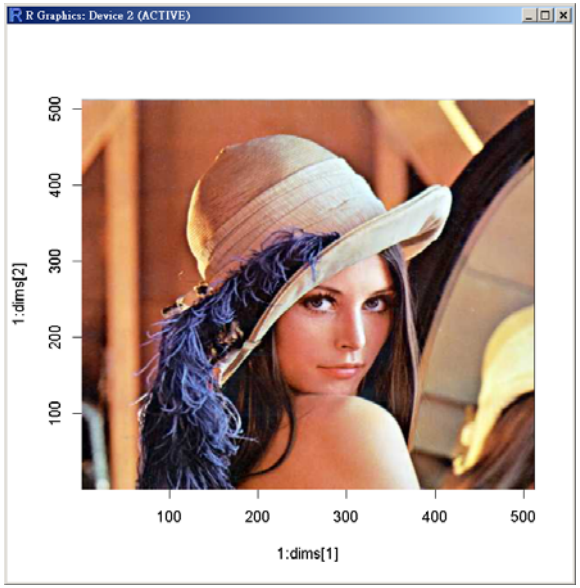
SVD: Making Approximations

```
> iris.sub <- iris[sample(1:150, 8),1:4]
> iris.sub
   Sepal.Length Sepal.Width Petal.Length Petal.Width
58          4.9         2.4          3.3         1.0
59          6.6         2.9          4.6         1.3
77          6.8         2.8          4.8         1.4
84          6.0         2.7          5.1         1.6
54          5.5         2.3          4.0         1.3
39          4.4         3.0          1.3         0.2
71          5.9         3.2          4.8         1.8
87          6.7         3.1          4.7         1.5
> M.svd <- svd(iris.sub)
> M.svd
$d
[1] 22.2553197  2.2360595  0.7611307  0.1773813

$u
           [,1]         [,2]         [,3]        [,4]
[1,] -0.2898553 -0.096733080 -0.007319459 -0.05013322
[2,] -0.3885172 -0.006908608  0.305429166 -0.28018114
[3,] -0.3992219  0.066823762  0.450619905  0.06954991
[4,] -0.3793864  0.327663490 -0.174978375 -0.69121320
[5,] -0.3275406  0.106859076  0.218964907  0.50428246
[6,] -0.2285027 -0.918407065 -0.136688043 -0.13248141
[7,] -0.3782377  0.154232634 -0.776519488  0.27425130
[8,] -0.3989561 -0.009386179  0.058068514  0.29884180

$v
           [,1]       [,2]       [,3]       [,4]
[1,] -0.7497994 -0.3154600  0.5318218  0.2354811
[2,] -0.3527468 -0.5480151 -0.7276317 -0.2140122
[3,] -0.5343751  0.7023730 -0.1376906 -0.4496184
[4,] -0.1667746  0.3268587 -0.4108028  0.8346201
```




```
> M.svd$u %*% (diag(M.svd$d) %*% t(M.svd$v))
     [,1] [,2] [,3] [,4]
[1,]  4.9  2.4  3.3  1.0
[2,]  6.6  2.9  4.6  1.3
[3,]  6.8  2.8  4.8  1.4
[4,]  6.0  2.7  5.1  1.6
[5,]  5.5  2.3  4.0  1.3
[6,]  4.4  3.0  1.3  0.2
[7,]  5.9  3.2  4.8  1.8
[8,]  6.7  3.1  4.7  1.5
>
> # use the first two values to approximate
> d.sub <- diag(M.svd$d[1:2])
> u.sub <- as.matrix(M.svd$u[, 1:2])
> v.sub <- as.matrix(M.svd$v[, 1:2])
> iris.sub.approx <- u.sub %*% d.sub %*% t(v.sub)
> iris.sub.approx
         [,1]     [,2]     [,3]      [,4]
[1,] 4.905057 2.394043 3.295235 1.0051334
[2,] 6.488070 3.058517 4.609664 1.4369796
[3,] 6.614690 3.052204 4.852772 1.5306008
[4,] 6.099701 2.576853 5.026535 1.6476201
[5,] 5.390302 2.440411 4.063166 1.2938078
[6,] 4.460863 2.919270 1.275109 0.1768745
[7,] 6.202869 2.780357 4.740493 1.5166003
[8,] 6.664012 3.143504 4.729919 1.4739142
>
> # compute the sum of squared errors
> sum((iris.sub - iris.sub.approx)^2)
[1] 0.610784
```

SVD: Image Compression (1/3)



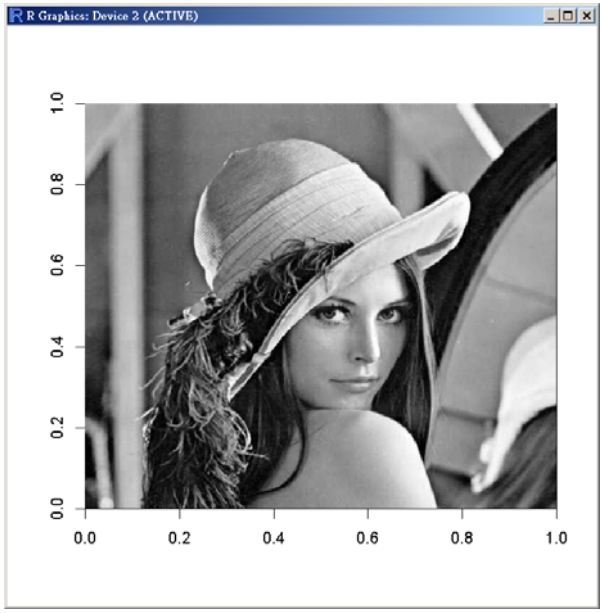
Lenna 97: A Complete Story of Lenna
http://www.ee.cityu.edu.hk/~lmpo/lenna/Lenna97.html
https://en.wikipedia.org/wiki/Lenna
This scan became one of the most used images in computer history.[4] In a 1999 issue of *IEEE Transactions on Image Processing* "Lena" was used in three separate articles,[5] and the picture continued to appear in scientific journals throughout the beginning of the 21st century. ... To explain Lenna's popularity, David C. Munson, editor-in-chief of IEEE Transactions on Image Processing, noted that it was a good test image because of its detail, flat regions, shading, and texture. However, he also noted that its popularity was largely because an image of an attractive woman appealed to the males in a male-dominated field

```
> # require packages: locfit, tiff, fftwtools
> library(EBImage) # (Repositories: BioC Software)
> lena <- readImage("lena.jpg")
> dims <- dim(lena)
> dims
[1] 512 512   3
>
> plot(c(0, dims[1]), c(0, dims[2]), type='n', xlab="", ylab="")
> rasterImage(lena, 0, 0, dims[1], dims[2])
```

```
if (!requireNamespace("BiocManager", quietly = TRUE))
    install.packages("BiocManager")
BiocManager::install("EBImage")
```

```
> library(jpeg) # install.packages("jpeg")
> lena <- readJPEG("lena.jpg")
```

SVD: Image Compression (2/3)




```
> lena.flip <- Image(flip(lena))
> # convert RGB to grayscale
> red.weight   <- .2989
> green.weight <- .587
> blue.weight  <- 0.114
>
> lena.gray <- red.weight   * imageData(lena.flip)[,,1] +
+              green.weight * imageData(lena.flip)[,,2] +
+              blue.weight  * imageData(lena.flip)[,,3]
> dim(lena.gray)
[1] 512 512
> lena.gray[1:5, 1:5]
           [,1]       [,2]       [,3]       [,4]       [,5]
[1,] 0.07128863 0.06344627 0.05952510 0.06736745 0.07913098
[2,] 0.07913098 0.06736745 0.06344627 0.07128863 0.08305216
[3,] 0.08697333 0.07520980 0.07128863 0.07913098 0.09089451
[4,] 0.09089451 0.08305216 0.07913098 0.08305216 0.09873686
[5,] 0.09570980 0.08786745 0.08002510 0.08786745 0.10355216
> image(lena.gray, col = grey(seq(0, 1, length = 256)))
```

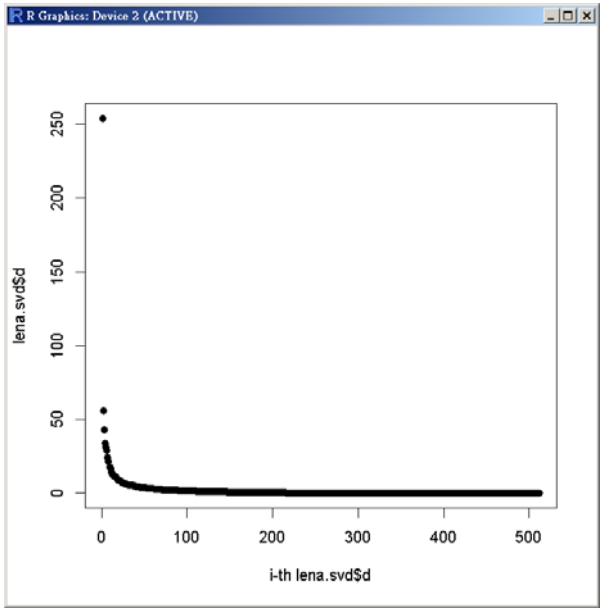
In 1972, at the age of 21. 67-year-old

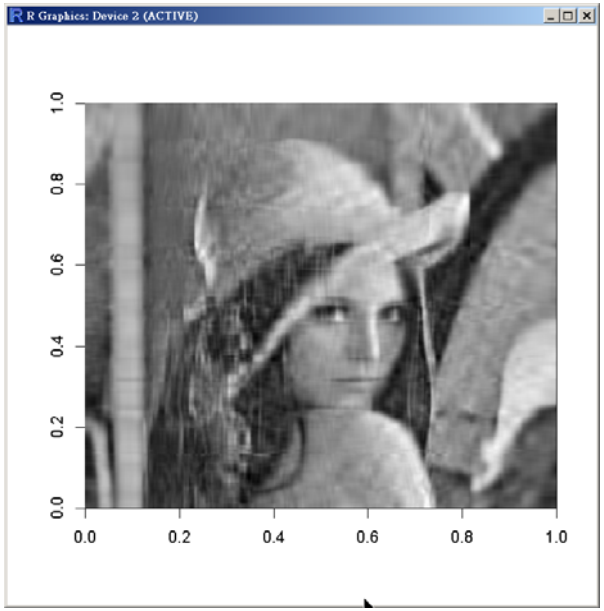
Converting RGB to grayscale/intensity
http://stackoverflow.com/questions/687261/converting-rgb-to-grayscale-intensity

工程師都愛的萊娜小姐　究竟是誰？(林一平 2019-12-06)
https://www.digitimes.com.tw/col/article.asp?id=1129

SVD: Image Compression (3/3)

```
> lena.svd <- svd(lena.gray)
> d <- diag(lena.svd$d)
> dim(d)
[1] 512 512
> u <- lena.svd$u
> v <- lena.svd$v
> plot(1:length(lena.svd$d), lena.svd$d, pch=19, xlab="i-th lena.svd$d", ylab="lena.svd$d")
>
> used.no <- 20
> u.sub <- as.matrix(u[, 1:used.no])
> v.sub <- as.matrix(v[, 1:used.no])
> d.sub <- as.matrix(d[1:used.no, 1:used.no])
> lena.approx <- u.sub %*% d.sub %*% t(v.sub)
> image(lena.approx, col = grey(seq(0, 1, length = 256)))
```



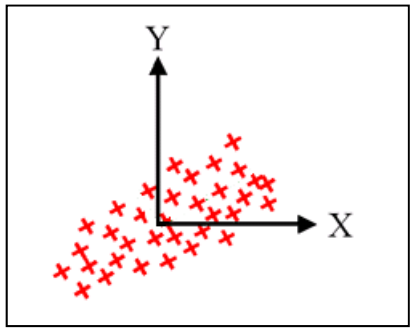


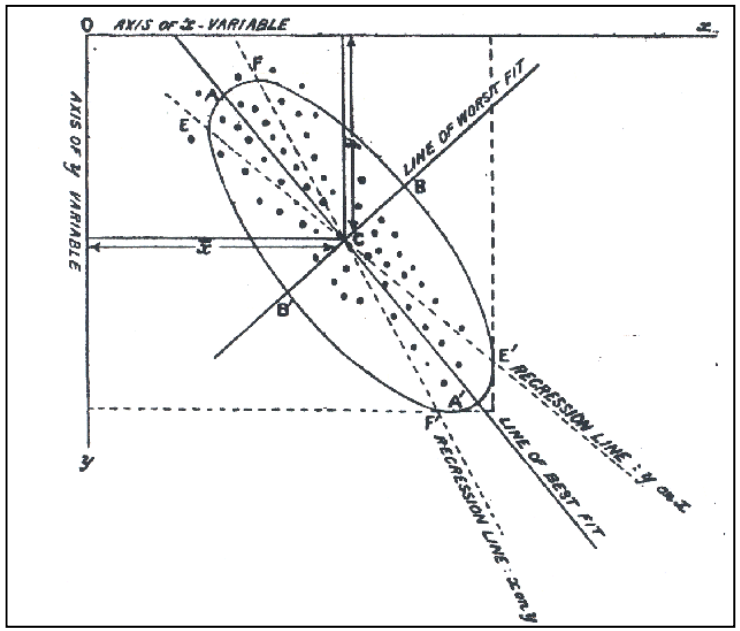
(3) Principal Component Analysis

Data Matrix

MA Table	exp01	exp02	exp03	exp04	exp05	exp•••	exp p
gene001	-0.48	-0.42	0.87	0.92	0.67		-0.35
gene002	-0.39	-0.56	1.08	1.21	0.52		-0.58
gene003	0.87	0.25	-0.17	0.18	-0.13		-0.13
gene004	1.57	1.03	1.22	0.31	0.16		-1.02
gene005	-1.15	-0.86	1.21	1.62	1.12		-0.44
gene006	0.04	-0.12	0.31	0.16	0.17		0.08
gene007	2.95	0.45	-0.40	-0.66	-0.59		-0.76
gene008	-1.22	-0.14	1.34	1.50	0.63		-0.55
gene009	-0.78	-1.06	-0.79	-0.02	0.16		0.03
gene010	-0.53	-0.40	0.18	0.58	-0.09		-0.45
gene011	-0.50	-0.42	0.66	1.05	0.68		0.01
gene012	-0.86	-0.29	0.42	0.46	0.30		-0.63
gene013	-0.16	0.29	0.17	-0.28	-0.02		-0.04
gene014	-0.36	-0.03	-0.08	-0.08	-0.23		-0.21
gene015	-0.72	-0.85	0.54	1.04	0.84		-0.64
gene016	-0.78	-0.32	0.26	0.20	0.48		0.27
gene017	0.60	-0.36	0.41	0.45	0.18		-1.02
gene018	-0.20	-0.07	0.13	0.10	0.38		0.05
gene019	-2.29	-0.64	0.77	1.60	0.53		-0.38
gene020	-1.45	-0.16	1.08	1.50	0.74		-0.70
gene021	-0.57	0.42	1.08	1.35	0.64		-0.40
gene022	-0.10	0.13	0.41	0.60	0.23		0.19
gene•••							
gene n	-1.79	0.94	2.18	1.75	0.23		-0.66

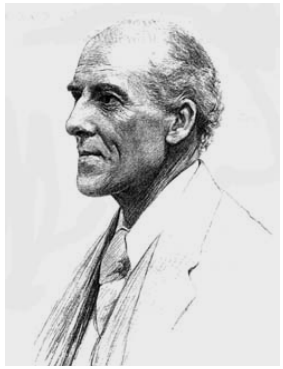
Karl Pearson 1901;
Hotelling 1933;
Jolliffe 2002





On lines and planes of closest fit to systems of points in space.
The London, Edinburgh and Dublin Philosophical Magazine and Journal of Science, 6 (2), 559-572, 1901.

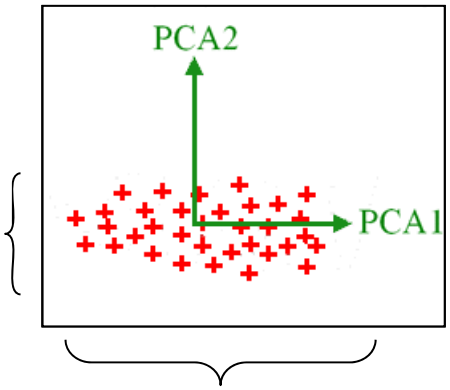
- As an exploratory tool to uncover unknown trends in the data.
- Make a visual inspection of the relationship between observations in a multi-dimensional matrix.
- PCA is a method that reduces data dimensionality by performing a covariance analysis between factors.
- PCA is to 'summarize' the data, it is not considered a clustering tool.



Karl Pearson (1857-1936)

PCA

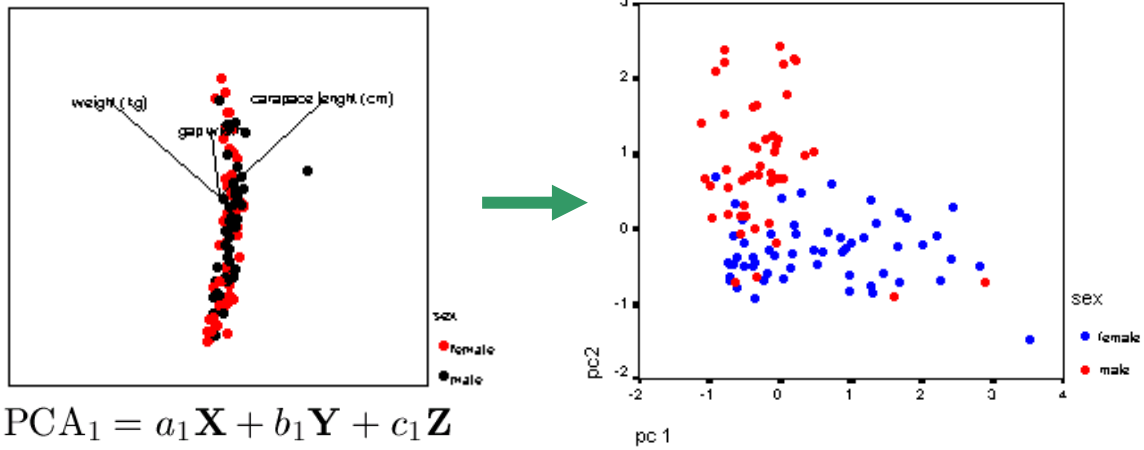
PCA is a method that reduces data dimensionality by finding the new variables (major axes, principal components).



$$\mathrm{PCA}_1 = a_1\mathbf{X} + b_1\mathbf{Y}$$

$$\mathrm{PCA}_2 = a_2\mathbf{X} + b_2\mathbf{Y}$$

Image source: 61BL4165 Multivariate Statistics, Department of Biological Sciences, Manchester Metropolitan University



$$\mathrm{PCA}_1 = a_1\mathbf{X} + b_1\mathbf{Y} + c_1\mathbf{Z}$$

$$\mathrm{PCA}_2 = a_2\mathbf{X} + b_2\mathbf{Y} + c_2\mathbf{Z}$$

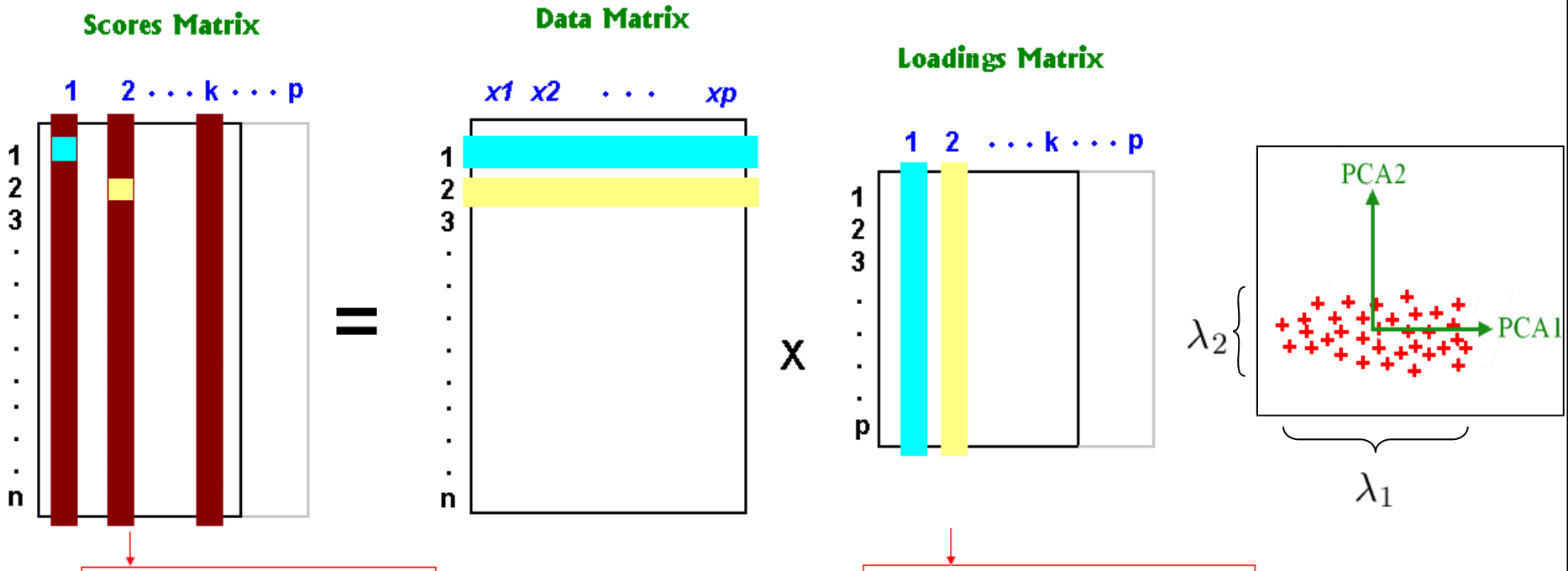
$$\mathrm{PCA}_1 = a_{11}\mathbf{X}_1 + a_{12}\mathbf{X}_2 + \cdots + a_{1p}\mathbf{X}_p$$

$$\mathrm{PCA}_2 = a_{21}\mathbf{X}_1 + a_{22}\mathbf{X}_2 + \cdots + a_{2p}\mathbf{X}_p$$

Amongst all possible projections, PCA finds the projections so that the maximum amount of information, measured in terms of variability, is retained in the smallest number of dimensions.

PCA: Loadings and Scores

$$Z = X \quad W$$



The *i*th principal component of $\mathbf{X}$ is $\mathbf{X}\mathbf{w}_i$, where $\mathbf{w}_i$ is the *i*th normalized eigenvector of $\Sigma_{\mathbf{x}}$ corresponding to the *i*th largest eigenvaules.

Eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p$

$$\text{proportion} = \frac{\sum_{i=1}^{k} \lambda_i}{\sum_{i=1}^{p} \lambda_i}$$

PCA is the spectral decomposition of the variance covariance matrix, ***S***, of the data matrix, ***X***. we can write $S=CDC^T$.

PCA: General Methodology (1/3)

- Find a low-dimensional space such that when x is projected there, information loss is minimized.
- PCA centers the sample and then rotates the axes to line up with the directions of highest variance.

The projection of $\boldsymbol{x}$ on the direction of $\boldsymbol{w}$ is: $z = \boldsymbol{w}^T\boldsymbol{x}$

Find $\boldsymbol{w}$ such that var(z) is maximized

$$\begin{aligned}\text{var}(z) &= \text{var}(\boldsymbol{w}^T\boldsymbol{x}) \\ &= E[(\boldsymbol{w}^T\boldsymbol{x} - \boldsymbol{w}^T\boldsymbol{\mu})^2] \\ &= E[\boldsymbol{w}^T(\boldsymbol{x} - \boldsymbol{\mu})^2\boldsymbol{w}] \\ &= E[\boldsymbol{w}^T(\boldsymbol{x} - \boldsymbol{\mu})(\boldsymbol{x} - \boldsymbol{\mu})^T\boldsymbol{w}] \\ &= \boldsymbol{w}^T E[(\boldsymbol{x} - \boldsymbol{\mu})(\boldsymbol{x} - \boldsymbol{\mu})^T]\boldsymbol{w}\end{aligned}$$

$$\begin{aligned}\text{var}(\boldsymbol{x}) &= E[(\boldsymbol{x} - \boldsymbol{\mu})^2] \\ &= E[(\boldsymbol{x} - \boldsymbol{\mu})(\boldsymbol{x} - \boldsymbol{\mu})^T] \\ &= \boldsymbol{\Sigma}\end{aligned}$$

```
?cov
x <- iris[, 1:4]
cov(x)
```

PCA: General Methodology (2/3)

$\text{var}(z) = w^T \Sigma w$ Maximize var(z) subject to ||w||=1

$$\mathcal{L}(\lambda, w_1) = w_1^T \Sigma w_1 - \lambda(w_1^T w_1 - 1)$$

Lagrangian method

拉格朗日

$$\max_{w_1} \mathcal{L}(\lambda, w_1) \rightarrow \begin{cases} \frac{\partial \mathcal{L}(\lambda, w_1)}{\partial \lambda} = 0 \rightarrow w_1^T w_1 - 1 = 0 \\ \frac{\partial \mathcal{L}(\alpha, w_1)}{\partial w_1} = 0 \rightarrow 2\Sigma w_1 - 2\lambda w_1 = 0 \end{cases}$$

$\rightarrow \Sigma w_1 = \lambda w_1$

$\rightarrow w_1$ is an eigenvector of Σ

λ is an eigenvalue associated with w_1

```
x <- iris[, 1:4]
(covx <- cov(x))
e <- eigen(covx)
V <- e$vectors
V.inverse <- solve(e$vectors)
covx.hat <- V %*% diag(e$values) %*% V.inverse
covx.hat # same with covx
```

$$\text{var}(z) = \text{var}(w_1^T x) = w_1^T \Sigma w_1 = w_1^T \lambda w_1 = \lambda w_1^T w_1 = \lambda$$

$\rightarrow \max \text{var}(z) = \max \lambda$

PCA: General Methodology (3/3)

Second principal component:

Max $\mathrm{var}(z_2)$, s.t., $\|w_2\|=1$ and orthogonal to w_1

$$\mathcal{L}(\lambda_2, \beta, w_1, w_2) = w_2^T \Sigma w_2 - \lambda_2 (w_2^T w_2 - 1) - \beta (w_2^T w_1 - 0)$$

$$\max_{w_2} \mathcal{L}(\lambda_2, \beta, w_1, w_2) \quad \rightarrow \quad \Sigma w_2 = \lambda_2 w_2$$

w_i is the eigenvector of S associated with the i^{th} largest eigenvalue.

$$\mathrm{var}(z_i) = \lambda_i$$

Proof (by induction – Assume true for i -1, then prove true for i)

- w_i's are uncorrelated (orthogonal)
- w_1 explains as much as possible of original variance in data set
- w_2 explains as much as possible of remaining variance, etc.

PCA: Solutions

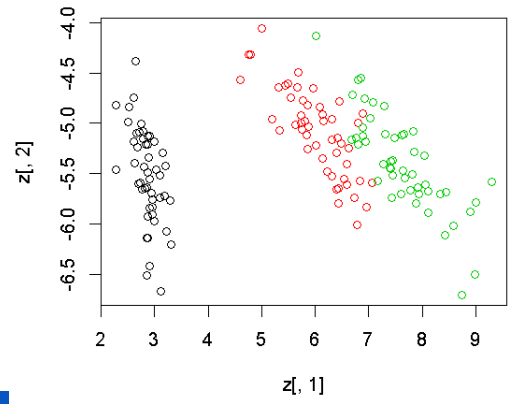
- If the dimensions are highly correlated, there will be a small number of eigenvectors with large eigenvalues, and ***k*** will be much smaller than ***d*** and a large reduction in dimensionality may be attained.

- If the dimensions are not correlated, ***k*** will be as large as ***d*** and there is no gain through PCA.

$$\text{var}(z) = w^T \Sigma w$$

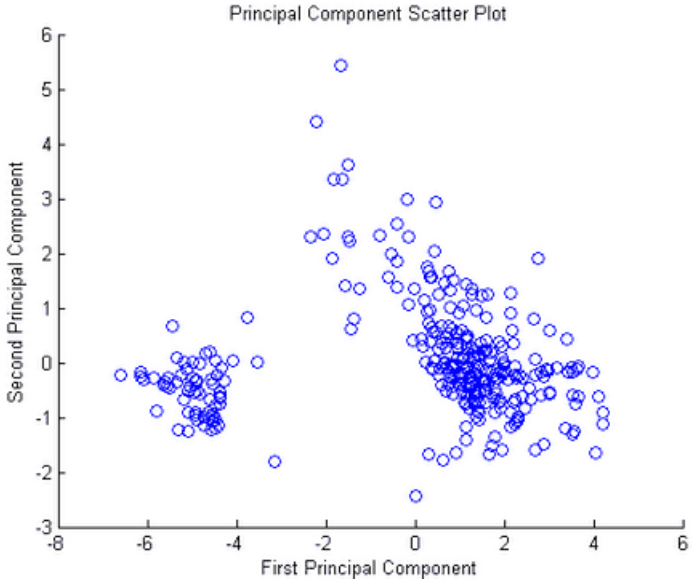
- ***S* is symmetric:** for two different eigenvalues, the eigenvectors are orthogonal.
- **If *S* is positive definite:** (***x'Sx>0, x!=null***): all eigenvalues are positive.
- **If *S* is singular:** then its rank, the effective dimension is $k < d$, and $\lambda_i = 0, i > k$.

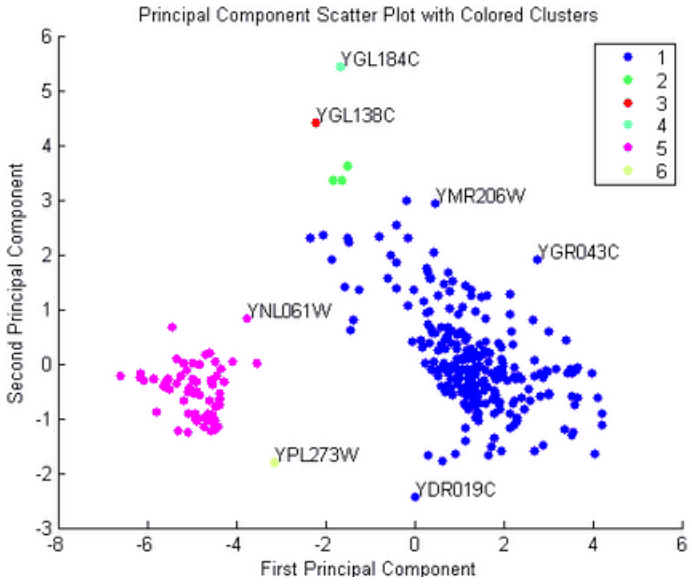
```
# PCA for iris data
z <- as.matrix(x) %*% e$vectors[, 1:2]
plot(z[, 1], z[, 2], col=iris[, 5])
```



When to use PCA?

- As an exploratory tool to uncover unknown trends in the data.
- PCA on genes provide a way to identify predominant gene expression patterns.
- PCA on conditions explore correlations between samples or conditions.
- PCA is to ‘summarize’ the data, it is not considered a clustering tool.





Yeast Microarray Data is from
DeRisi, JL, Iyer, VR, and Brown, PO.(1997). "Exploring the metabolic and genetic control of gene expression on a genomic scale"; Science, Oct 24;278(5338):680-6.

How Many Components to Use?

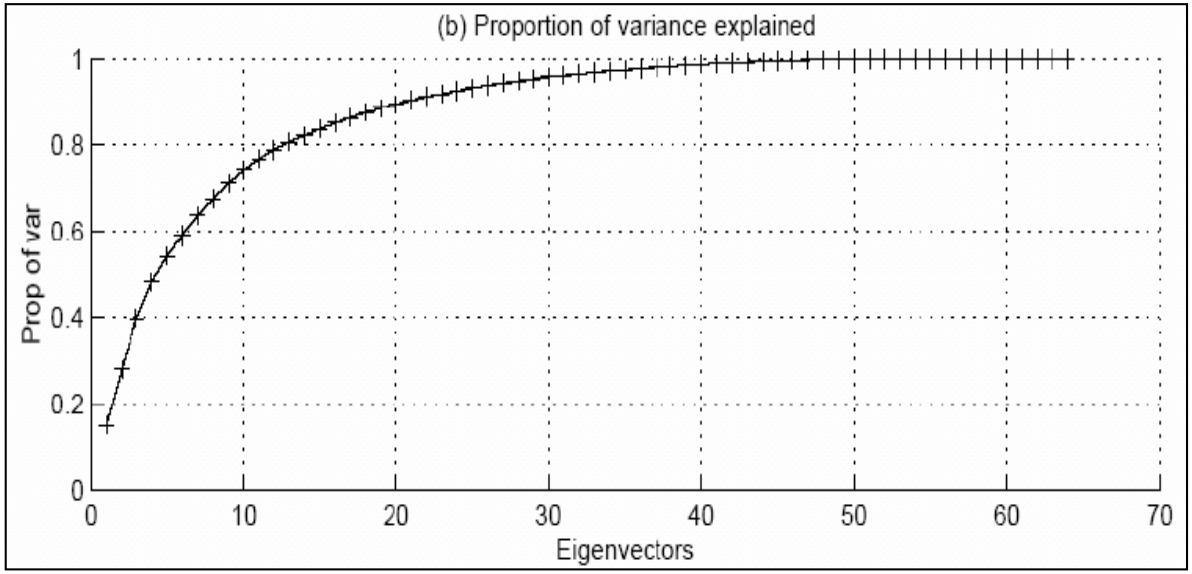
- The proportion of Variance explained by the first k principal components

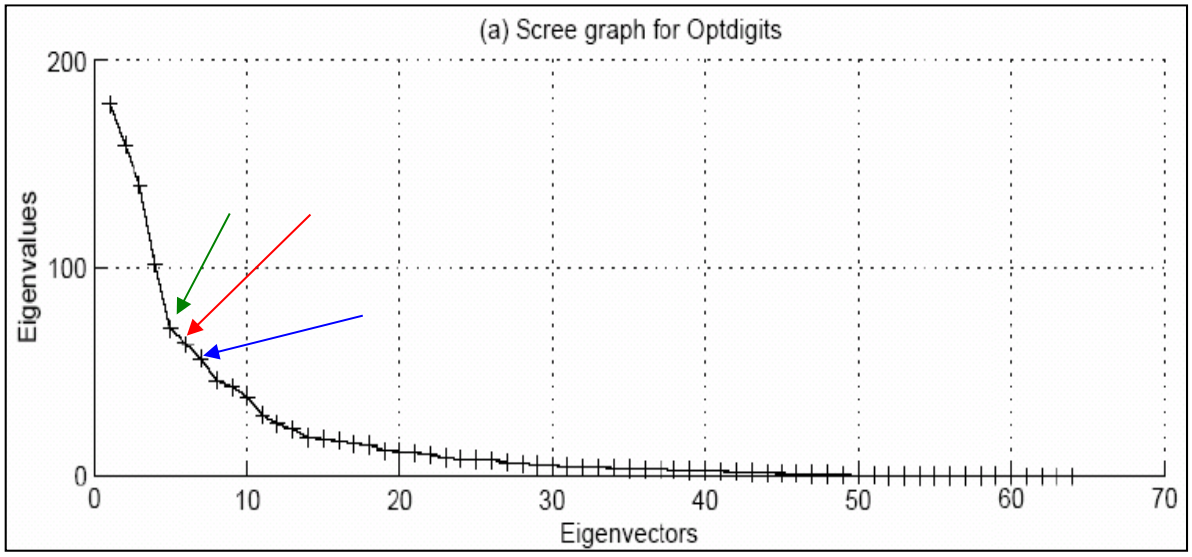
$$\frac{\lambda_1 + \lambda_2 + \cdots + \lambda_k}{\lambda_1 + \lambda_2 + \cdots + \lambda_k + \cdots + \lambda_d} \qquad \frac{\lambda_k}{\sum_{j=1}^{r} \lambda_j} = \frac{\lambda_k}{\mathrm{tr}(\Sigma)}.$$

- If $\lambda_j < 1$ then component explains less variance than original variable (correlation matrix).
- Use 2 components (or 3) for visual ease.
- Keep only the eigenvectors with eigenvalues greater than **average eigenvalue**.
- Keep only those which have higher than the **average input variance**.

Scree Diagram

At the elbow, adding another eigenvector does not significantly increase the variance explained.





PCA: Scaling (1/2)

- Different variables have completely different scaling.
  - Eigenvalues of the matrix is scale dependent.
  - (If we would multiply one column of the data matrix ***X*** by some scale factor (say ***s***) then variance of this variable would increase by ***s2*** and this variable can dominate whole covariance matrix and hence whole eigenvalue and eigenvectors.)

- Covariance Matrix
  - Variables must be in same units.
  - Emphasizes variables with most variance.
  - Mean eigenvalue > 1.0

- Correlation Matrix
  - Variables are standardized (mean=0.0, SD=1.0)
  - Variables can be in different units.
  - All variables have same impact on analysis.
  - Mean eigenvalue = 1.0

PCA: Scaling (2/2)

- **Bring all data to the same scale:** If scale of the data is unknown then it is better to use correlation matrix instead of the covariance matrix.
- The interpretation of the principal components derived by these two methods (**Covariance Matrix and Correlation Matrix**) can be completely different.
- If the variance of the original ***xi*** dimensions vary considerably, they affect the directions of the principal components more than the correlations.
  - Standardized data by columns, mean=0, sd=1,
  - PCA on correlation matrix, for the correlations to be effective and not the individual variances.

PCA: Potential Problems

- Sensitive to outliers
  - Robust estimation
  - Discarding the isolated data points that are far away.
- Lack of Independence
  - NO PROBLEM
- Lack of Normality
  - Normality desirable but not essential
- Lack of Precision
  - Precision desirable but not essential
- Many Zeroes in Data Matrix
  - Problem (use Correspondence Analysis)

This works better than taking the average because we take into account correlations and differences in variances.

Example:

average

	A	B	C	D	E	F	平均	PCA1
1	學號	小考1	期中考	小考2	期末考	報告		
2	A01	69	92	85	45	62		
3	A02	66	90	83	36	90		
4	A03	72	92	80	62	70		
5	A04	68	90	60	37	95		
6	A05	74	60	86	54	70		
7	A06	77	90	88	88	95		
8	A07	73	88	77	51	95		
9	A08	61	90	84	40	82		
10	A09	66	88	82	39	80		
11	A10	76	75	87	72	80		
12	A11	64	90	90	26	95		
13	A12	75	90	60	55	70		
14	A13	92	90	83	90	95		

Circle of Correlations

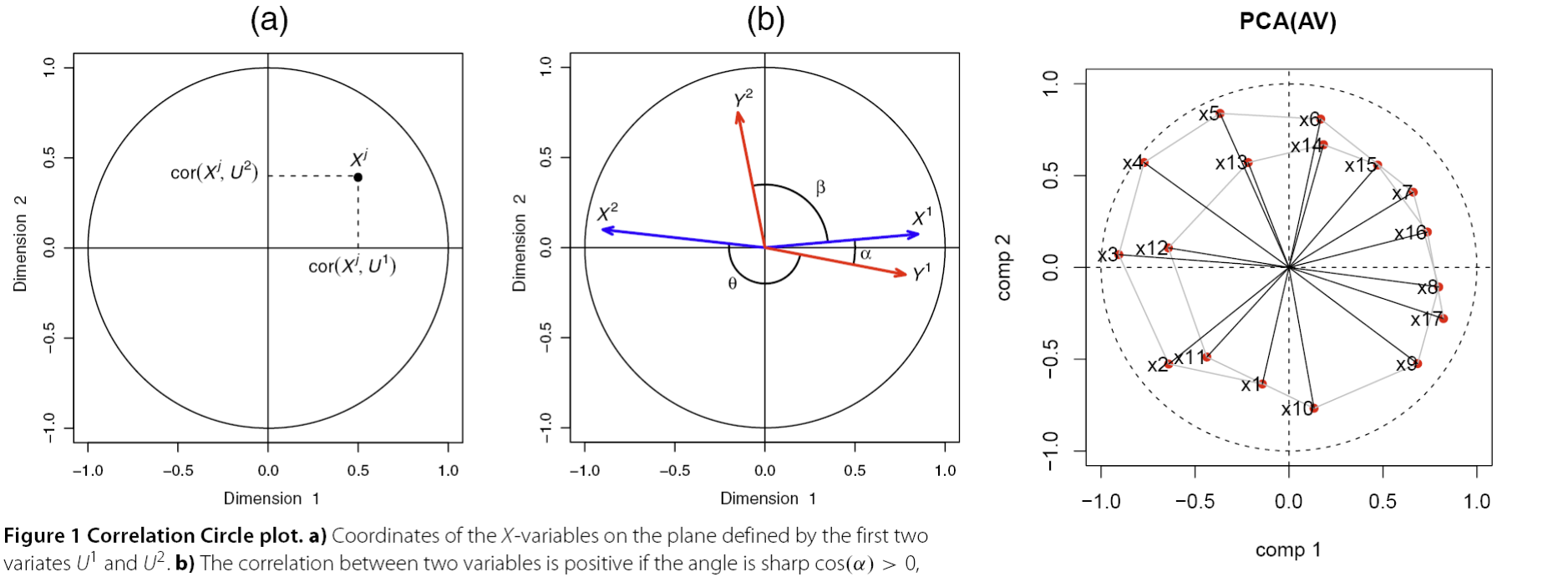


Figure 1 Correlation Circle plot. a) Coordinates of the X-variables on the plane defined by the first two variates U^1 and U^2. **b)** The correlation between two variables is positive if the angle is sharp $\cos(\alpha) > 0$, negative if the angle is obtuse $\cos(\theta) < 0$, and null if the vectors are perpendicular $\cos(\beta) \approx 0$.

González *et al. BioData Mining* 2012, **5**:19
http://www.biodatamining.org/content/5/1/19

the input variables, X_j,

the DR components, Z_k,

$$\rho_{jk} = \mathrm{Corr}(X_j; Z_k) = \frac{\mathrm{Cov}(X_j, Z_k)}{\sqrt{\mathrm{Var}(X_j)\mathrm{Var}(Z_k)}}.$$

Circles of correlations associated with the first two DR components based on the applied vector and path point approaches applied to the microarray data of the yeast cell cycle.

Principal Components Analysis and SVD

The principal components are equal to the **right singular values** if the variables of data is scaled. (subtract the mean, divide by the standard deviation).

```
> m1 <- matrix(sample(1:16,16),4,4)
> m1
     [,1] [,2] [,3] [,4]
[1,]   15    1   16    7
[2,]    8    9    2   10
[3,]   13    4   12    3
[4,]    5   14   11    6
> m1.scale.svd <- svd(scale(m1))
> m1.scale.svd
$d
[1] 2.827057e+00 1.759769e+00 9.544443e-01 4.258869e-17

$u
           [,1]       [,2]       [,3] [,4]
[1,] -0.5580839 -0.3507292  0.5617218  0.5
[2,]  0.5716314 -0.5999038 -0.2517003  0.5
[3,] -0.4320314  0.2946885 -0.6902952  0.5
[4,]  0.4184839  0.6559445  0.3802737  0.5

$v
           [,1]       [,2]       [,3]        [,4]
[1,] -0.5663183 -0.3664762 -0.1512544  0.72256547
[2,]  0.5395013  0.4585555  0.1574801  0.68837872
[3,] -0.5008709  0.3789166  0.7772586 -0.03767775
[4,]  0.3706081 -0.7154329  0.5900773  0.05112996
```

```
> m1.pca <- prcomp(m1, scale=T)
> m1.pca
Standard deviations:
[1] 1.6322e+00 1.016003e+00 5.510487e-01 2.458859e-17

Rotation:
            PC1        PC2        PC3         PC4
[1,] -0.5663183 -0.3664762 -0.1512544  0.72256547
[2,]  0.5395013  0.4585555  0.1574801  0.68837872
[3,] -0.5008709  0.3789166  0.7772586 -0.03767775
[4,]  0.3706081 -0.7154329  0.5900773  0.05112996
```

```
> pca2 <- princomp(m1, cor=T)
> pca2$scores
        Comp.1     Comp.2     Comp.3        Comp.4
[1,]  1.821811  0.7126839  0.6190721  6.227657e-16
[2,] -1.866036  1.2190081 -0.2773982 -9.020562e-16
[3,]  1.410325 -0.5988089 -0.7607725 -1.804112e-16
[4,] -1.366101 -1.3328832  0.4190986  4.649059e-16
> pca2$loadings

Loadings:
     Comp.1 Comp.2 Comp.3 Comp.4
[1,]  0.566  0.366 -0.151  0.723
[2,] -0.540 -0.459  0.157  0.688
[3,]  0.501 -0.379  0.777
[4,] -0.371  0.715  0.590

               Comp.1 Comp.2 Comp.3 Comp.4
SS loadings      1.00   1.00   1.00   1.00
Proportion Var   0.25   0.25   0.25   0.25
Cumulative Var   0.25   0.50   0.75   1.00
```

Source: Singular Value Decomposition, João Neto, http://www.di.fc.ul.pt/~jpn/r/svd/svd.html

PCA in R

- 5 functions to do Principal Components Analysis in R (by Gaston Sanchez): **`prcomp{stats}; princomp{stats}; PCA{FactoMineR}; dudi.pca{ade4}; acp{amap}; epPCA{ExPosition}`**
  (http://gastonsanchez.com/blog/how-to/2012/06/17/PCA-in-R.html)

- **STHDA**: Statistical tools for high-throughput data analysis
  - Principal component analysis in R : **`prcomp()`** vs. **`princomp()`** - R software and data mining

  http://www.sthda.com/english/wiki/principal-component-analysis-in-r-prcomp-vs-princomp-r-software-and-data-mining
  - **`FactoMineR`** and **`factoextra`** : Principal Component Analysis Visualization - R software and data mining

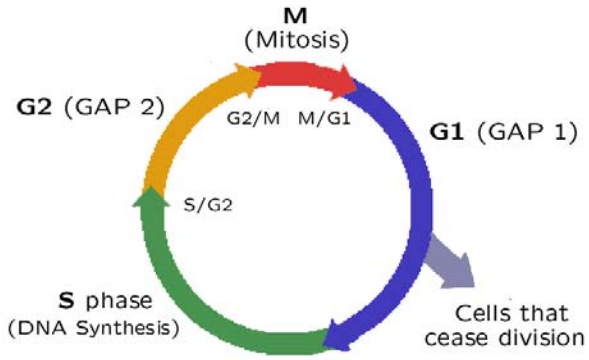
  http://www.sthda.com/english/wiki/factominer-and-factoextra-principal-component-analysis-visualization-r-software-and-data-mining

- Gregory B. Anderson, principal component analysis in R
  https://www.ime.usp.br/~pavan/pdf/MAE0330-PCA-R-2013

- R Package "**`bigpca`**": Title PCA, Transpose and Multicore Functionality for '**`big.matrix`**'
  https://cran.r-project.org/web/packages/bigpca/

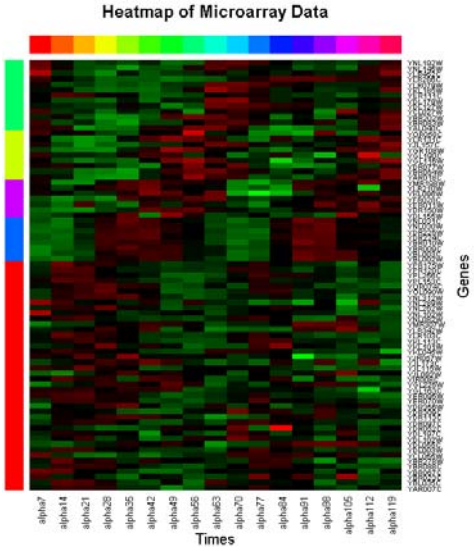
範例: Microarray Data of Yeast Cell Cycle

- Synchronized by alpha factor arrest method (Spellman et al. 1998; Chu et al. 1998)
- 103 known genes: every 7 minutes and totally 18 time points. (remove NA's: 79 genes)



Microarray Data Matrix

MA Table	exp01	exp02	exp03	exp04	exp05	exp•••	exp p
gene001	-0.48	-0.42	0.87	0.92	0.67		-0.35
gene002	-0.39	-0.58	1.08	1.21	0.52		-0.58
gene003	0.87	0.25	-0.17	0.18	-0.13		-0.13
gene004	1.57	1.03	1.22	0.31	0.16		-1.02
gene005	-1.15	-0.86	1.21	1.62	1.12		-0.44
gene006	0.04	-0.12	0.31	0.16	0.17		0.08
gene007	2.95	0.45	-0.40	-0.66	-0.59		-0.76
gene008	-1.22	-0.74	1.34	1.50	0.63		-0.55
gene009	-0.73	-1.06	-0.79	-0.02	0.16		0.03
gene010	-0.58	-0.40	0.13	0.58	-0.09		-0.45
gene011	-0.50	-0.42	0.66	1.05	0.68		0.01
gene012	-0.86	-0.29	0.42	0.46	0.30		-0.63
gene013	-0.16	0.29	0.17	-0.28	-0.02		-0.04
gene014	-0.36	-0.03	-0.03	-0.08	-0.23		-0.21
gene015	-0.72	-0.85	0.54	1.04	0.84		-0.64
gene016	-0.78	-0.52	0.26	0.20	0.48		0.27
gene017	0.60	-0.55	0.41	0.45	0.18		-1.02
gene018	-0.20	-0.67	0.13	0.10	0.38		0.05
gene019	-2.29	-0.64	0.77	1.60	0.53		-0.38
gene020	-1.46	-0.76	1.08	1.50	0.74		-0.70
gene021	-0.57	0.42	1.03	1.35	0.64		-0.40
gene022	-0.11	0.13	0.41	0.60	0.23		0.19
gene•••							
gene n	-1.79	0.94	2.13	1.75	0.23		-0.66

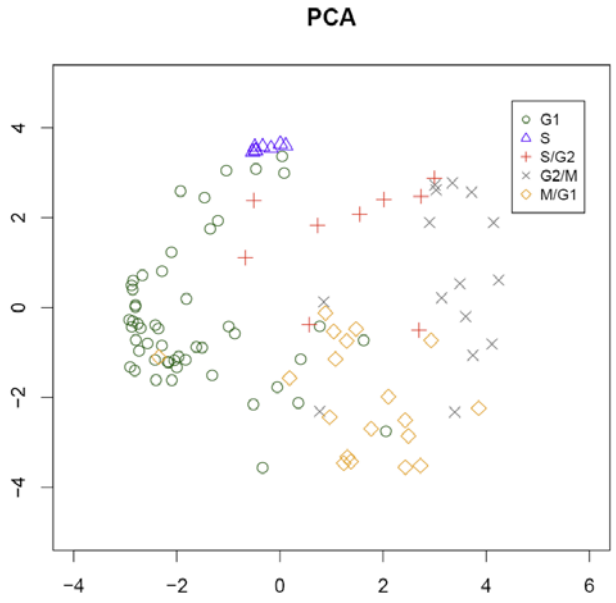


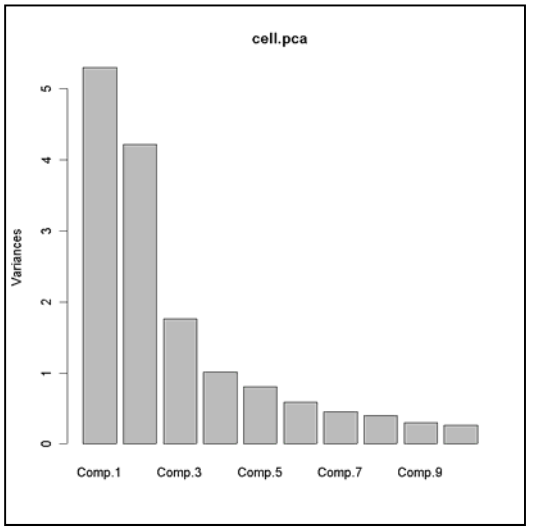

```
cell.matrix  <- read.table("YeastCellCycle_alpha.txt", header=TRUE, row.names=1)
n <- dim(cell.matrix)[1]
p <- dim(cell.matrix)[2]-1
cell.data <- cell.matrix[,2:p+1]
gene.phase <- cell.matrix[,1]
phase <- unique(gene.phase)
phase.name <- c("G1", "S", "S/G2", "G2/M", "M/G1")
cell.sdata <- t(scale(t(cell.data)))
rc <- rainbow(5)[as.integer(gene.phase)]
cc <- rainbow(ncol(cell.sdata))
hv <- heatmap(cell.sdata, col = GBRcol, scale = "column", Colv=NA, Rowv=NA,
              RowSideColors = rc, ColSideColors = cc, margins = c(5,10),
              xlab = "Times", ylab =  "Genes", main = "Heatmap of Microarray Data")
```

PCA on Conditions

```
cell.pca <- princomp(cell.sdata, cor=TRUE, scores=TRUE)
# 2D plot for first two components
pca.dim1 <- cell.pca$scores[,1]
pca.dim2 <- cell.pca$scores[,2]
plot(pca.dim1, pca.dim2, main="PCA for Cell Cycle Data on Genes", xlab="1st PCA
  Component", ylab="2nd PCA Component",col=c(phase), pch=c(phase))
legend(3, 4, phase.name, pch=c(phase), col=c(phase))

# shows a screeplot.
plot(cell.pca)
biplot(cell.pca)
```

MA Table	PCA-1	PCA-2	PCA-3
gene001	-0.18	-0.11	-0.03
gene002	0.51	-0.53	0.54
gene003	-0.35	-0.39	0.26
gene004	-0.18	-1.08	0.41
gene005	-0.62	-0.8	0.13
gene006	-0.09	-0.23	0.77
gene007	-0.38	-0.32	1.08
gene008	-0.88	-0.55	1.03
gene009	-1.26	0.45	0.41
gene010	0.12	-0.36	-0.16
gene011	-0.28	-0.44	2.13
gene012	-0.45	-0.23	0.82
gene013	-0.2	-0.43	0.44
gene014	0.03	-0.26	-0.68
gene015	-0.7	-0.76	0.5
gene016	-0.61	0.07	-0.04
gene017	-0.23	-0.71	0.01
gene018	0.1	0.1	0.11
gene019	-0.94	-0.97	0.24
gene020	-0.55	-0.53	0.86
gene021	-0.47	-0.87	-0.02
gene022	-0.34	-1.1	0.51
gene•••	-0.49	-0.2	0.91
gene n	-0.15	-1.04	-0.01



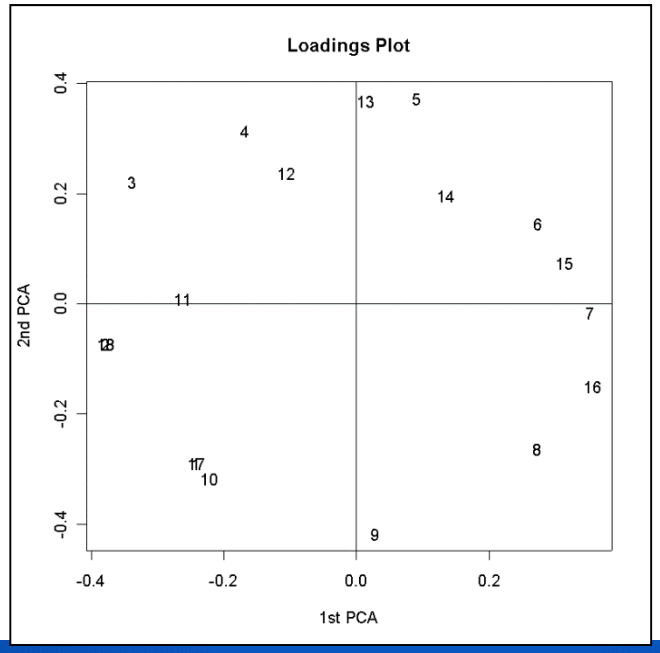


Loadings Plot

```
# loadings plot
plot(loadings(cell.pca)[,1], loadings(cell.pca)[,2], xlab="1st PCA",
ylab="2nd PCA", main="Loadings Plot", type="n")
text(loadings(cell.pca)[,1], loadings(cell.pca)[,2], labels=paste(1:p))
abline(h=0)
abline(v=0)
```

```
> summary(cell.pca)
Importance of components:
                          Comp.1    Comp.2    Comp.3     Comp.4     Comp.5        Comp.15
Standard deviation     2.3012110 2.0542795 1.3300507 1.00895544 0.90053289    0.308577283
Proportion of Variance 0.3309732 0.2637540 0.1105647 0.06362444 0.05068497 ... 0.005951246
Cumulative Proportion  0.3309732 0.5947272 0.7052919 0.76891637 0.81960134    1.000000000
```

```
# print loadings
loadings(cell.pca)
summary(cell.pca)
```



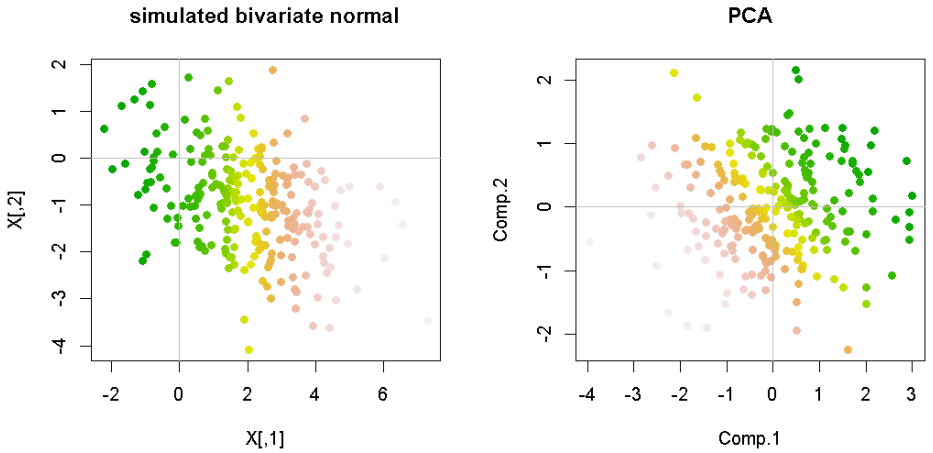
Loadings:	Comp.1	Comp.2	Comp.3	Comp.4
alpha14	-0.283	-0.21	0.283	0.136
alpha21	-0.374	0.211	-0.135	-0.16
alpha28	-0.26	0.298	0.161	-0.168
alpha35	-0.102	0.372	0.165	-0.321
alpha42	0.161	0.355	0.2	-0.317
alpha49	0.287	0.167	0.116	-0.515
alpha56	0.35	0.172	-0.274	-0.115
alpha63	0.251	-0.258	-0.275	-0.37
alpha70	-0.372	-0.217	-0.382	-0.159
alpha77	-0.253	-0.221	-0.321	-0.32
alpha84	-0.249	-0.437	-0.309	-0.256
alpha91	-0.115	0.279	-0.436	0.114
alpha98	0.36	-0.284	0.186	-0.138
alpha105	0.16	0.257	-0.283	-0.125
alpha112	0.347	0.319	-0.178	-0.276
alpha119	0.348	-0.164	-0.201	0.11

範例: two-dimensional simulated data

Example 2.3 The two-dimensional **simulated data** consist of 250 vectors $\mathbf{X}_i$ from the bivariate normal distribution with mean $[2, -1]^T$ and covariance matrix Σ as

$$\Sigma = \begin{pmatrix} 2.4 & -0.5 \\ -0.5 & 1 \end{pmatrix}.$$

```
> library(MASS)
> mu <- c(2, -1)
> Sigma <- matrix(c(2.4, -0.5, -0.5, 1), 2)
> n <- 250
> X <- mvrnorm(n, mu, Sigma)
>
> mycol <- terrain.colors(n)
> sorted.x1 <- sort(X[,1])
> order.x1 <- order(X[,1])
> id <- 1:n
> sorted.id <- id[order.x1]
> x1.col <- mycol[order(sorted.id)]
>
> par(mfrow=c(1, 2))
> plot(X, col=x1.col, pch=16,
+  main="simulated bivariate normal")
> abline(h=0, v=0, col="gray")
> X.pca <- princomp(X, cor = TRUE)
> X.pca$sdev
   Comp.1    Comp.2
1.1875339 0.7679605
```



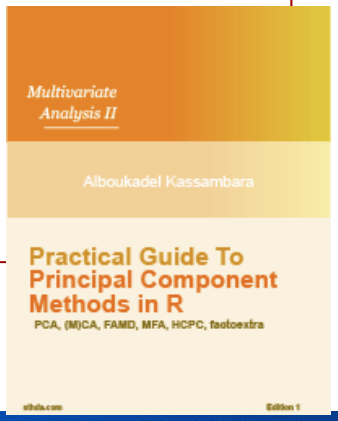

```
> X.pca$loadings

Loadings:
     Comp.1 Comp.2
[1,] -0.707 -0.707
[2,]  0.707 -0.707

                Comp.1 Comp.2
SS loadings        1.0    1.0
Proportion Var     0.5    0.5
Cumulative Var     0.5    1.0
> plot(X.pca$scores, col=x1.col, pch=16, main="PCA")
> abline(h=0, v=0, col="gray")
```

範例: decathlon2 {factoextra}: Athletes' performance in decathlon

use **FactoMineR** for the analysis and **factoextra** for ggplot2-based visualization.

```
> pca.pkg <- c("FactoMineR", "factoextra", "corrplot")
> install.packages(pca.pkg)
> lapply(pca.pkg, library, character.only=TRUE)
> data(decathlon2) # 十項全能
> head(decathlon2) # 100米, 跳遠, 鉛球, 跳高, 400米, 110米跨欄, 鐵餅, 撐竿跳高, 標槍, 1500米
          X100m Long.jump Shot.put High.jump X400m X110m.hurdle Discus
SEBRLE    11.04      7.58    14.83      2.07 49.81        14.69  43.75
CLAY      10.76      7.40    14.26      1.86 49.37        14.05  50.72
BERNARD   11.02      7.23    14.25      1.92 48.93        14.99  40.87
YURKOV    11.34      7.09    15.19      2.10 50.42        15.31  46.26
ZSIVOCZKY 11.13      7.30    13.48      2.01 48.62        14.17  45.67
McMULLEN  10.83      7.31    13.76      2.13 49.91        14.38  44.41
          Pole.vault Javeline X1500m Rank Points Competition
SEBRLE           5.02    63.19  291.7    1   8217    Decastar
CLAY             4.92    60.15  301.5    2   8122    Decastar
BERNARD          5.32    62.77  280.1    4   8067    Decastar
YURKOV           4.72    63.44  276.4    5   8036    Decastar
ZSIVOCZKY        4.42    55.37  268.0    7   8004    Decastar
McMULLEN         4.42    56.37  285.1    8   7995    Decastar
> dim(decathlon2)
[1] 27 13
> # standardization # x <- scale(x)
> x <- decathlon2[,1:10]
> # (default, PCA {FactoMineR} standardizes the data automatically
```

FactoMineR: Multivariate Exploratory Data Analysis and Data Mining



Practical Guide to Principal Component Methods in R
http://www.sthda.com/english/articles/31-principal-component-methods-in-r-practical-guide/112-pca-principal-component-analysis-essentials/

範例: PCA {FactoMineR}

```
> # PCA(X, scale.unit = TRUE, ncp = 5, graph = TRUE)
> x.pca <- PCA(x, graph = FALSE)
> class(x.pca)
[1] "PCA"   "list "
> str(x.pca)
List of 5
 $ eig : num [1:10, 1:3] 3.75 1.745 1.518 1.032 0.618 ...
  ..- attr(*, "dimnames")=List of 2
 ...
  ..$ call      : language PCA(X = x, graph = FALSE)
 - attr(*, "class")= chr [1:2] "PCA" "list "
> print(x.pca)
**Results for the Principal Component Analysis (PCA)**
The analysis was performed on 27 individuals, described by 10 variables
*The results are available in the following objects:

   name               description
1  "$eig"             "eigenvalues"
2  "$var"             "results for the variables"
3  "$var$coord"       "coord. for the variables"
4  "$var$cor"         "correlations variables - dimensions"
...
15 "$call$col.w"      "weights for the variables"
```

FactoMineR (version 2.3)

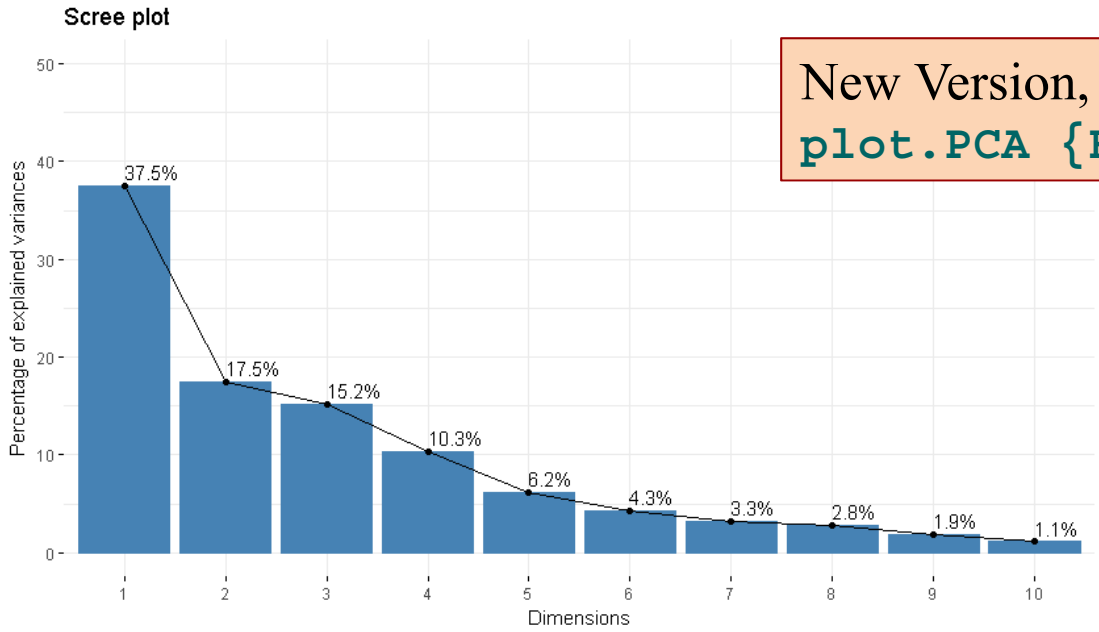
```
x.pca$eig
x.pca$ind
x.pca$var
```

(OLD version)

- `get_eigenvalue(x.pca)`: Extract the eigenvalues/variances of principal components
- `fviz_eig(x.pca)`: Visualize the eigenvalues
- `get_pca_ind(x.pca), get_pca_var(x.pca)`: Extract the results for individuals and variables.
- `fviz_pca_ind(x.pca), fviz_pca_var(x.pca)`: Visualize the results individuals and variables.
- `fviz_pca_biplot(x.pca)`: Make a biplot of individuals and variables.

Eigenvalues/Variances, scree plot

```
> # Eigenvalues/Variances
> eig.val <- get_eigenvalue(x.pca)
> eig.val
       eigenvalue variance.percent cumulative.variance.percent
Dim.1   3.7499727        37.499727                    37.49973
Dim.2   1.7451681        17.451681                    54.95141
Dim.3   1.5178280        15.178280                    70.12969
Dim.4   1.0322001        10.322001                    80.45169
Dim.5   0.6178387         6.178387                    86.63008
...
Dim.10  0.1122959         1.122959                   100.00000
> # scree plot
> fviz_eig(x.pca, addlabels = TRUE, ylim = c(0, 50))
```

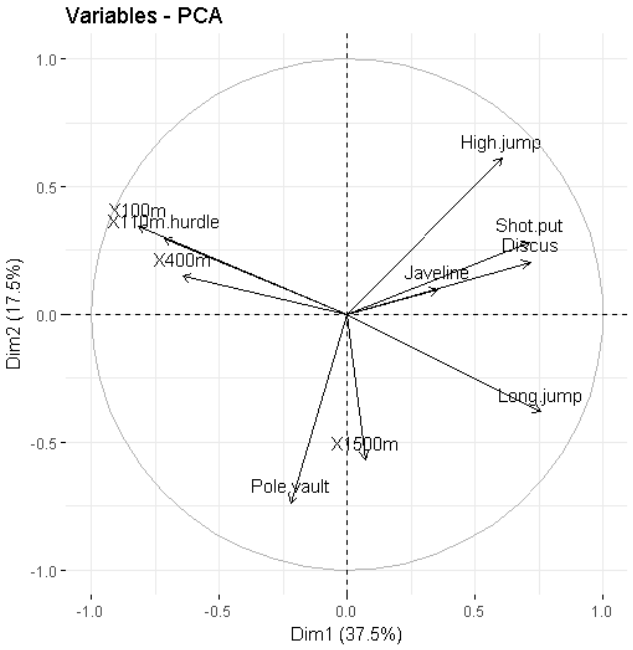


New Version, See
`plot.PCA {FactoMineR}`

Correlation Circles

```
> var <- get_pca_var(x.pca)
> var
Principal Component Analysis Results for variables
 ===================================================
  Name       Description
1 "$coord"   "Coordinates for the variables"
2 "$cor"     "Correlations between variables and dimensions"
3 "$cos2"    "Cos2 for the variables"
4 "$contrib" "contributions of the variables"
> # Coordinates of variables
> head(var$coord, 4)
              Dim.1      Dim.2       Dim.3       Dim.4      Dim.5
X100m     -0.8189521  0.3427787  0.100864539  0.10134200 -0.2198061
Long.jump  0.7588985 -0.3814931 -0.006261254 -0.18542415
Shot.put   0.7150783  0.2821167  0.473854591  0.03610404
High.jump  0.6084933  0.6113542  0.004605966  0.07124353
> # Correlation circle, variable correlation plots
> fviz_pca_var(x.pca, col.var = "black")
```

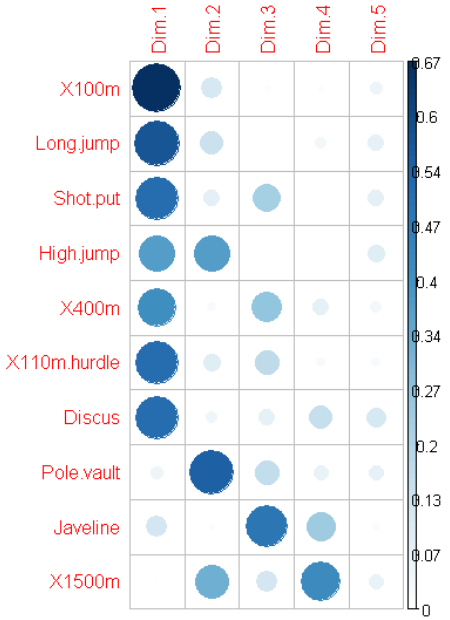
# **var$cos2**: quality of representation for variables on the factor map.
var.cos2 = var.coord * var.coord.
# **var$contrib**: the contributions of the variables to the principal components.
(var.cos2*100) / (total cos2 of the component).

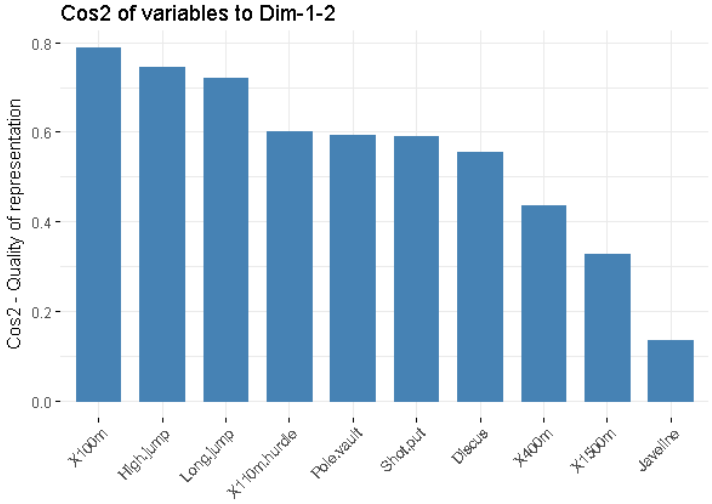


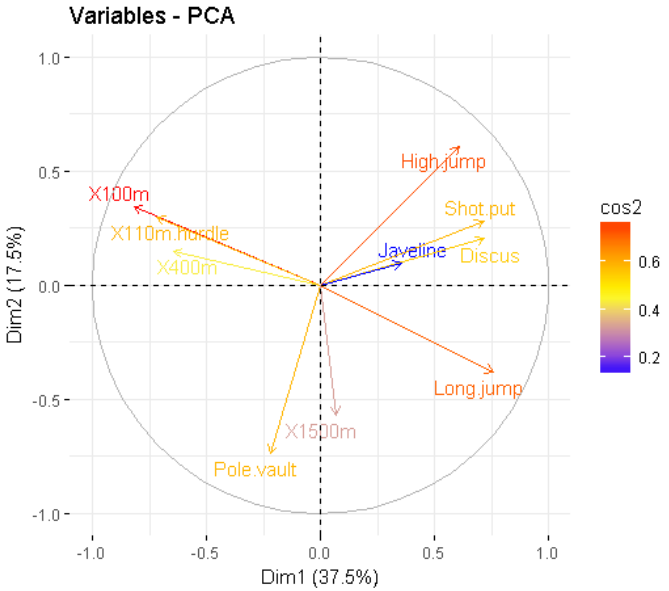
Positively correlated variables are grouped together.
Negatively correlated variables are positioned on opposite sides of the plot origin (opposed quadrants).
The distance between variables and the origin measures the quality of the variables on the factor map. Variables that are away from the origin are well represented on the factor map.

Quality of representation: square cosine (cos2 values) plot

```
> head(var$cos2, 4)
              Dim.1      Dim.2        Dim.3       Dim.4      Dim.5
X100m     0.6706825 0.11749725 1.017366e-02 0.010270201 0.04831474
Long.jump 0.5759270 0.14553701 3.920330e-05 0.034382115 0.06954513
Shot.put  0.5113370 0.07958983 2.245382e-01 0.001303502 0.07763857
High.jump 0.3702640 0.37375400 2.121493e-05 0.005075641 0.09035233
> corrplot(var$cos2, is.corr=FALSE)
> fviz_cos2(x.pca, choice = "var", axes = 1:2)
> # variables with low/mid/high cos2 values will be colored in blue/yellow/red
> fviz_pca_var(x.pca, col.var = "cos2",
+              gradient.cols = c("blue", "yellow", "red"),
+              repel = TRUE) # Avoid text overlapping
```

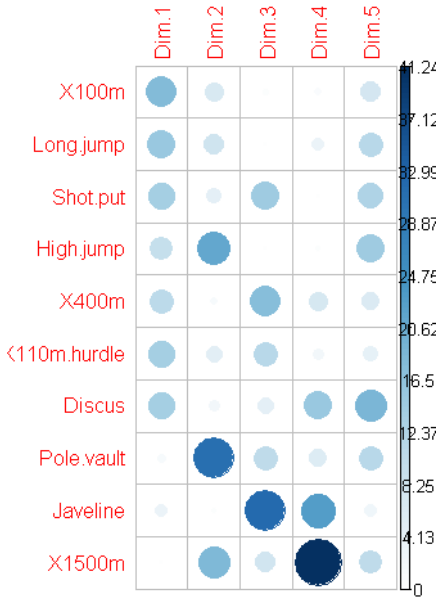


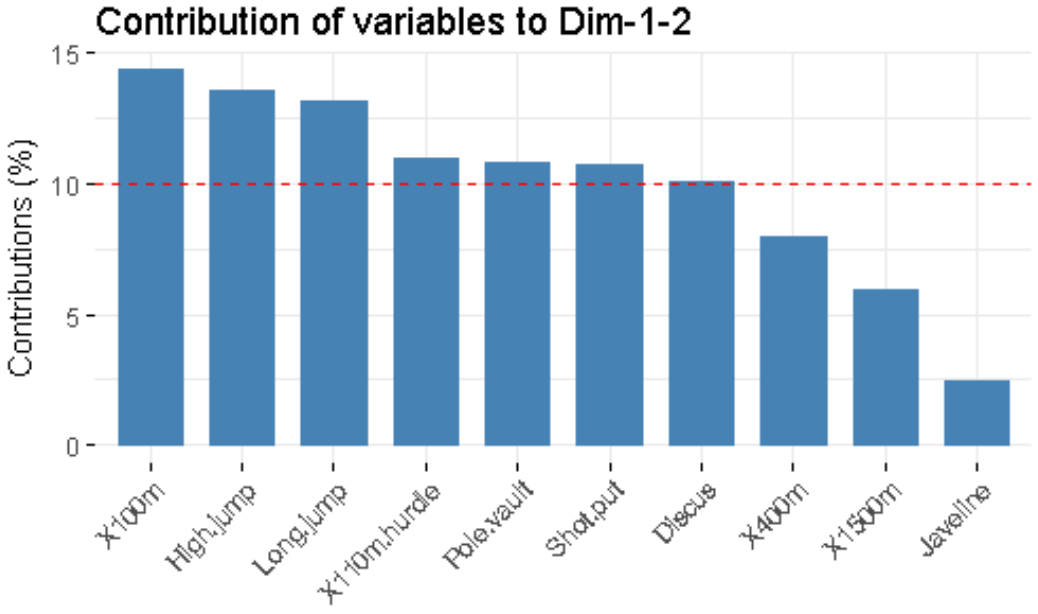




Contributions of variables to PCs

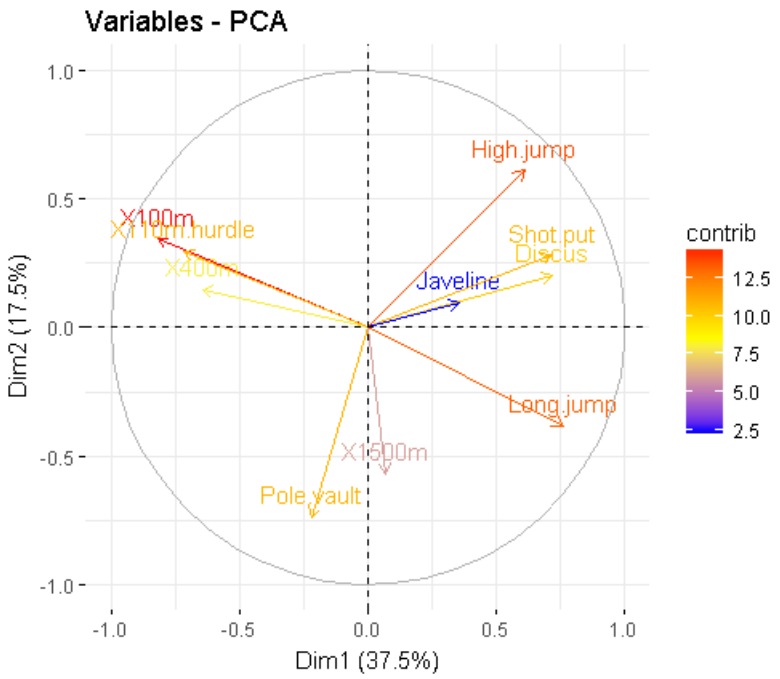
```
> head(var$contrib, 4)
             Dim.1     Dim.2        Dim.3     Dim.4    Dim.5
X100m     17.88500  6.732718  0.670277238 0.9949816  7.81996
Long.jump 15.35817  8.339426  0.002582856 3.3309545 11.25620
Shot.put  13.63575  4.560583 14.793387670 0.1262838 12.56616
High.jump  9.87378 21.416504  0.001397716 0.4917303 14.62394
> corrplot(var$contrib, is.corr=FALSE)
> # Contributions of variables to PC1
> fviz_contrib(x.pca, choice = "var", axes = 1, top = 10)
> # Contributions of variables to PC2
> fviz_contrib(x.pca, choice = "var", axes = 2, top = 10)
> # The total contribution to PC1 and PC2:
> fviz_contrib(x.pca, choice = "var", axes = 1:2, top = 10)
```

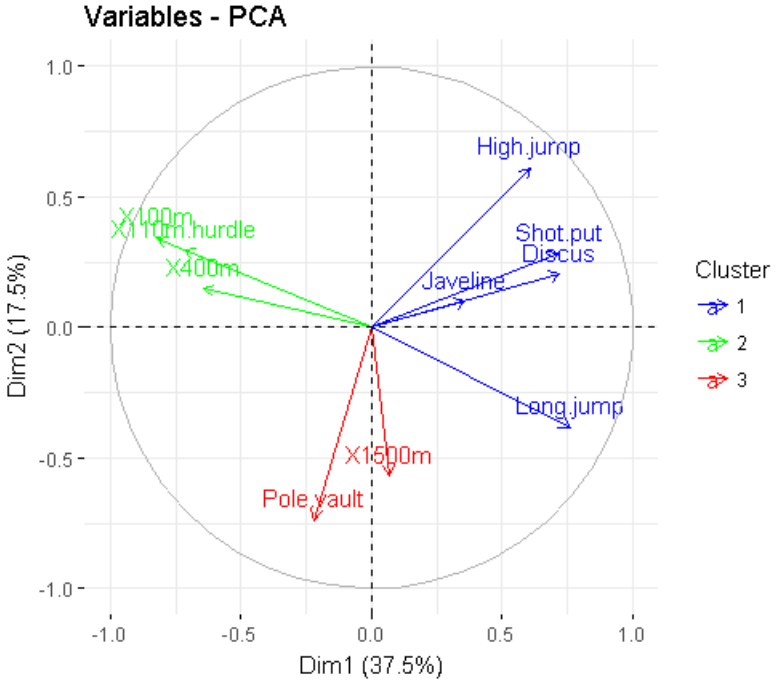




Highlight the most important variables

```
> fviz_pca_var(x.pca, col.var = "contrib",
+              gradient.cols = c("blue", "yellow", "red"))
> set.seed(123)
> var.kms <- kmeans(var$coord, centers = 3, nstart = 25)
> kms.grp <- as.factor(var.kms$cluster)
> # Color variables by kmeans' result
> fviz_pca_var(x.pca, col.var = kms.grp, palette = c("blue", "green", "red"),
+              legend.title = "Cluster")
```





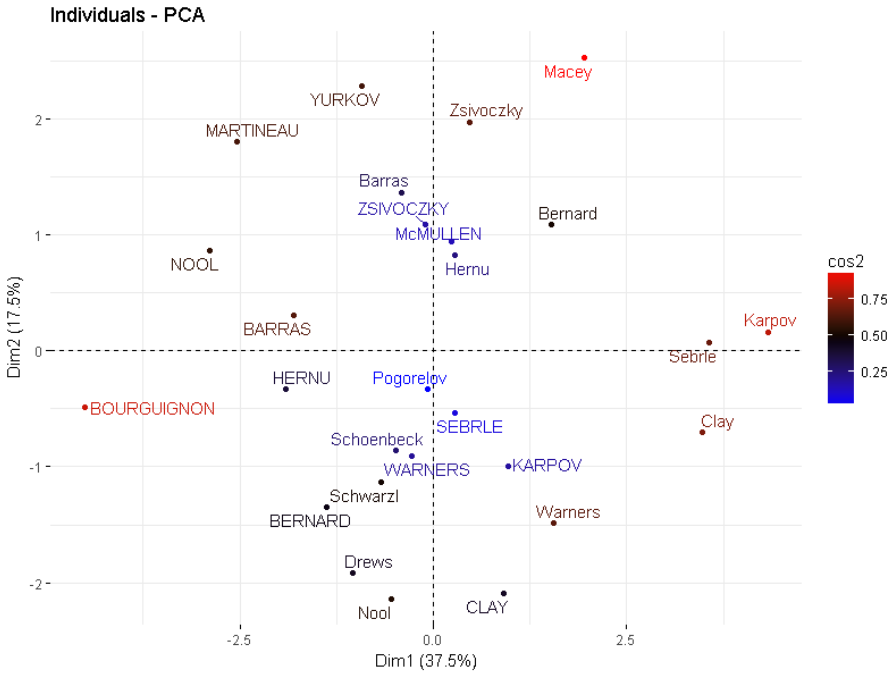
Obtain PCA results for individuals

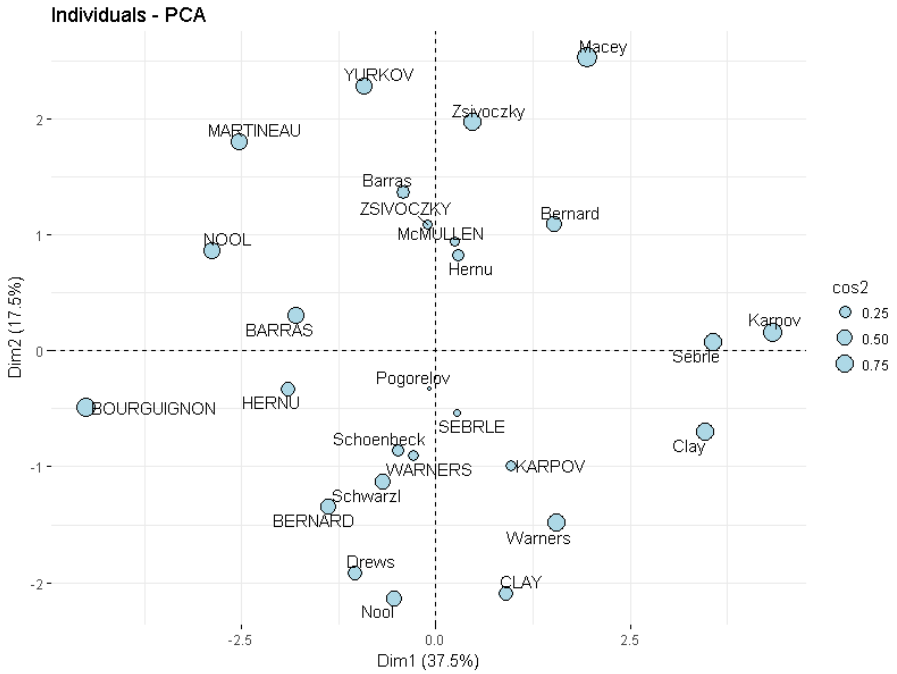
```
> ind <- get_pca_ind(x.pca)
> ind
Principal Component Analysis Results for individuals
 ===================================================
  Name       Description
1 "$coord"   "Coordinates for the individuals"
2 "$cos2"    "Cos2 for the individuals"
3 "$contrib" "contributions of the individuals"
> # Coordinates of individuals
> head(ind$coord, 3)
              Dim.1      Dim.2      Dim.3       Dim.4       Dim.5
SEBRLE     0.2779582 -0.5364345  1.5852390  0.10582254  1.07462350
CLAY       0.9048536 -2.0942803  0.8406848  1.85071783 -0.40864484
BERNARD   -1.3722659 -1.3481155  0.9619317 -1.49307179 -0.18266695
> # Quality of individuals
> head(ind$cos2, 3)
               Dim.1      Dim.2      Dim.3        Dim.4        Dim.5
SEBRLE    0.015446507 0.05753138 0.50241310 0.0022388646 0.2308788213
CLAY      0.065574226 0.35127414 0.05660346 0.2743196867 0.0133742243
BERNARD   0.232236641 0.22413434 0.11411498 0.2749258382 0.0041150408
> # Contributions of individuals
> head(ind$contrib, 3)
              Dim.1      Dim.2     Dim.3       Dim.4       Dim.5
SEBRLE    0.07630746  0.6107062  6.132015  0.04018174  6.92267277
CLAY      0.80865774  9.3082618  1.724567 12.29002506  1.00104404
BERNARD   1.85987901  3.8570314  2.257887  7.99896372  0.20002354
```

cos2 (Quality of individuals): https://personal.utdallas.edu/~herve/abdi-awPCA2010.pdf

Graph of individuals

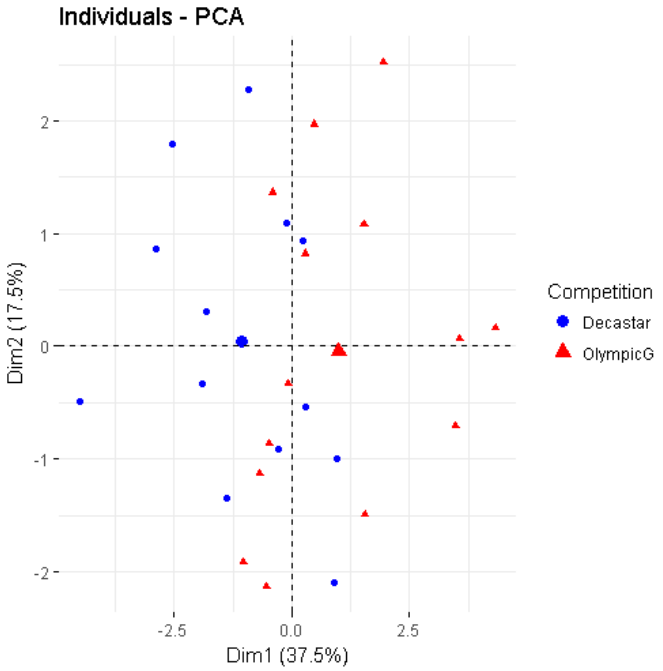
```
> # color individuals by their cos2 values
> fviz_pca_ind(x.pca, col.ind = "cos2", gradient.cols = c("blue", "black", "red"),
+              repel = TRUE)
>
> # change the point size according the cos2 of the corresponding individuals
> fviz_pca_ind(x.pca, pointsize = "cos2", pointshape = 21, fill = "lightblue",
+              repel = TRUE)
```

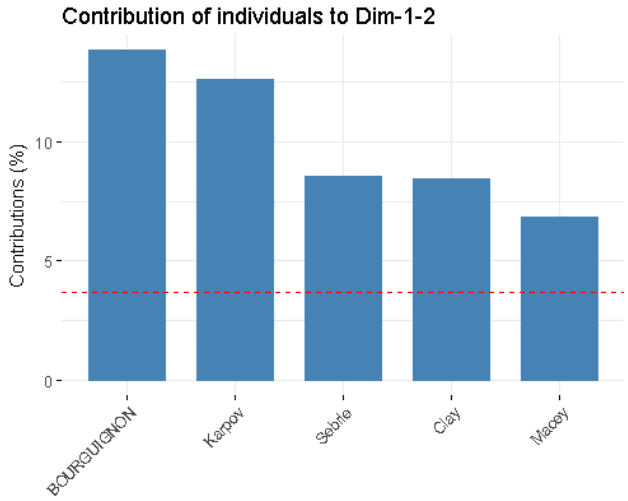


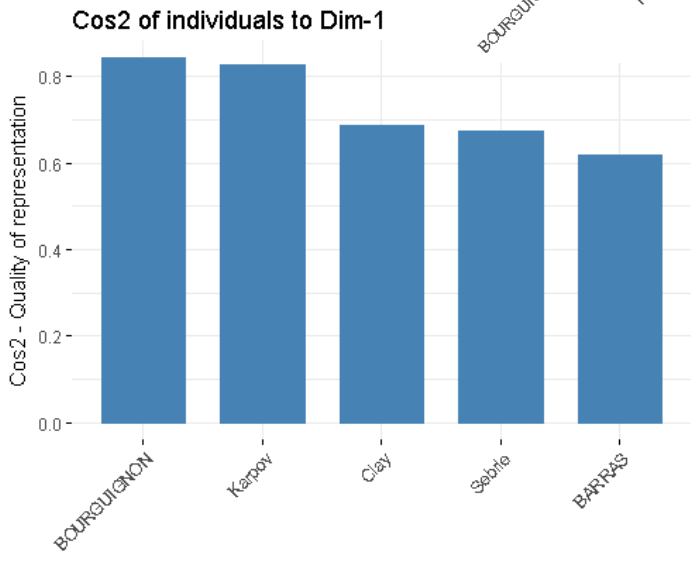


Graph of individuals

```
> fviz_pca_ind(x.pca, geom.ind = "point", col.ind = decathlon2[,13],
+              palette = c("blue", "red"), legend.title = "Competition")
>
> # quality of representation (cos2) of individuals on the factor map
> fviz_cos2(x.pca, choice = "ind", top = 5)
>
> # Total contribution of individuals on PC1 and PC2
> fviz_contrib(x.pca, choice = "ind", axes = 1:2, top = 5)
```







get eigenvectors
`x.pca$svd$V`

(4) The Biplot

The data matrix can be factored:

$$\mathbf{X} = \mathbf{AB}'$$

$\mathbf{X}_{n\times p}$: data matrix.
$\mathbf{A}_{n\times k}$: the coordinates for the n observations points along k rectangular axes.
$\mathbf{B}_{p\times k}$: the coordinates for the p variables along the same k axes.

To obtain $\mathbf{A}$ and $\mathbf{B}$, using Singular Value Decomposition (SVD)

$$\mathbf{X} = \mathbf{UDV}'$$

$\mathbf{A}_{[2]}$: the $n \times 2$ matrix of biplot coordinates for the observation points.
$\mathbf{B}_{[2]}$: the $p \times 2$ matrix of biplot coordinates for the variables.

$$\mathbf{A}_{[2]} = \mathbf{U}_{[2]}\mathbf{D}^{c}_{[2]}$$

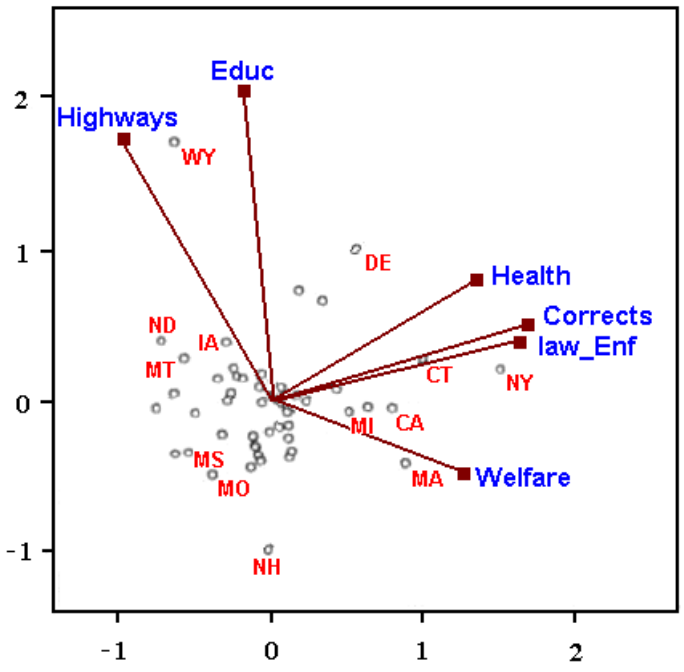
$$\mathbf{B}_{[2]} = \mathbf{V}_{[2]}\mathbf{D}^{1-c}_{[2]}$$

$\mathbf{U}_{[2]}$: the first two columns of $\mathbf{U}$.
$\mathbf{V}_{[2]}$: the first two columns of $\mathbf{V}$.
$\mathbf{D}_{[2]}$: the diagonal matrix formed by the first two singular values.

$$\mathbf{X}_{[2]} = \mathbf{A}_{[2]}\mathbf{B}'_{[2]}$$

Each row of $\mathbf{A}_{[2]}$ is plotted as a point in a two-axis coordinate system.
The rows of $\mathbf{B}_{[2]}$ are also plotted within the same space.
Goodness of fit measure R (s_r : singular values)

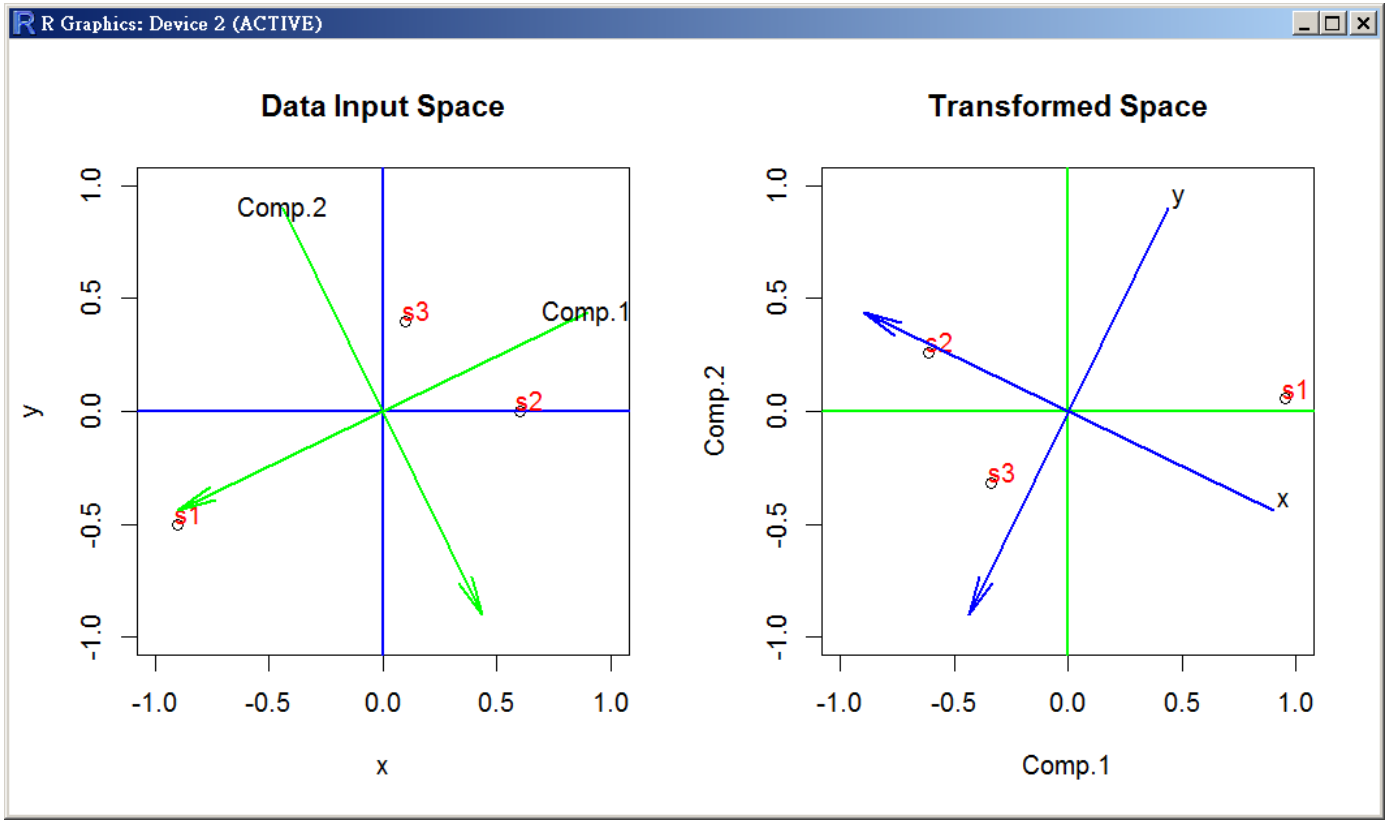
$$R = \frac{s_1^2 + s_2^2}{\sum_{r=1}^{p} s_s^2}$$



Biplot of 1992 State Policy Spending

- K. R. Gabriel (1971). The biplot graphical display of matrices with application to principal component analysis. Biometrika 58, 453–467.
- J.C. Gower and D. J. Hand (1996). Biplots. Chapman & Hall.

Moving Towards the Biplot: Rotation of axes




```
x <- c(-0.9, 0.6, 0.1)
y <- c(-0.5, 0, 0.4)
plot(x, y, xlim=c(-1, 1), ylim=c(-1, 1), main="Data Input Space")
abline(h=0, v=0, col="blue", lwd=2)
text(x+0.05, y+0.05, c("s1", "s2", "s3"), col="red")
pca <- princomp(cbind(x, y)); ab <- pca$loadings
arrows(-ab[1,1], -ab[2,1], ab[1,1], ab[2,1], col="green", angle = 10, lwd=2)
text(-ab[1,1], -ab[2,1], "Comp.1")
arrows(-ab[1,2], -ab[2,2], ab[1,2], ab[2,2], col="green", angle = 10, lwd=2)
text(-ab[1,2], -ab[2,2], "Comp.2")
```

Graphical Display of Matrix Multiplication

$A(4, 2)$ $B(2, 3)$ $P(4, 3)$

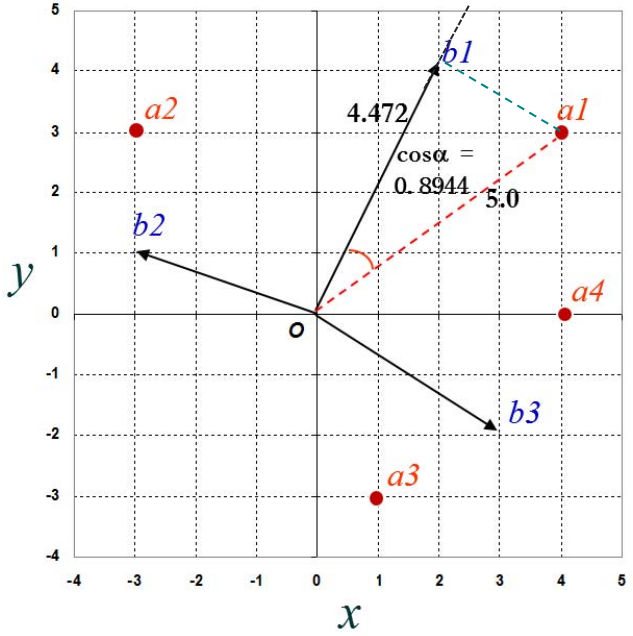
$$\begin{array}{c} \\ a1 \\ a2 \\ a3 \\ a4 \end{array}\begin{array}{c} \begin{array}{cc} x & y \end{array} \\ \begin{bmatrix} 4 & 3 \\ -3 & 3 \\ 1 & -3 \\ 4 & 0 \end{bmatrix} \end{array} \times \begin{array}{c} \\ x \\ y \end{array}\begin{array}{c} \begin{array}{ccc} b1 & b2 & b3 \end{array} \\ \begin{bmatrix} 2 & -3 & 3 \\ 4 & 1 & -2 \end{bmatrix} \end{array} = \begin{array}{c} \\ a1 \\ a2 \\ a3 \\ a4 \end{array}\begin{array}{c} \begin{array}{ccc} b1 & b2 & b3 \end{array} \\ \begin{bmatrix} 20 & -9 & 6 \\ 6 & 12 & -15 \\ -10 & -6 & 9 \\ 8 & -12 & 12 \end{bmatrix} \end{array}$$

Inner product property: $\mathbf{x}^{\mathrm{T}}\mathbf{y} = \|\mathbf{x}\| \cdot \|\mathbf{y}\| \cdot \cos(\theta)$

- $P_{ij} = OA_i \times OB_j \times cos\alpha_{ij}$
- Implies the product matrix

(Source) Modified from: Biplot Analysis of Multi-Environment Trial Data, Weikai Yan, May 2006

$P_{11} = 5 \times 4.472 \times 0.8944 = 20$



- The *biplot points* can be projected onto the *biplot axes*, and their projections, multiplied by the length of the corresponding biplot vectors, give the scalar products which are equal to the elements of the target matrix.

- The cosines of the angles between the variables approximate the pairwise correlation coefficients.

Source: Biplots in Practice, Michael Greenacre.

Singular Value Decomposition (SVD) & Singular Value Partitioning (SVP)

The 'rank' of Y, i.e., the minimum number of PC required to fully represent Y

Matrix characterising the rows

"Singular values"

Matrix characterising the columns

SVD:

$$P_{ij} \xrightarrow{SVD} \sum_{k=1}^{r} a_{ik} \lambda_k b_{kj}$$

SVP:

$$\xrightarrow{SVP} \sum_{k=1}^{r} (a_{ik} \lambda_k^{f})(\lambda_k^{1-f} b_{kj}) \qquad (0 \le f \le 1)$$

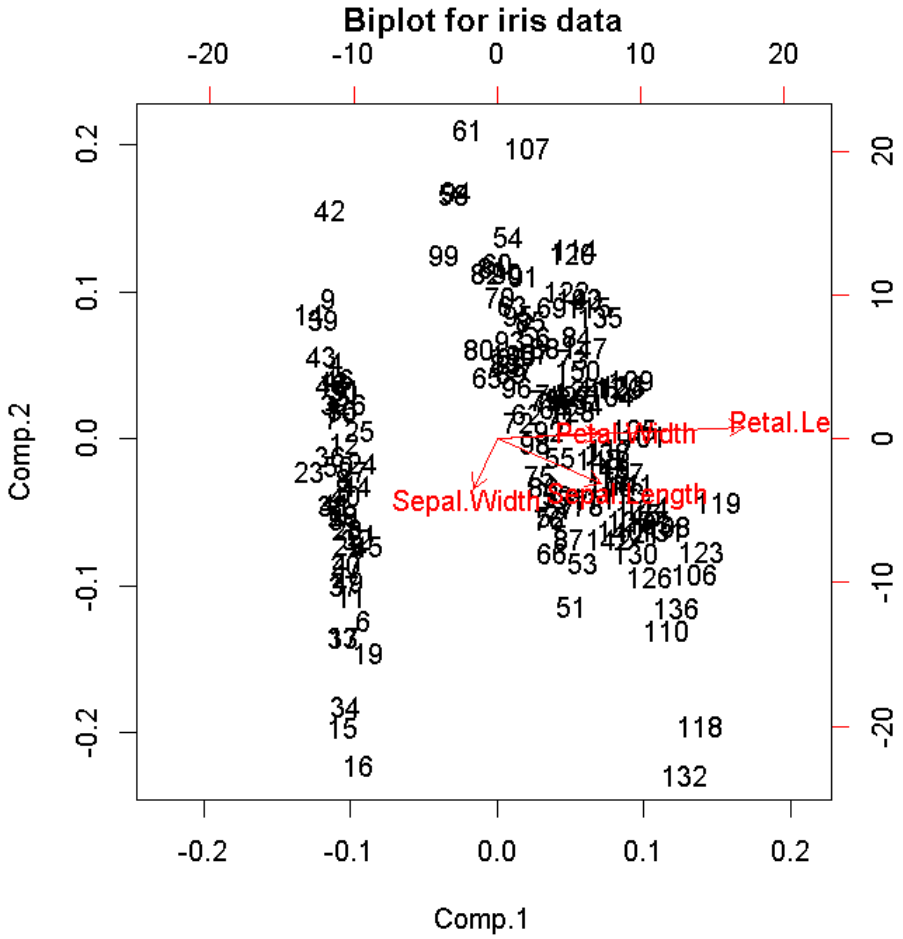
Rows scores — Column scores

Plot — Biplot — Plot

(Source) from: Biplot Analysis of Multi-Environment Trial Data, Weikai Yan, May 2006

biplot {stats}:
Biplot of Multivariate Data

```
iris.pca <- princomp(iris[,1:4])
biplot(iris.pca, main="Biplot for iris data")
```



Interpretation of Biplot

- **Interpreting Points**: the relative location of the points can be interpreted.
  - Points that are close together correspond to observations that have similar scores on the components displayed in the plot.
  - To the extent that these components fit the data well, the points also correspond to observations that have similar values on the variables.
- **Interpreting Vectors**: both the direction and length of the vectors can be interpreted.
  - A vector points in the direction which is most like the variable represented by the vector. This is the direction which has the highest squared multiple correlation with the principal components.
  - The length of the vector is proportional to the squared multiple correlation between the fitted values for the variable and the variable itself.
  - *The fitted values for a variable are the result of projecting the points in the space orthogonally onto the variable's vector (to do this, you must imagine extending the vector in both directions).*
  - The observations whose points project furthest in the direction in which the vector points are the observations that have the most of whatever the variable measures. Those points that project at the other end have the least. Those projecting in the middle have an average amount.
  - Thus, vectors that point in the same direction correspond to variables that have similar response profiles, and can be interpreted as having similar meaning in the context set by the data.

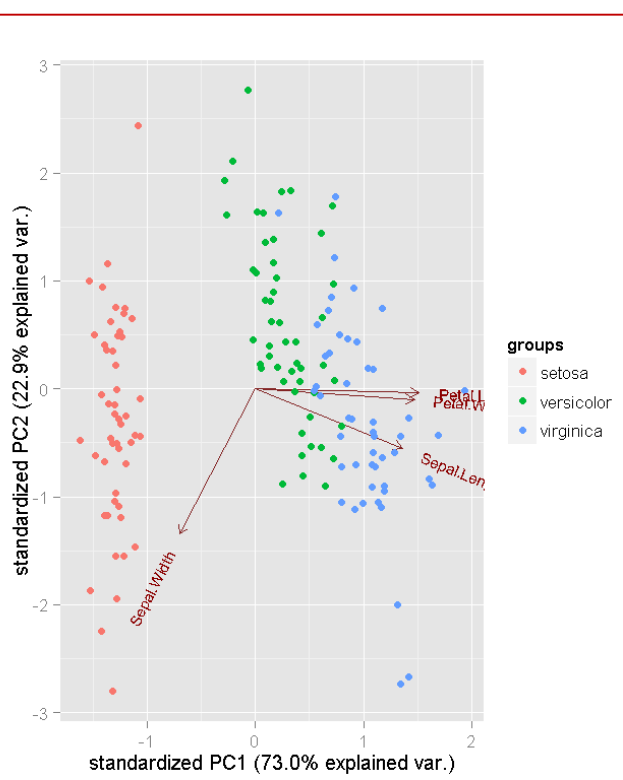
Source: Principal Components: BiPlots, Forrest Young's Notes
http://forrest.psych.unc.edu/research/vista-frames/help/lecturenotes/lecture13/biplot.html

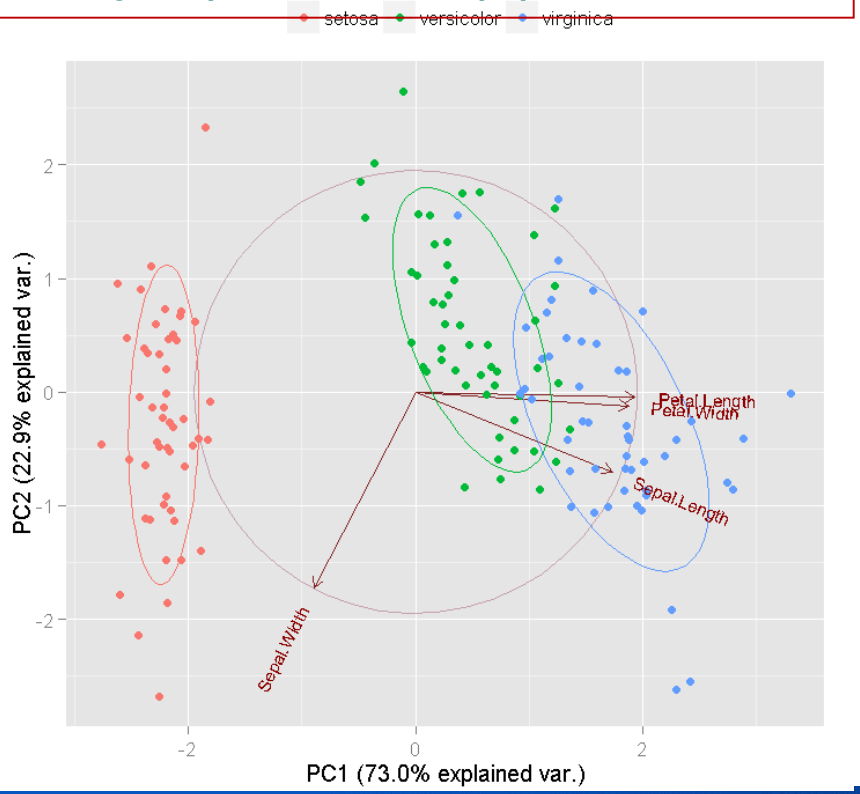
Biplot in R

- **biplot {stats}**: Biplot of Multivariate Data
  https://stat.ethz.ch/R-manual/R-devel/library/stats/html/biplot.html
- **biplot.princomp {stats}**: Biplot for Principal Components:
  https://stat.ethz.ch/R-manual/R-devel/library/stats/html/biplot.princomp.html
- ggbiplot: https://github.com/vqv/ggbiplot
- **biplot.rda {vegan}**: http://cc.oulu.fi/~jarioksa/softhelp/vegan/html/biplot.rda.html
- **biplot.psych {psych}**: http://www.personality-project.org/r/html/biplot.psych.html
  https://cran.r-project.org/web/packages/psych/
- **bpca**: Biplot of Multivariate Data Based on Principal Components Analysis
  https://cran.r-project.org/web/packages/bpca/index.html
- **dynBiplotGUI**: Full Interactive GUI for Dynamic Biplot in R
  https://cran.r-project.org/web/packages/dynBiplotGUI/index.html
- The BiplotGUI package homepage: http://biplotgui.r-forge.r-project.org/
- **BiplotGUI**: Interactive Biplots in R: https://cran.r-project.org/web/packages/BiplotGUI/index.html
- **biplotbootGUI**: Bootstrap on Classical Biplots and Clustering Disjoint Biplot:
  https://cran.r-project.org/web/packages/biplotbootGUI/index.html
- **GGEBiplotGUI**: GGEBiplotGUI: Interactive GGE Biplots in R:
  https://cran.r-project.org/web/packages/GGEBiplotGUI/index.html
- **multibiplotGUI**: Multibiplot Analysis in R:
  https://cran.r-project.org/web/packages/multibiplotGUI/index.html
- **MultBiplot** In R: http://biplot.dep.usal.es/classicalbiplot/multbiplot-in-r/
- **NominalLogisticBiplot**: Biplot representations of categorical data
  https://cran.r-project.org/web/packages/NominalLogisticBiplot/index.html
- **OrdinalLogisticBiplot**: Biplot representations of ordinal variables
  https://cran.r-project.org/web/packages/OrdinalLogisticBiplot/index.html
- **PLSbiplot1**: The Partial Least Squares (PLS) Biplot
  https://cran.r-project.org/web/packages/PLSbiplot1/index.html
- **PCABiplot**: Principal Components Analysis Biplots
  http://biplot.usal.es/ClassicalBiplot/multbiplot-in-r/pcabiplot-manual.pdf

ggbiplot for Iris Data

```
> library(devtools)
> install_github("vqv/ggbiplot")
>
> library(ggbiplot)
> iris.prcomp <- prcomp(iris[,1:4], scale. = TRUE)
> ggbiplot(iris.prcomp, groups = iris[,5])
> ggbiplot(iris.prcomp, obs.scale = 1, var.scale = 1,
+   groups = iris[,5], ellipse = TRUE, circle = TRUE) +
+   scale_color_discrete(name = '') +
+   theme(legend.direction = 'horizontal', legend.position = 'top')
```





Creating A Biplot Using SVD (1/3)

```
> library(lattice)
> state.spending <- read.table("StatePolicySpending.txt", header = T, row.names=1)
> head(state.spending)
   Education Welfare Highways HealthCare Corrections LawEnforcement
AL     0.863   0.448    0.168      0.284       0.044          0.183
AR     0.887   0.492    0.241      0.150       0.044          0.141
AZ     0.765   0.473    0.249      0.112       0.090          0.364
CA     0.916   0.817    0.142      0.170       0.104          0.425
CO     0.782   0.415    0.188      0.108       0.076          0.282
CT     0.764   0.742    0.251      0.323       0.128          0.347
> spend <- scale(state.spending)
> spend.svd <- svd(spend, nu=2, nv=2)
>
> D <- spend.svd$d[1:2]
> V <- spend.svd$v[,1:2]
> U <- spend.svd$u[,1:2]
>
> # Create matrices for variables and observations by weighting singular vectors with
> # the square roots of the first two singular values. These will be used to construct
> # a symmetric biplot.
>
> spend.var <- V * (rep(1, length(V[,1])) %*% t(D^.5))
> spend.obs <- U * (rep(1, length(U[,1])) %*% t(D^.5))
> row.names(spend.var) <- colnames(spend)
> row.names(spend.obs) <- row.names(spend)
```

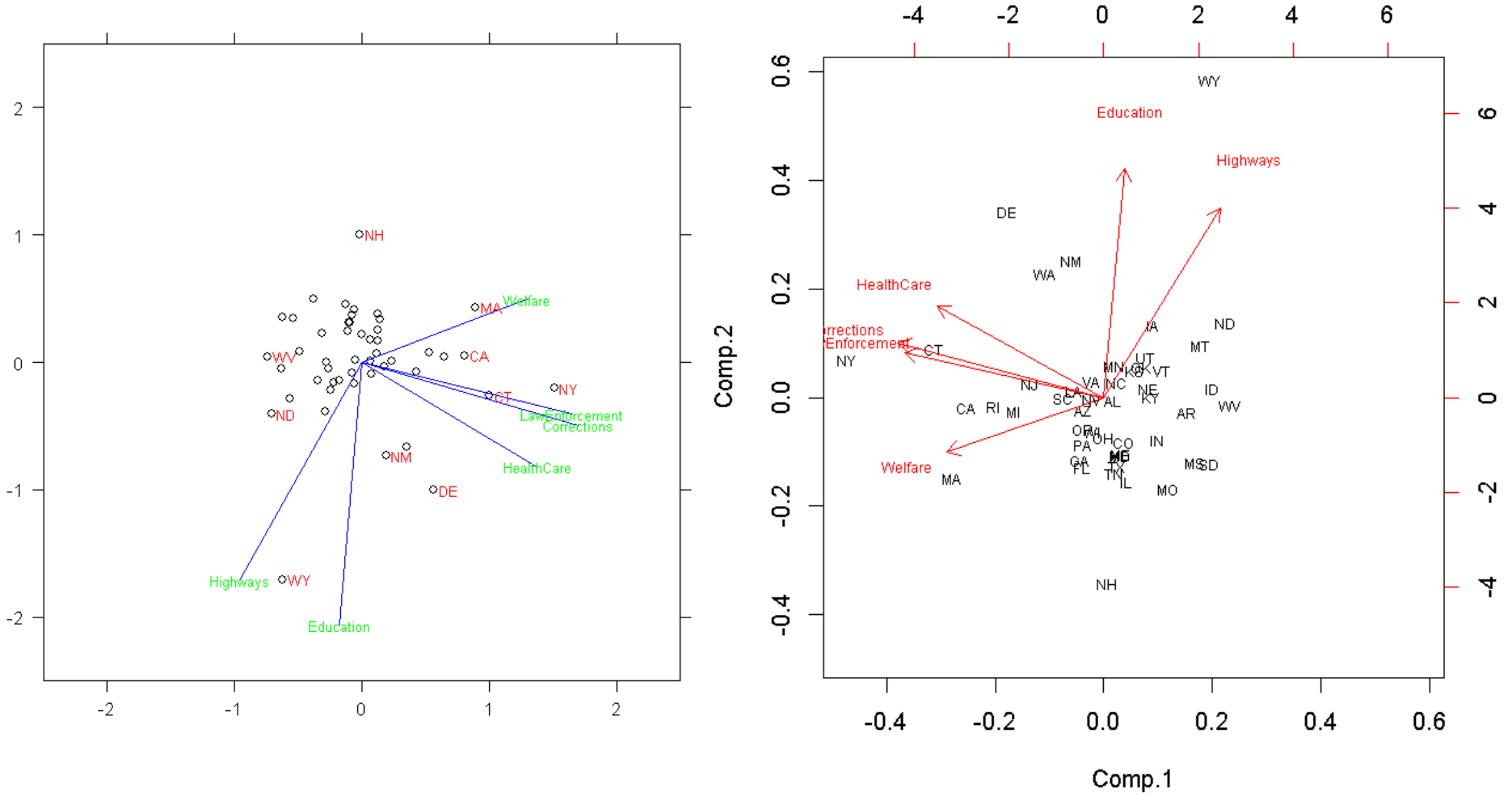
Source: Measurement, Scaling, and Dimensional Analysis, Bill Jacoby Summer 2015

Creating A Biplot Using SVD (2/3)

```
> # Within the panel function, "panel.xyplot" draws the observation points and
> # "panel.segments" draws the variable vectors. The first "panel.text" labels the vectors,
> # and the second "panel.text" provides labels for relatively extreme observation points.
> xyplot(spend.obs[,2] ~ spend.obs[,1],
+        aspect = 1,
+        panel = function(x, y) {
+                    panel.xyplot(x, y, col = "black")
+                    panel.segments(rep(0, length(spend.var[,1])),
+                                   rep(0, length(spend.var[,1])),
+                                   spend.var[,1], spend.var[,2], lty = 1, col = "blue")
+                    panel.text(spend.var[,1], spend.var[,2],
+                               row.names(spend.var), cex = .7, col = "green")
+                    panel.text(x[abs(x)>.7 | abs(y)>.7]+.04, y[abs(x)>.7 | abs(y)>.7],
+                               row.names(spend.obs)[abs(x)>.7 | abs(y)>.7], cex = .7,
+                               adj = 0, col= "red")
+                },
+       xlim = c(-2.5, 2.5), ylim = c(-2.5, 2.5),
+       xlab = " ", ylab = " ")
>
> # Calculate proportion of variance explained by
> # first two pairs of singular vectors
> var.explained <- sum(D^2)/sum(spend.svd$d^2)
> var.explained
[1] 0.6233372
```

Creating A Biplot Using SVD (3/3)

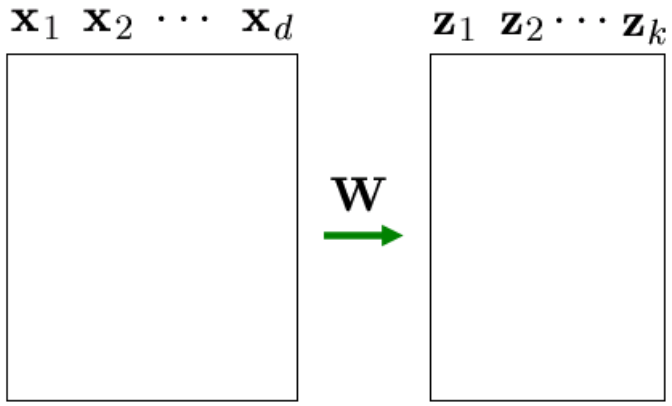
```
biplot(princomp(scale(state.spending)), cex=0.6)
```



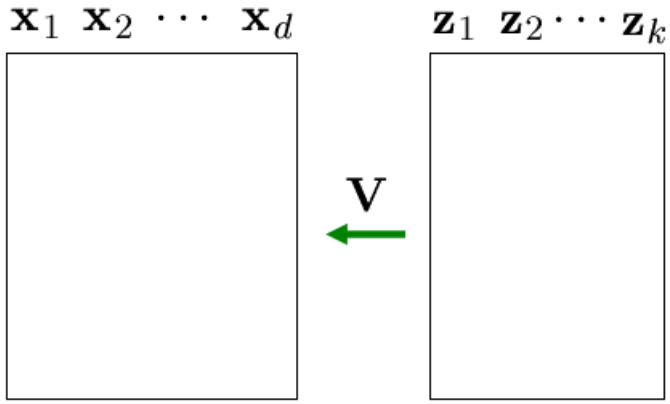
(5) Factor Analysis (1/4)

- There is a set of unobservable, latent factors z_j, $j=1,\ldots,k$, which when acting in combination generate $\boldsymbol{x}$.
- **Goal:** to characterize the dependency among the observed variables by means of a smaller number of factors (groupings).
- A few factors can represent the groups of variables.
- FA always partitions the variables into factor clusters.

PCA $\mathbf{z} = \mathbf{W}^T(\mathbf{x} - \mu)$



FA $\mathbf{x} - \mu = \mathbf{V}\mathbf{z} + \mathbf{e}$



Factor Analysis (2/4)

- FA assumes that each input dimension can be written as a weighted sum of the ***k*** factors, plus the residual term.

$$x_i - \mu_i = \sum_{j=1}^{k} v_{ij} z_j + \epsilon_i, \quad i = 1, \cdots, d$$

$$\text{Var}(x_i) = \sum_{j=1}^{k} v_{ij}^2 + \psi_i$$

Factor loadings

Model: $\mathbf{x} - \mu = \mathbf{V}\mathbf{z} + \mathbf{E}$

$[d \times 1] \quad [d \times k]\,[k \times 1]\,[d \times 1]$

The variance explained by the common factor and unique factor

Sample

$$\mathbf{X} = \{\mathbf{x}^t\}_{t=1}^{N}$$

$$E[\mathbf{x}^t] = \mu$$

$$\text{Cov}[\mathbf{x}^t] = \Sigma$$

Common Factors

$$E[z_i] = 0, \quad i = 1, \cdots, k$$

$$\text{Var}(z_i) = 1$$

$$\text{Cov}(z_i, z_j) = 0, i \neq j$$

Unique Factors

$$E[\epsilon_i] = 0, \quad i = 1, \cdots, k$$

$$\text{Var}(\epsilon_i) = \psi_i$$

$$\text{Cov}(\epsilon_i, \epsilon_j) = 0, i \neq j$$

$$\text{Cov}(\epsilon_i, z_j) = 0, \forall i, j$$

Factor Analysis (3/4)

$$\mathbf{x} - \mu = \mathbf{V}\mathbf{z} + \mathbf{E}$$

$$\begin{aligned}\Sigma &= \mathrm{Cov}(\mathbf{x}) \\ &= \mathrm{Cov}(\mathbf{V}\mathbf{z} + \mathbf{E}) \\ &= \mathrm{Cov}(\mathbf{V}\mathbf{z}) + \mathrm{Cov}(\mathbf{E}) \\ &= \mathbf{V}\mathrm{Cov}(\mathbf{z})\mathbf{V}^T + \Psi \\ &= \mathbf{V}\mathbf{V}^T + \Psi\end{aligned}$$

$$\Psi = \mathrm{diag}[\psi_i]_{i=1}^{d}$$

Example: two factors

$$\mathrm{Cov}(x_1, x_2) = v_{11}v_{21} + v_{12}v_{22}$$

- If x_1 and x_2 have high covariance, then they are related through a factor.
- 1st factor => v_{11}, v_{21} high
- 2nd factor => v_{12}, v_{22} high
- In either case, the sum will be high.
- If x_1 and x_2 have low covariance, then they depend on different factors and in the products in the sum.
- One term will be high, the other will be low, the sum will be low.

Variance Component:

$$x_1 = v_{11}\, z_1 + v_{12}\, z_2 + \epsilon_1$$

$$\mathrm{Cov}(x_1, z_2) = \mathrm{Cov}(v_{12}z_2, z_2) = v_{12}\mathrm{Var}(z_2) = v_{12} \quad \rightarrow \quad \mathrm{Cov}(\mathbf{x}, \mathbf{z}) = \mathbf{V}$$

The loadings represent the correlations of variables with the factors.

Factor Analysis (4/4)

Model: $\mathbf{x} - \mu = \mathbf{V}\mathbf{z} + \mathbf{E}$

Variance Component: $\Sigma = \mathbf{V}\mathbf{V}^T + \Psi$ → $\Psi = \text{diag}[\psi_i]_{i=1}^d$

$\mathbf{S} = \mathbf{V}\mathbf{V}^T + \Psi$

$\Psi = \psi\mathbf{I}$ Probabilistic PCA

$\Psi = 0\mathbf{I}$ Conventional PCA

To find $\mathbf{V} = [d \times k]$

- If there are only a few factors (***V*** has few columns), then we have a simplified structure for ***S***.
- Finding factor loadings and the specific variances.

$$\mathbf{S} = \mathbf{C}\mathbf{D}\mathbf{C}^T = \mathbf{C}\mathbf{D}^{1/2}\mathbf{D}^{1/2}\mathbf{C}^T = (\mathbf{C}\mathbf{D}^{1/2})(\mathbf{C}\mathbf{D}^{1/2})^T$$

$$\text{Var}(x_i) = \sum_{j=1}^{k} v_{ij}^2 + \psi_i \quad \rightarrow \quad \psi_i = s_i^2 - \sum_{j=1}^{k} v_{ij}^2$$

$\mathbf{C} = [d \times k]$

$\mathbf{D} = [k \times k]$

$\mathbf{V} = \mathbf{C}\mathbf{D}^{1/2}$

Two Uses of Factor Analysis

- It can be used for knowledge extraction when we find the loadings and try to express the variables using fewer factors.
- It can also be used for dimension reduction when $k < d$.

- Find the factor scores z_j from x_i.
- Find the loadings w_{ji} such that

$$x_i - \mu_i = \sum_{j=1}^{k} v_{ij} z_j + \epsilon_i, \quad i = 1, \cdots, d$$

$$z_j = \sum_{j=1}^{d} w_{ji} x_i + \epsilon_i, \quad j = 1, \cdots, k$$

$$\mathbf{z}^t = \mathbf{W}^T \mathbf{x}^t + \mathbf{e}, \quad \forall t = 1, \cdots, N$$

NOTE: For dimension reduction, FA offers no advantage over PCA except the interpretability of factors allowing the identification of common causes, a simple explanation, and knowledge extraction.

$$\mathbf{Z} = \mathbf{XW} + \mathbf{E} \rightarrow \mathbf{W} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T Z$$

$$\mathbf{Z} = [N \times k]$$

$$\mathbf{W} = (N-1)(\mathbf{X}^T\mathbf{X})^{-1}\frac{\mathbf{X}^T Z}{N-1}$$

$$\mathbf{X} = [N \times d]$$

$$\mathbf{E} = [N \times k]$$

$$\mathbf{W} = (\frac{\mathbf{X}^T\mathbf{X}}{N-1})^{-1}\frac{\mathbf{X}^T Z}{N-1} \qquad \mathrm{Cov}(\mathbf{x}, \mathbf{z}) = \mathbf{V}$$

$$\mathbf{W} = \mathbf{S}^{-1}\mathbf{V} \rightarrow \hat{\mathbf{Z}} = \mathbf{XW} = \mathbf{XS}^{-1}\mathbf{V}$$

FA: Rotation

- When V is multiplied with any orthogonal matrix ($TT^T = I$), the solution is not unique.

$$\mathbf{S} = \mathbf{V}\mathbf{V}^T + \Psi \longrightarrow \mathbf{S} = (\mathbf{V}\mathbf{T})(\mathbf{V}\mathbf{T})^T = \mathbf{V}\mathbf{T}\mathbf{T}^T\mathbf{V}^T = \mathbf{V}\mathbf{I}\mathbf{V}^T = \mathbf{V}\mathbf{V}^T$$

- If T is an orthogonal matrix, the distance to the origin does not change.

$$\mathbf{z}^T\mathbf{z} = (\mathbf{T}\mathbf{x})^T(\mathbf{T}\mathbf{x}) = \mathbf{x}^T\mathbf{x}$$

- Multiplying with an orthogonal matrix has the effect of rotating the axes which allows us to choose the set of axes most interpretable.

$$\mathbf{T} = \begin{bmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{bmatrix}$$

Rotates the axes by phi

- **Orthogonal rotation**: the factor are still orthogonal after the rotation.
  - **Varimax**: tries to maximize variance of squared loadings for each factor (orthogonal):
    - lines up factors with original variables.
    - improves interpretability of factors.
  - **Quartimax**: maximizes the variance of the squared loadings within the variables.
- **Oblique rotation**: the factors are allowed to become correlated.

R: factanal

```
data(iris3)
Iris <- data.frame(rbind(iris3[,,1], iris3[,,2], iris3[,,3]),
Species = rep(c("setosa","versicolor","virginica"), rep(50,3)))

## FA
data <- Iris[,1:4]
class <- Iris[,5]
iris.fa <-  factanal(data, factors=1)
fa.dim1 <- as.matrix(data)%*%iris.fa$loadings[,1]
```

```
> library(stats)

> help(factanal)
```

```
Call:
factanal(x = data, factors = 1)

Uniquenesses:
Sepal.L. Sepal.W. Petal.L. Petal.W.
   0.240    0.822    0.005    0.069

Loadings:
         Factor1
Sepal.L.  0.872
Sepal.W. -0.422
Petal.L.  0.998
Petal.W.  0.965

               Factor1
SS loadings      2.864
Proportion Var   0.716

Test of the hypothesis that 1 factor is sufficient.
The chi square statistic is 85.51 on 2 degrees of freedom.
The p-value is 2.7e-19
```

```
> factanal(data, factors=2)
Error in factanal(data, factors = 2) : 2 factors is too many for 4 variables
```

(6) Multidimensional Scaling (MDS)

(Torgerson 1952; Cox and Cox 2001)

http://www.lib.utexas.edu/maps/united_states.html

■ Classical MDS takes a set of dissimilarities and returns a set of points such that the distances between the points are approximately equal to the dissimilarities.

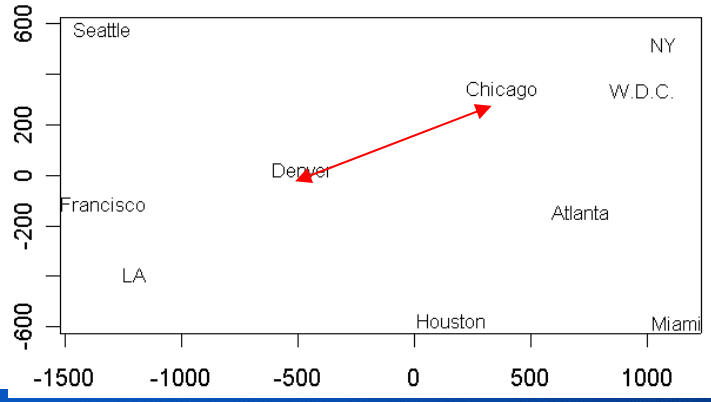
■ projection from some unknown dimensional space to 2-d dimension.

Flying Mileages Between Ten U.S. Cities

0										Atlanta
587	0									Chicago
1212	920	0								Denver
701	940	879	0							Houston
1936	1745	831	1374	0						Los Angeles
604	1188	1726	968	2339	0					Miami
748	713	1631	1420	2451	1092	0				New York
2139	1858	949	1645	347	2594	2571	0			San Francisco
2182	1737	1021	1891	959	2734	2408	678	0		Seattle
543	597	1494	1220	2300	923	205	2442	2329	0	Washington D.C.

?

MDS



MDS: Metric and Non-Metric Scaling

- Given the distance between pairs of points, we don't know the exact coordinates of the points, or their dimensionality, or how the distances are calculated.
- MDS is the method for placing these points in a low space such that the Euclidean distance between them in the two-dimensional space is as close as possible to the given distances in the original space.

Question: Given a *dissimilarity matrix* D of certain objects, can we construct points in k-dimensional (often 2-dimensional) space such that

Goal of metric scaling
the Euclidean distances between these points approximate the entries in the dissimilarity matrix?

$$S = \sum_{i,j} (\hat{d}_{ij} - d_{ij})^2$$

Goal of non-metric scaling
the order in distances coincides with the order in the entries of the dissimilarity matrix approximately?

$$Stress = \sqrt{\frac{\sum_{i,j} (\hat{d}_{ij} - d_{ij})^2}{\sum_{i,j} d_{ij}^2}}$$

Mathematically: for given k, compute points $x_1,\ldots,x_n$ in k-dimensional space such that the object function is minimized.

MDS: General Methodology (1/3)

Constraint: center the data at the origin and assume

$$\mathbf{X} = \{\mathbf{x}_t\}_{t=1}^{N} \quad \mathbf{x} \in \mathcal{R}^d$$

$$\sum_{i=1}^{N} x_{ij} = 0, \ \forall j = 1, \cdots, d$$

$$\begin{aligned} d_{rs}^2 &= \| \mathbf{x}_r - \mathbf{x}_s \|^2 \\ &= \sum_{j=1}^{d} (x_{rj} - x_{sj})^2 \\ &= \sum_{j=1}^{d} x_{rj}^2 + 2\sum_{j=1}^{d} x_{rj}x_{sj} + \sum_{j=1}^{d} x_{sj}^2 \\ &= b_{rr} + b_{ss} - 2b_{rs} \end{aligned}$$

$$\sum_{r=1}^{N} d_{rs}^2 = T + Nb_{ss}$$

$$\sum_{s=1}^{N} d_{rs}^2 = T + Nb_{rr}$$

$$\sum_{r=1}^{N}\sum_{s=1}^{N} d_{rs}^2 = 2NT$$

$$T \equiv \sum_{i=1}^{N} b_{ii} = \sum_{i=1}^{N}\sum_{j=1}^{d} x_{ij}^2$$

$$d_{.s}^2 \equiv \frac{1}{N}\sum_{r=1}^{N} d_{rs}^2$$

$$d_{r.}^2 \equiv \frac{1}{N}\sum_{s=1}^{N} d_{rs}^2$$

$$d_{..}^2 \equiv \frac{1}{N^2}\sum_{r=1}^{N}\sum_{s=1}^{N} d_{rs}^2$$

$$b_{rs} \equiv \sum_{j=1}^{d} x_{rj}x_{sj}$$

$$b_{rs} = \frac{1}{2}(d_{r.}^2 + d_{.s}^2 - d_{..}^2 - d_{rs}^2)$$

MDS: General Methodology (2/3)

- The new coordinates of instance *t* are given by the *t*-th elements of the eigenvectors, c_j, j=1,…,k, after normalization.

Only Distance Matrix is Needed

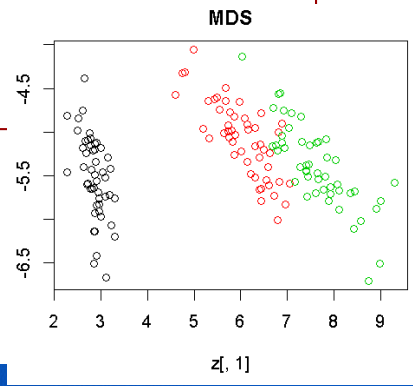
$$d_{rs}^2 = b_{rr} + b_{ss} - 2b_{rs}$$

$$b_{rs} \equiv \sum_{j=1}^{d} x_{rj} x_{sj} \quad \rightarrow \quad b_{rs} = \frac{1}{2}(d_{r.}^2 + d_{.s}^2 - d_{..}^2 - d_{rs}^2)$$

$$\mathbf{B} = \mathbf{X}\mathbf{X}^T \quad [N \times N] \qquad \text{Spectral Decomposition} \qquad \mathbf{X} = \mathbf{C}\mathbf{D}^{1/2}$$

C: columns are the eigenvectors of **B**.
D: diagonals are the eigenvalues of **B**.

```
> x <- as.matrix(iris[, 1:4])
> B <- x %*% t(x)
> d <- 2
> eB <- eigen(B)
> C <- eB$vectors
> D <- eB$values
> Z <- C[, 1:d] %*% diag(D[1:d])
> plot(z[,1], z[,2],
+  col=iris[,5], main="MDS")
```



$$\mathbf{Z} \equiv \hat{\mathbf{X}} = \underset{[N \times k]}{\hat{\mathbf{X}}} = \begin{matrix} c_1 \cdots c_k \cdots c_N \\ \mathbf{C} \end{matrix} \quad \begin{matrix} \sqrt{\lambda_1} & & \\ & \ddots & \\ & & \sqrt{\lambda_k} \end{matrix} \mathbf{D} \quad \begin{matrix} & & \\ & \ddots & \\ & & \sqrt{\lambda_N} \end{matrix}$$

$$z_{tj} = \sqrt{\lambda_j} c_{tj} \qquad \begin{matrix} j = 1, \cdots, k \\ t = 1, \cdots, N \end{matrix}$$

MDS: General Methodology (3/3)

- The map is centered on the origin, we can get any rotated or mirror image version.
- MDS can be used for dimension reduction by calculating pairwise Euclidean distances in the d-dimensional x space and giving this as input to MDS, which then projects it to a lower-dimensional space so as to preserve these distance.

$$\mathbf{B} = \mathbf{X}\mathbf{X}^T \qquad [N \times N]$$

$$\mathbf{C} = \mathbf{X}^T\mathbf{X} \qquad [d \times d]$$

- Chatfield and Collins, 1980: Eigenvalues of (XX^T) are the same as those of (X^TX) and eigenvectors are related by a simple linear transformation.
- PCA does the same work with MDS.
- PCA done on the correlation matrix equals doing MDS with standardized Euclidean distance where each variable has unit variance.

General Case of MDS

- The linear mapping

$$\mathbf{z} = g(\mathbf{x}|\theta) \qquad \mathbf{z} \in \mathcal{R}^k \qquad \mathbf{x} \in \mathcal{R}^d$$

$g(\mathbf{x}|\theta)$: the mapping function from d to k dimensions

Classical MDS: $\mathbf{z} = g(\mathbf{x}|\theta) = \mathbf{W}^T\mathbf{x}$

- **The nonlinear mapping: Sammon mapping**
- Sammon stress: the normalized error in the mapping

$$E[\theta|\mathbf{X}] = \sum_{r,s}^{N} \frac{(\| \mathbf{z}_r - \mathbf{z}_s \| - \| \mathbf{x}_r - \mathbf{x}_s \|)^2}{\| \mathbf{x}_r - \mathbf{x}_s \|^2}$$

$$= \sum_{r,s}^{N} \frac{(\| g(\mathbf{x}_r|\theta) - g(\mathbf{x}_s|\theta) \| - \| \mathbf{x}_r - \mathbf{x}_s \|)^2}{\| \mathbf{x}_r - \mathbf{x}_s \|^2}$$

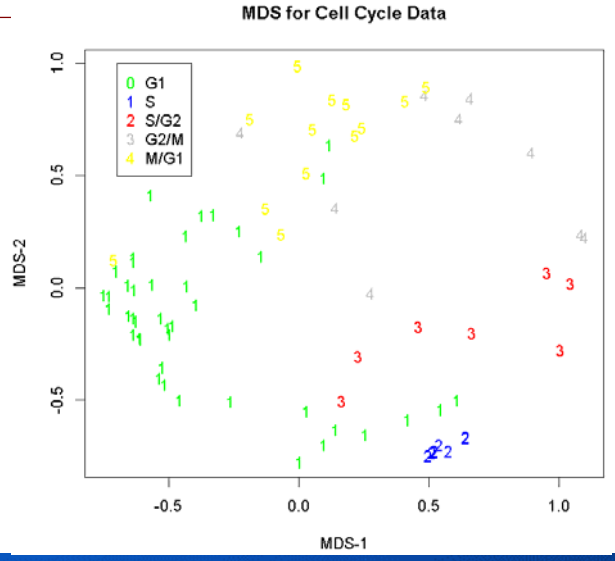
- Nonlinear dimensionality reduction
- Use regression method for g(.|theta)

- In the case of classification, one can include class information in the distance (Webb, 1999) as $d'_{rs} = (1-\alpha)d_{rs} + \alpha c_{rs}$

c_{rs}: the distance between the classes $\mathbf{x}_r$ and $\mathbf{x}_s$ belong to.

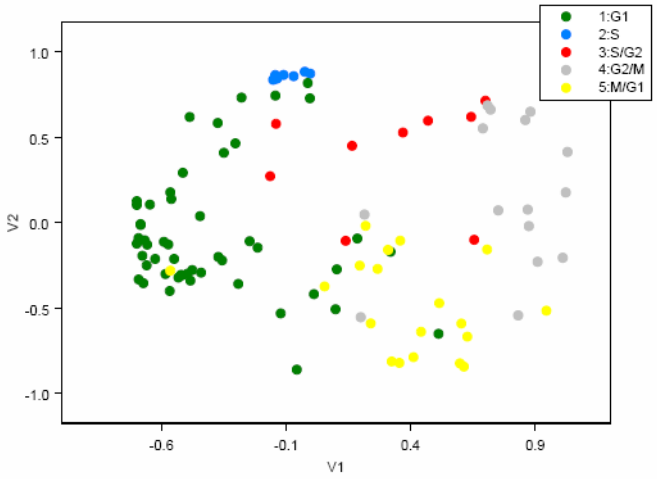
MDS to Microarray Data

```
cell.matrix  <- read.table("YeastCellCycle_alpha.txt", header=TRUE, row.names=1)
n <- dim(cell.matrix)[1]
p <- dim(cell.matrix)[2]-1
cell.data <- cell.matrix[,2:p+1]
gene.phase <- cell.matrix[,1]
phase.name <- c("G1", "S", "S/G2", "G2/M", "M/G1")
cell.sdata <- t(scale(t(cell.data)))
cell.cor <- cor(t(cell.sdata))
cell.dist <- sqrt(2*(1-cell.cor))
cell.mds <- cmdscale(cell.dist)
plot(cell.mds[,1], cell.mds[,2], type="n", xlab="MDS-1", ylab="MDS-2", main="MDS for
Cell Cycle Data")
number <- c(1, 4, 5, 2, 3)[as.integer(gene.phase)]
phase.color <- c("green", "blue", "red", "gray", "yellow")
text(cell.mds[,1], cell.mds[,2], number, col= phase.color[number])
legend(-0.7, 1.0, phase.name, pch="01234", col=phase.color)
```

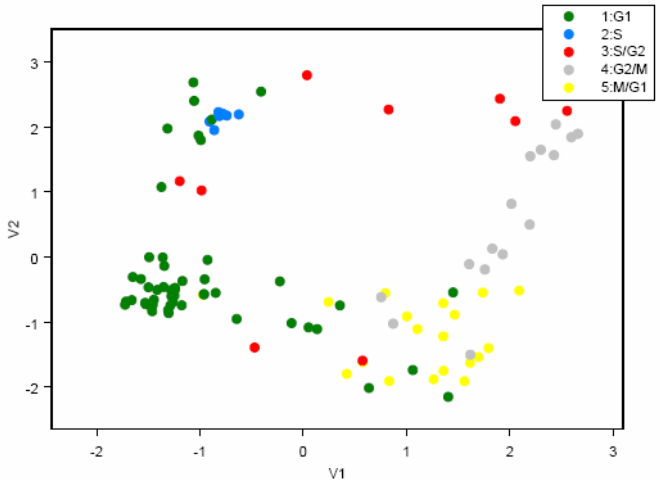


Using Different Features

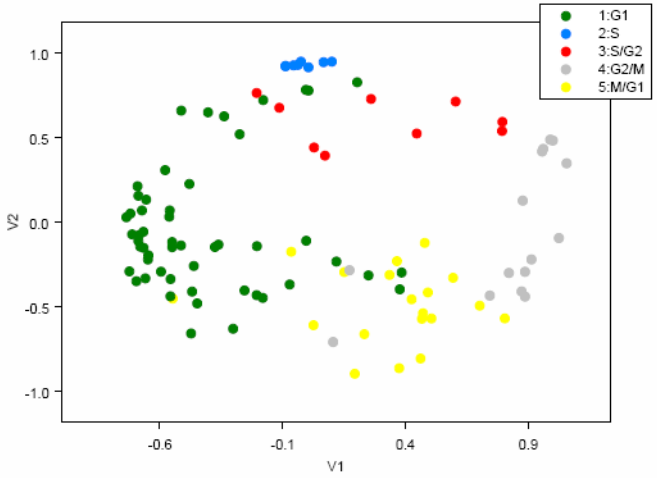
(a) MDS



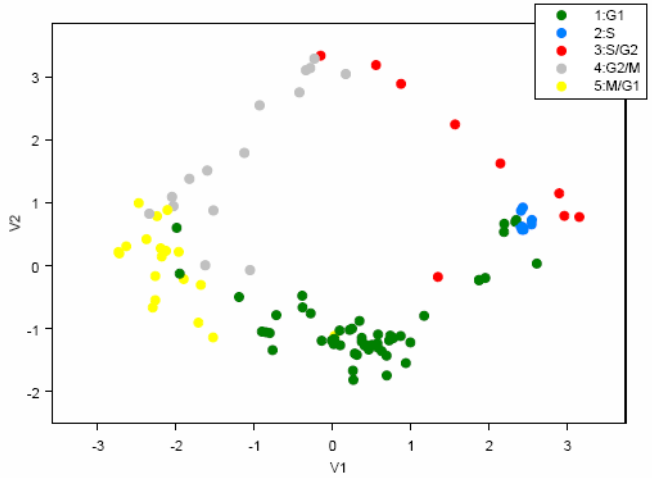
(c) Isomap



(b) MDS+DWT



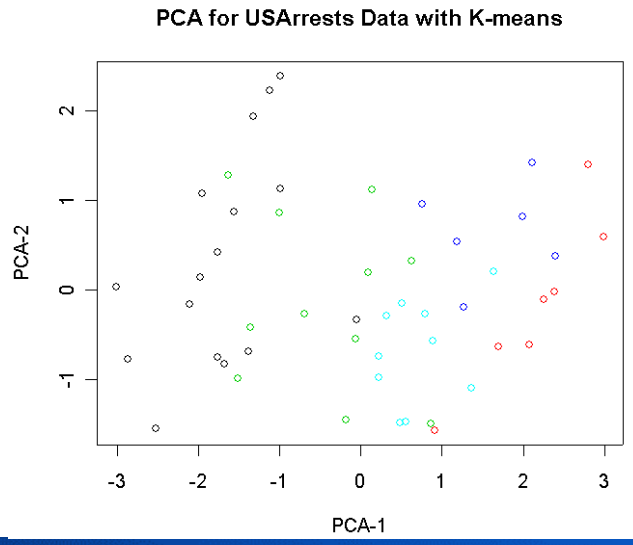
(d) Isomap+DWT

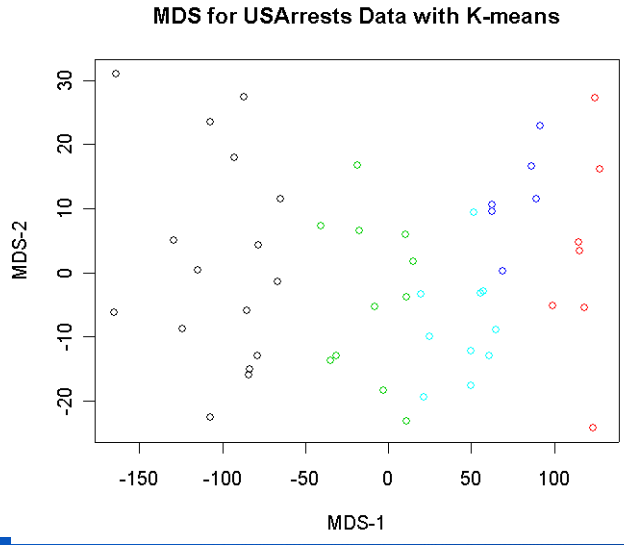


R: PCA, MDS with K-means

```
> library(stats)
```

```
no.group <- 5
no.iter <- 20
USArrests.kmeans <- kmeans(USArrests, no.group, no.iter)
plot(USArrests, col = USArrests.kmeans$cluster, main = "K-means: USArrests data")
# PCA
USArrests.pca <- princomp(USArrests, cor=TRUE, scores=TRUE)
pca.dim1 <- USArrests.pca$scores[,1]; pca.dim2 <- USArrests.pca$scores[,2]
plot(pca.dim1, pca.dim2,  main="PCA for USArrests Data with K-means", xlab="PCA-1",
ylab="PCA-2", col=USArrests.kmeans$cluster)
# MDS
USArrests.mds<- cmdscale(dist(USArrests))
mds.dim1 <- USArrests.mds[,1]; mds.dim2 <- USArrests.mds[,2]
plot(mds.dim1, mds.dim2, xlab="MDS-1", ylab="MDS-2", main="MDS for USArrests Data with K-
means", col = USArrests.kmeans$cluster)
```





(7) Isometric Mapping (Isomap)

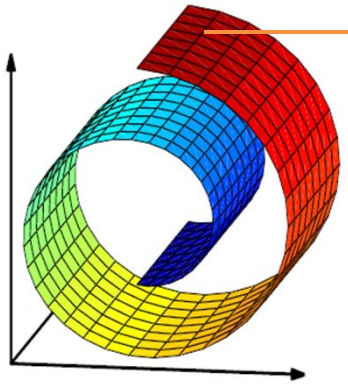
Manifolds (流形) and Nonlinearity:

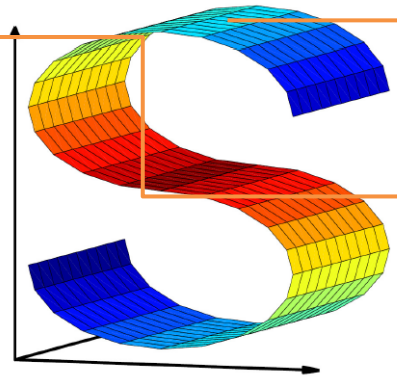
A manifold is a mathematical geometric space and in which the local space is Euclidean space.

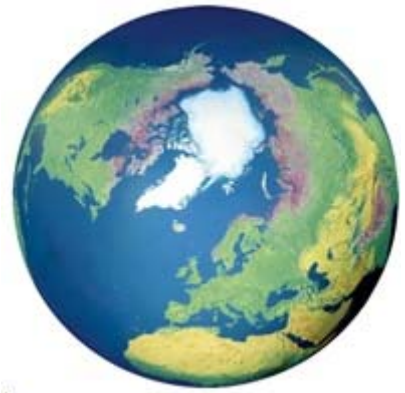
Swissroll

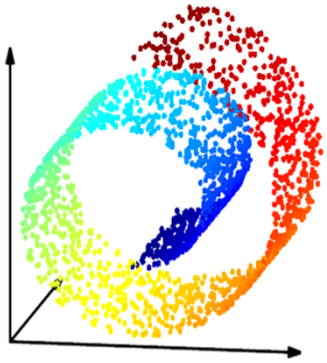
S-curve

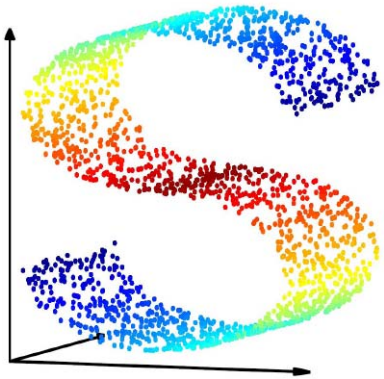
Locally Euclidean



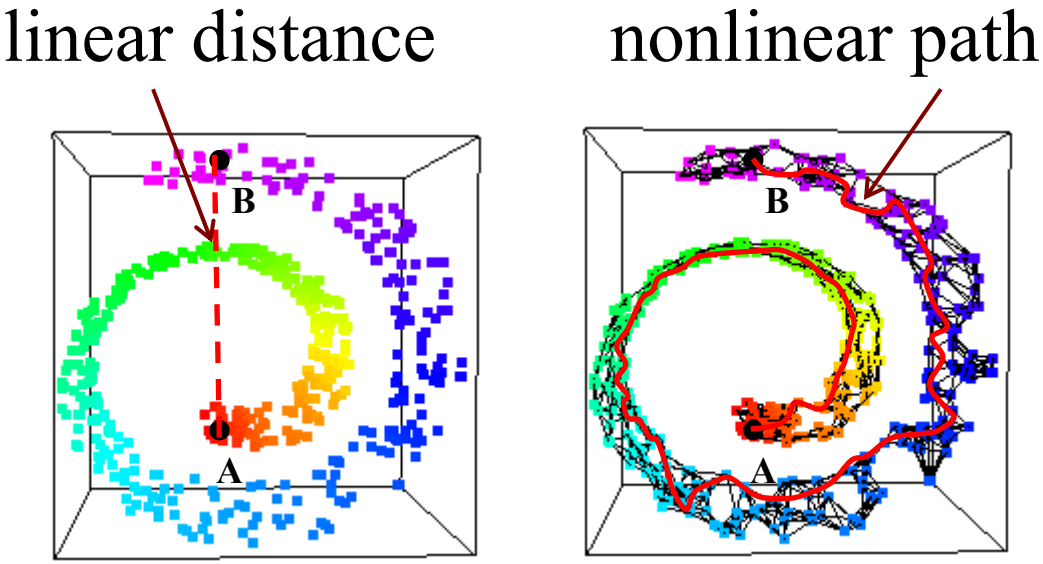








Nonlinear Structure



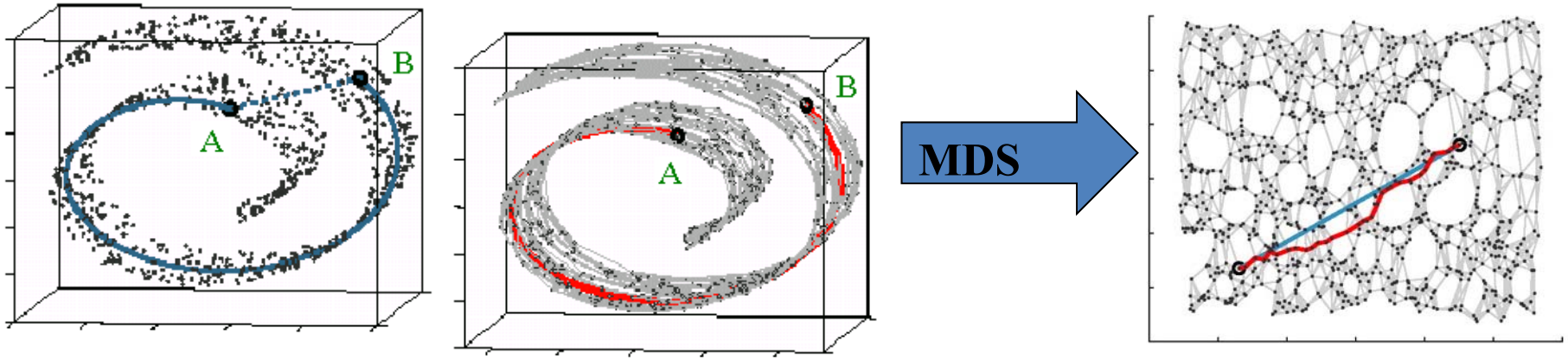
Machine learning for nonlinear dimension reduction (NLDR) and manifold learning

- **ISOMAP** (Tenenbaum, de Silva and Langford, 2000)
- Local linear embedding (**LLE**)(Roweis and Saul, 2000)
- **Hessian eigenmaps** (Donoho and Grimes, 2003)
- **Laplacian eigenmaps** (Belkin and Niyogi, 2003)
- **Diffusion maps** (Coifman et al., 2005) and their variants.

Isometric Mapping (Isomap)

Tenenbaum , J. B., Silva, V. de, and Langford, J. C. (2000). A Global Geometric Framework for Nonlinear Dimensionality Reduction, *Science* 290, 2319-2323.

Isomap finds the projection that preserves the global, nonlinear geometry of the data by preserving the geodesic manifold interpoint distances.

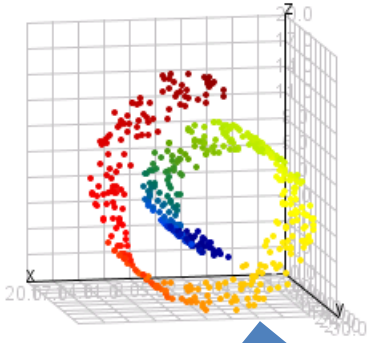


What is important is the geodesic distance!

Isometric Feature Mapping (ISOMAP)

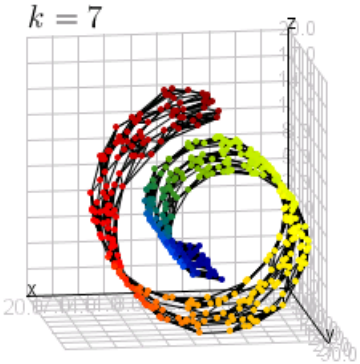
Tenenbaum, J.B., Silva, V.d., Langford, J.C.: A Global Geometric Framework for Nonlinear Dimensionality Reduction. Science **290** (2000) 2319–2323

Geodesic Distance Approximation

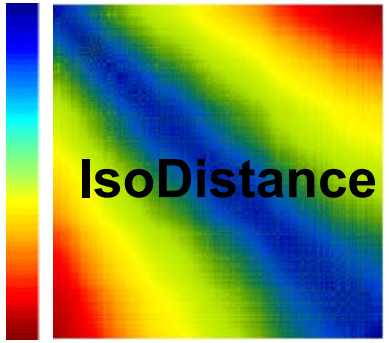


nx3

K-nearest neighbors (KNN)

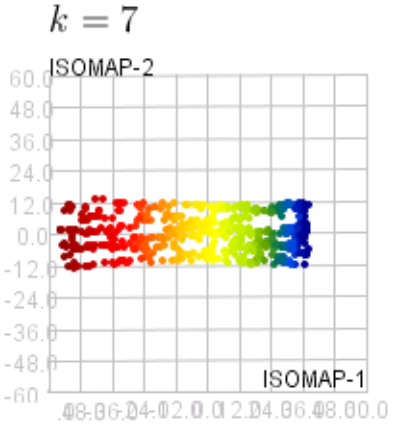


nx3



nxn

Nonlinear Dimension Reduction



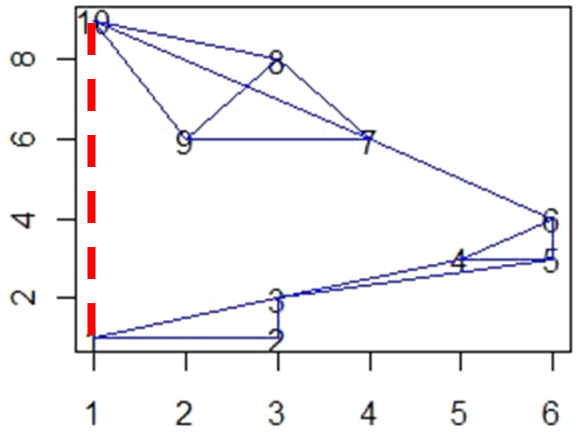
nx2

Multidimensional Scaling (MDS)

Geodesic Distance

Euclidean Distance

samples = 10, neighbors = 3



$$d_G(i,j) = \min\{\ d_G(i,j),\ d_G(i,l) + d_G(l,j)\ \}$$

IsoDistance

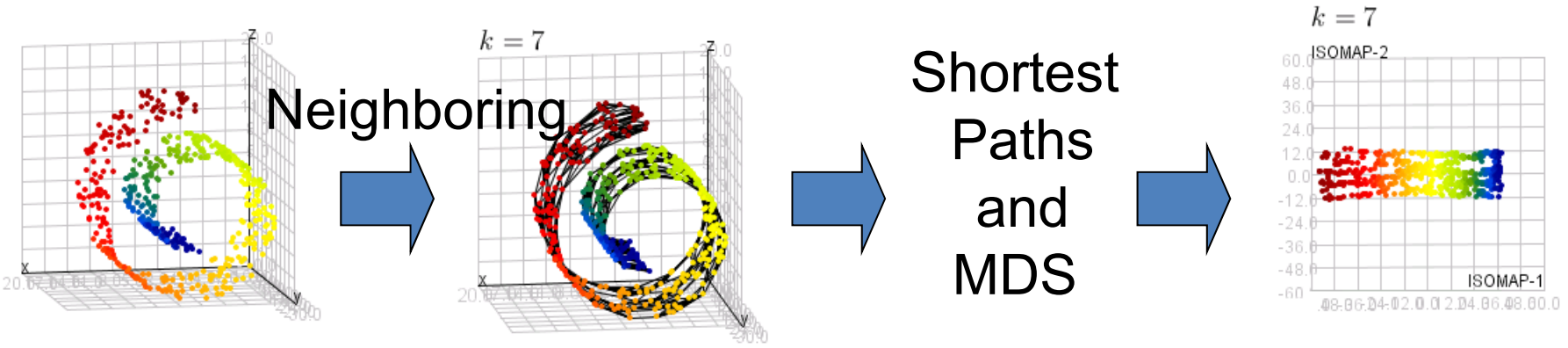
	1	2	3	4	5	6	7	8	9	10
1	0	2	2.236	4.472						?
2	2	0	1	2.828						
3	2.236	1	0	2.236						
4			2.236	0	1	1.414				
5			3.162	1	0	1				
6				1.414	1	0	2.828			
7						2.828	0	2.236	2	
8							2.236	0	2.236	2.236
9							2	2.236	0	3.162
10							4.243	2.236	3.162	0

12.957

The shortest path by point 1 to point 10: 1 →3 →4 →6 →7 →8 →10

	1	2	3	4	5	6	7	8	9	10
1	0	2	2.236	4.472	5.398	5.886	8.715	10.951	10.715	12.957
2	2	0	1	2.828	3.828	4.243	7.071	9.307	9.071	11.314
3	2.236	1	0	2.236	3.162	3.65	6.479	8.715	8.479	10.721
4	4.472	2.828	2.236	0	1	1.414	4.243	6.479	6.243	8.485
5	5.398	3.828	3.162	1	0	1	3.828	6.064	5.828	8.071
6	5.886	4.243	3.65	1.414	1	0	2.828	5.064	4.828	7.071
7	8.715	7.071	6.479	4.243	3.828	2.828	0	2.236	2	4.243
8	10.951	9.307	8.715	6.479	6.064	5.064	2.236	0	2.236	2.236
9	10.715	9.071	8.479	6.243	5.828	4.828	2	2.236	0	3.162
10	12.957	11.314	10.721	8.485	8.071	7.071	4.243	2.236	3.162	0

Algorithm of Isomap



Algorithm of Isomap (Tenenbaum *et al.*, 2000)

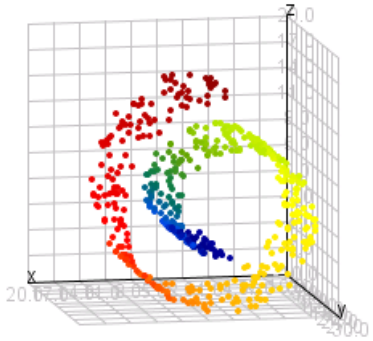
1. Calculate the distance $d_X(i,j)$ between all pairs i,j from n data points in the p-dimensional input space.
2. Construct the graph by determining the neighbors for each data point with ϵ-Isomap or k-Isomap.
3. Pursue the shortest paths in the graph G.
   Initialize $d_G(i,j) = d_X(i,j)$ if i,j are neighbors; otherwise, set $d_G(i,j) = \infty$. For each value of $l = 1, 2, \cdots, n$ and for all i,j, $d_G(i,j)$ are replaced by $\min\{d_G(i,j), d_G(i,l) + d_G(l,j)\}$.
4. Apply classical MDS to D_G.

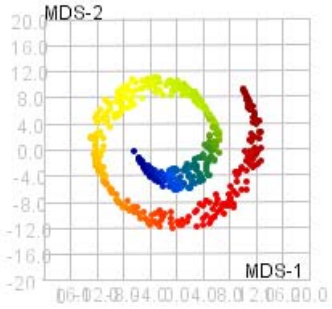
Notes

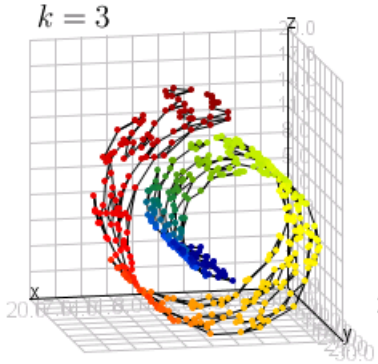
- For neighboring points Euclidean distance is a good approximation to the geodesic distance.
  - For faraway points estimate the distance by a series of short hops between neighboring points.
  - Find shortest paths in a graph with edges connecting neighboring data points.
  - Once we have all pairwise geodesic distances use classical metric MDS.

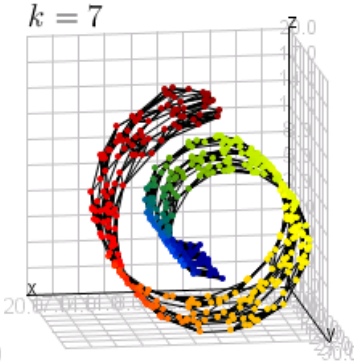
- Balasubramanian et al. (2002), *Science*:
  "What is new about the Isomap algorithm is how it defines the connectivity of each data point via its nearest Euclidean neighbors in the high-dimensional space."

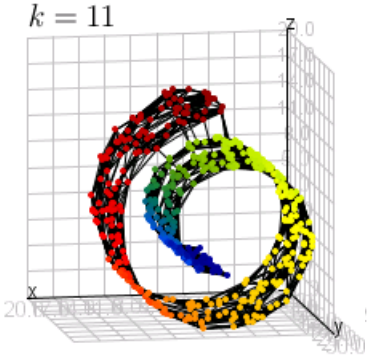
The Pinch and Short-Circuit Problem

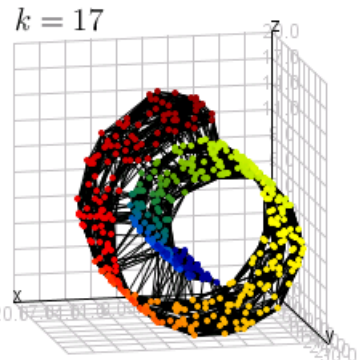


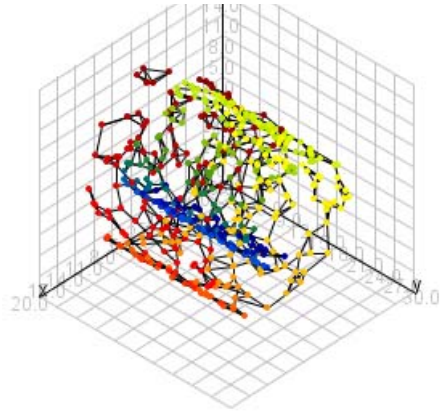


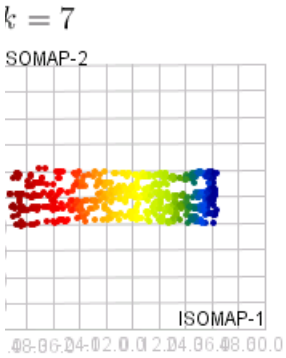


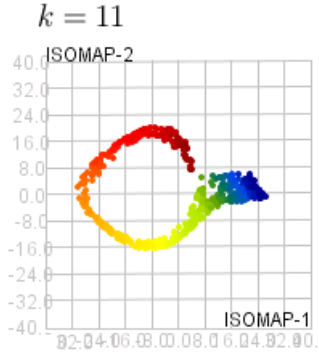


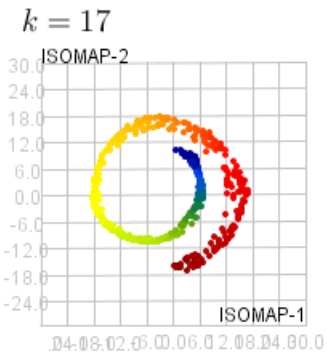


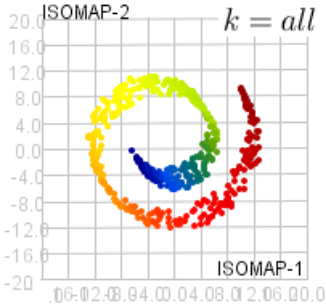




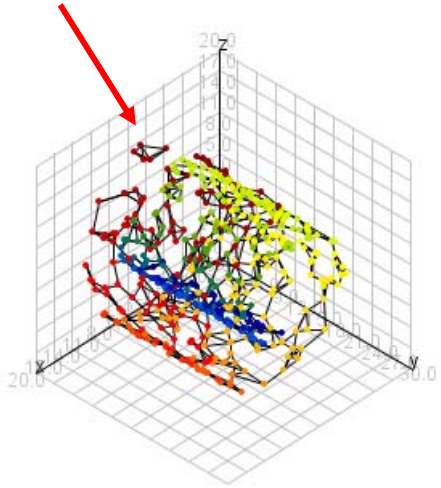


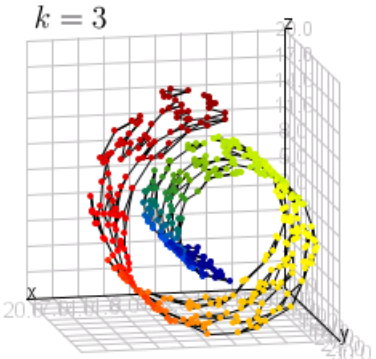




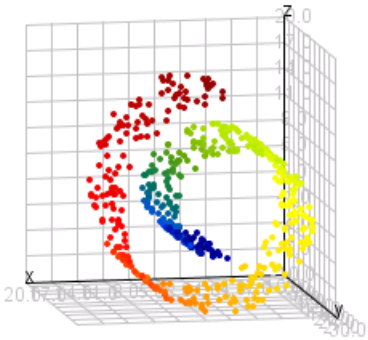


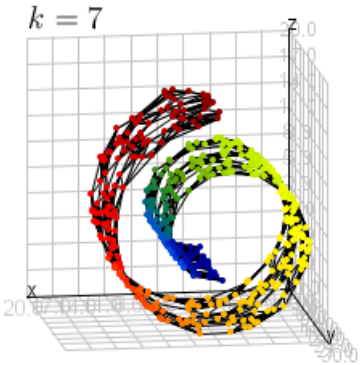
Short-Circuit Problem

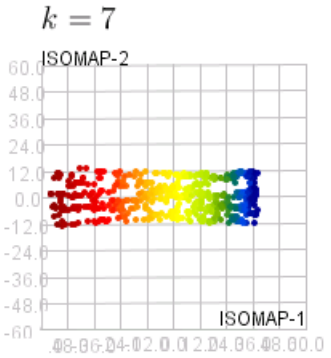




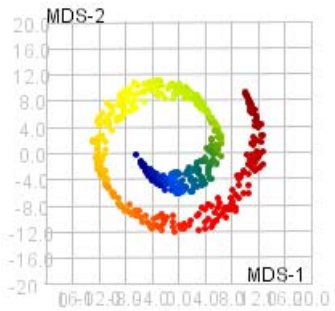
3D ScatterPlot

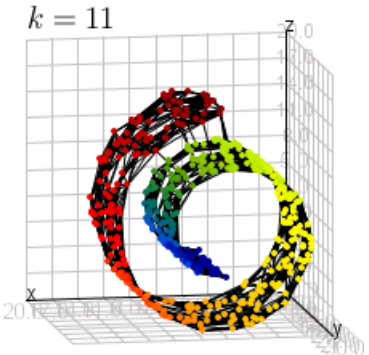


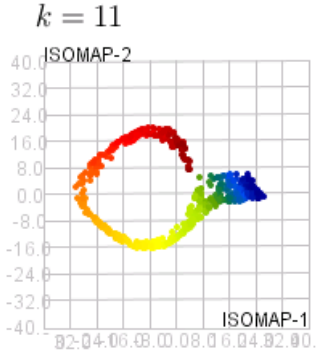




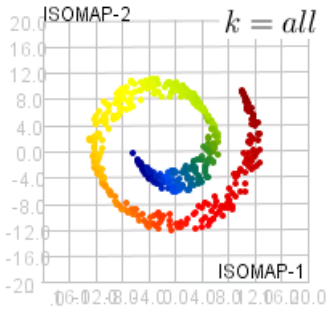
2D MDS

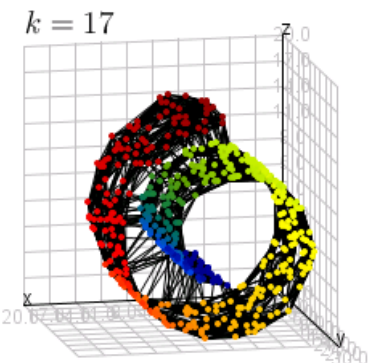


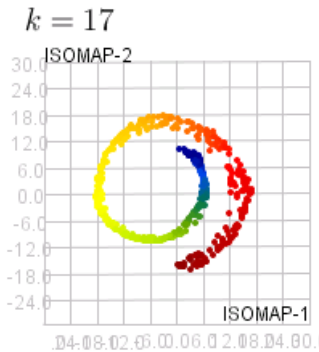




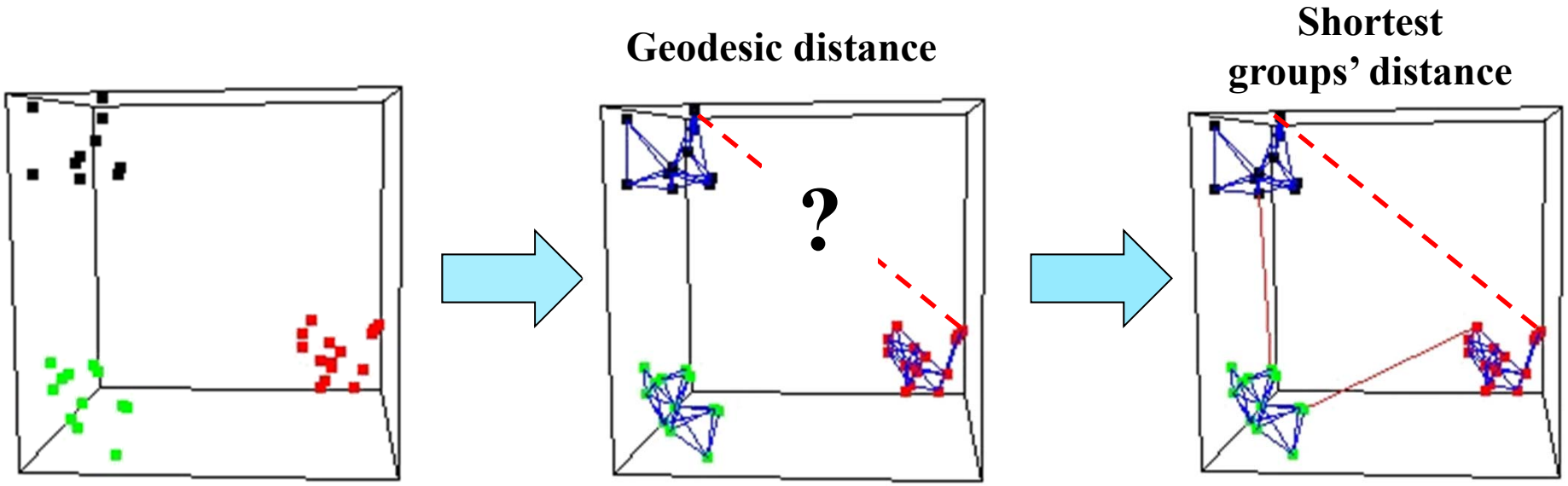
2D ISOAMP







Solving The Pinch and Short-Circuit Problem



K-nearest neighbors Single-linkage

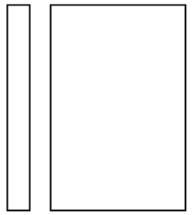
Benefit: A small number of neighbors in computing geodesic distance.

Example

lymphoma dataset

Alizadeh *et al.* (2000)

96 samples



854 genes

9 diagnostic classes

defined by Alizadeh *et al.* (2000).

- DLBCL
- Germinal Centre B
- NI Lymph Node/Tonsil
- Activated blood B
- Resting/activated T
- Transformed cell lines
- Follicular lymphoma
- Resting blood B
- CLL

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Approximate geodesic distances reveal biologically relevant structures in microarray data

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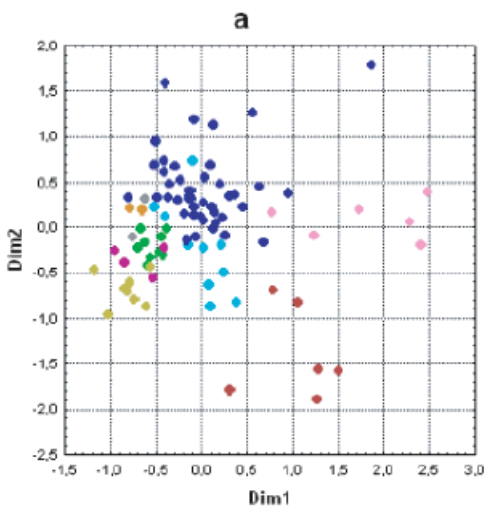
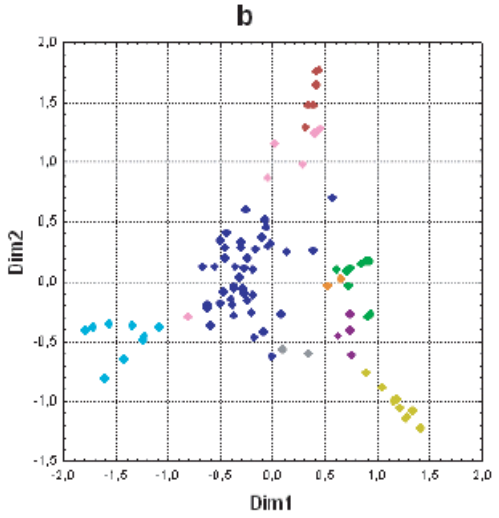
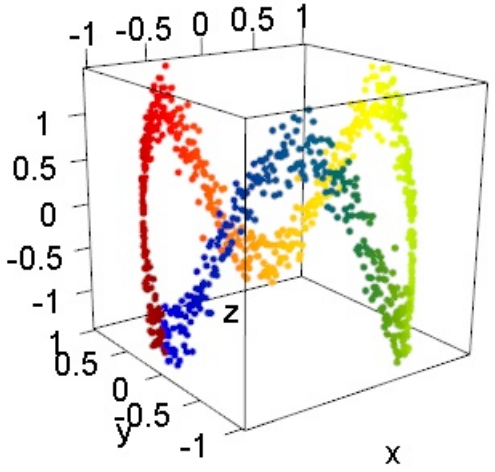
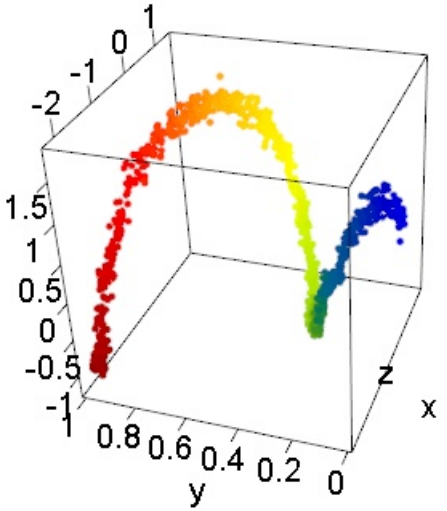




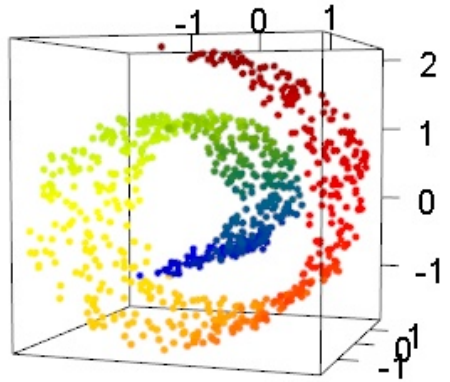
Some Nonlinear Manifold Data Sets



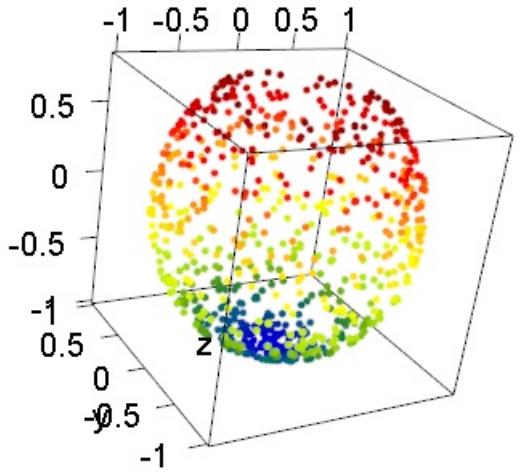
Trigcircle



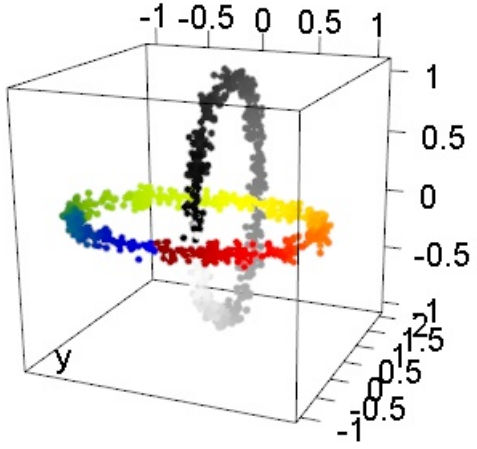
Spiral



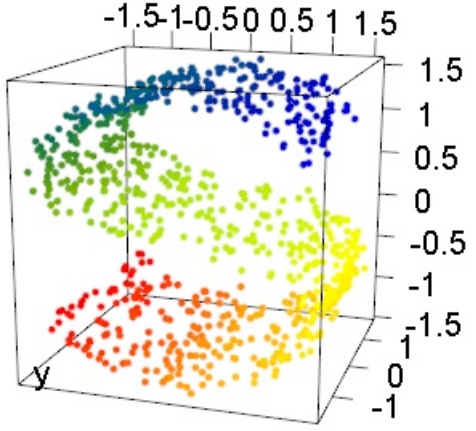
Swiss roll



Fishbowl



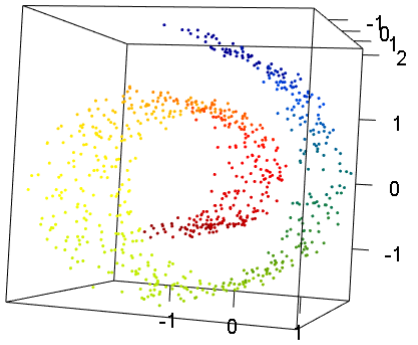
Chainlink

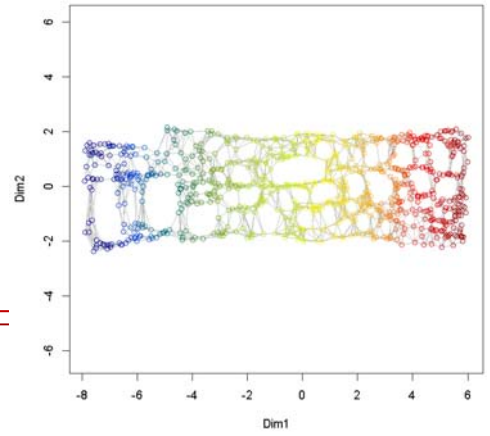


S curve

Simulation of Swiss Roll Data Set

```
swissroll <- function(n, sigma=0.05){

          angle <- (3*pi/2)*(1+2*runif(n));
          height <- runif(n);
          xdata <-  cbind(angle*cos(angle), height, angle*sin(angle))

          # angle <-  seq((1.5*pi): (4.5*pi), length.out=n);
          # height <- sample(0:21, n, replace = TRUE);
          # xdata <-  cbind(angle*cos(angle), height, angle*sin(angle))

          xdata <- scale(xdata) + matrix(rnorm(n*3, 0, sigma), n, 3)

          order.angle <- order(angle)
          sort.angle <- sort(order.angle, index.return=TRUE)
          col.id <- rainbow130(n)
          my.color <- col.id[sort.angle$ix]

          colnames(xdata) <- paste("x", 1:3, sep="")

    return(list(xdata=xdata, angle=angle, color=my.color))
}
```

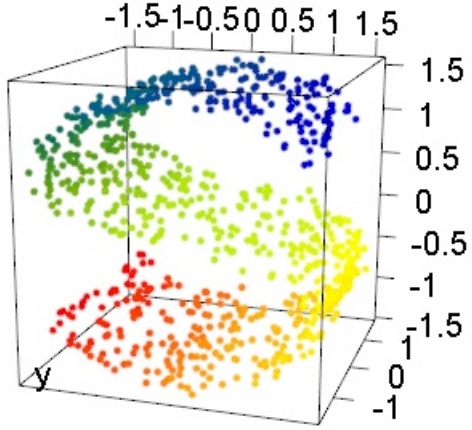





```
source("rainbow130.r")
sr <-  swissroll(800)
library(rgl); open3d()
plot3d(sr$xdata[,1], sr$xdata[,2], sr$xdata[,3], col=sr$color, size=3,
  xlab="", ylab="", zlab="", axes = T)
library(vegan)
sr.isomap <-  isomap(dist(sr$xdata), ndim=2, k=7) # try different k
plot(sr.isomap, col=sr$color)
```

Simulation of S Curve Data Set

```
Scurve <- function(n){
    # upper half S curve
    theta1 <- runif((n/2), min=-0.9*(pi), max=(pi)/2)
    z1 <- runif((n/2), min=0, max=5)
    x1 <- -cos(theta1)
    y1 <- 2-sin(theta1)
    side.upper <- matrix(0, ncol=4, nrow=(n/2))
    for(i in 1:(n/2)){
        side.upper[i,1] <- x1[i]
        side.upper[i,2] <- y1[i]
        side.upper[i,3] <- z1[i]
        side.upper[i,4] <- theta1[i]
    }
    order.theta1 <- order(theta1)
    sort.theta1 <- sort(order.theta1, method="qu", index=TRUE)
    upper.color <- sort.theta1$ix

    # lower half S curve
    theta2 <- runif((n/2), min=(pi)/2, max=1.9*(pi))
    z2 <- runif((n/2), min=0, max=5)
    x2 <- cos((pi)-theta2)
    y2 <- sin((pi)-theta2)
    side.lower <- matrix(0, ncol=4, nrow=(n/2))

    for(i in 1:(n/2)){
        side.lower[i,1] <- x2[i]
        side.lower[i,2] <- y2[i]
        side.lower[i,3] <- z2[i]
        side.lower[i,4] <- theta2[i]
    }
    order.theta2 <- order(theta2)
    sort.theta2 <- sort(order.theta2, method="qu", index=TRUE)
    lower.color <- sort.theta2$ix
```

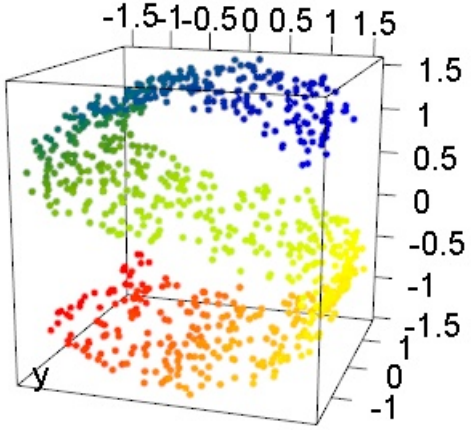


接續

Simulation of S Curve Data Set

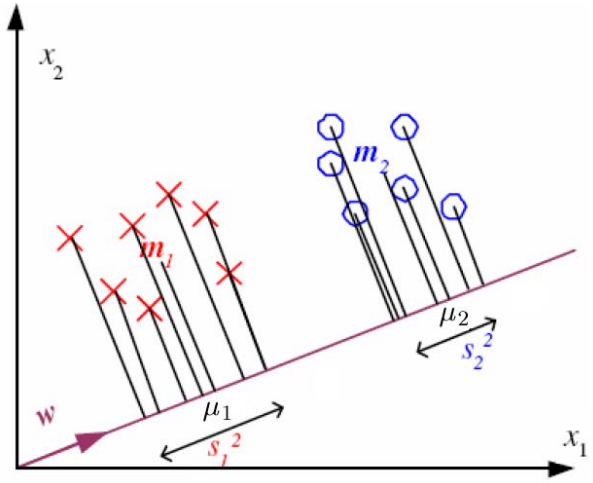
```
    xdata <- rbind(side.upper[,c(1,3,2)], side.lower[,c(1,3,2)])
    xdata <- scale(xdata) + matrix(rnorm(n*3,0, 0.05), n, 3)

    angle <- c(side.upper[,4], side.lower[,4])
    S.color <- c(upper.color, (n/2 + lower.color))
    my.color <- (rainbow130((1.2)*n)[S.color])[1:n]

    scatterplot3d(xdata, color=my.color,
                  xlab="x", ylab="y", zlab="z",
                  pch=20, angle=30)

    open3d()
    plot3d(xdata[,1], xdata[,2], xdata[,3], col=my.color, size=5,
           xlab="x", ylab="y", zlab="z")

    return(list(xdata=xdata, angle=angle, color=my.color))

}
```

Use *rgl* package to plot the simulated data.



(8) Linear Discriminant Analysis (LDA)

- LDA (Fisher, 1936) finds the linear combinations $w^T x$ of $x = (x_1, \ldots, x_p)$ with large ratios of between-groups to within-groups sum of squares.
- LDA is a supervised method for dimension reduction for classification problem.
- Given samples from two classes *C1* and *C2*, we want to find the direction, as defined by a vector w, such that when the data are projected onto *w*, the examples from the two classes are as well separated as possible.



LDA: Methodology (1/3)

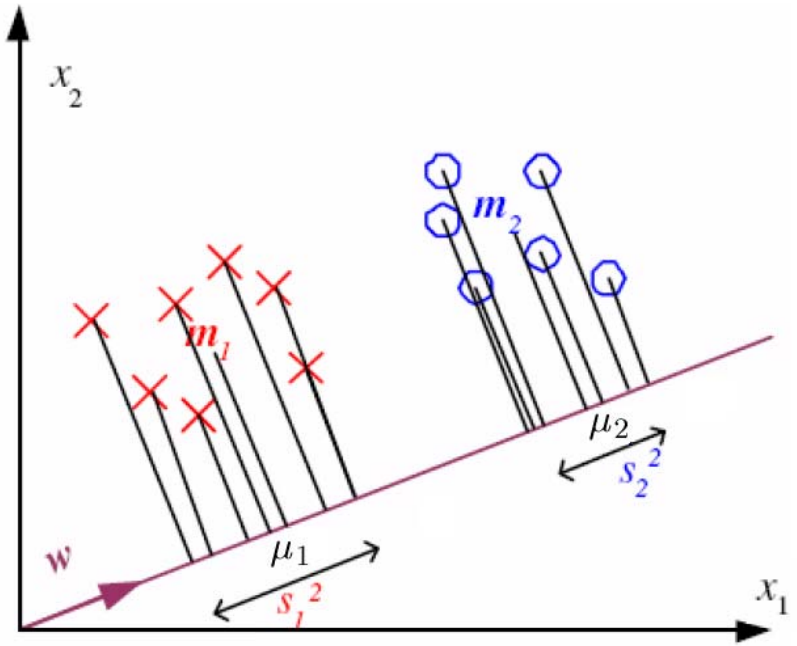
$z = \mathbf{w}^T \mathbf{x}$

the projection of $\mathbf{x}$ onto $\mathbf{w}$ and thus is a dimension reduction from d to 1.

$X = \{\mathbf{x}^t, r^t\}$, $r^t = 1$, if $\mathbf{x}^t \in C_1$ $r^t = 0$, if $\mathbf{x}^t \in C_2$

$\mathbf{m}_1 \in \mathcal{R}^d$: the means of samples from C_1 before projection

$\mu_1 \in \mathcal{R}^1$: the means of samples from C_1 after projection



LDA: Methodology (2/3)

$$\mu_1 = \frac{\sum_t^N \mathbf{w}^T\mathbf{x}^t r^t}{\sum_t^N r^t} = \mathbf{w}^T\mathbf{m}_1 \qquad \mu_2 = \frac{\sum_t^N \mathbf{w}^T\mathbf{x}^t (1-r^t)}{\sum_t^N (1-r^t)} = \mathbf{w}^T\mathbf{m}_2$$

$$s_1^2 = \sum_t (\mathbf{w}^T\mathbf{x}^t - \mu_1)^2 r^t \qquad s_2^2 = \sum_t (\mathbf{w}^T\mathbf{x}^t - \mu_2)^2 (1-r^t)$$

$$J(\mathbf{w}) = \frac{\mathbf{w}^T\mathbf{S}_B\mathbf{w}}{\mathbf{w}^T\mathbf{S}_W\mathbf{w}}$$

Want $|\mu_1 - \mu_2|$ to be large and $s_1^2 + s_2^2$ to be small

$$J(\mathbf{w}) = \frac{(\mu_1 - \mu_2)^2}{s_1^2 + s_2^2}$$

$$\begin{aligned}(\mu_1 - \mu_2)^2 &= (\mathbf{w}^T\mathbf{m}_1 - \mathbf{w}^T\mathbf{m}_2)^2 \\ &= \mathbf{w}^T(\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^T\mathbf{w} \\ &= \mathbf{w}^T\mathbf{S}_B\mathbf{w}\end{aligned}$$

$$\mathbf{S}_B = (\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^T$$

Between-class scatter matrix

$$\begin{aligned}s_1^2 &= \sum_t (\mathbf{w}^T\mathbf{x}^t - \mu_1)^2 r^t \\ &= \sum_t \mathbf{w}^T(\mathbf{x}^t - \mathbf{m}_1)(\mathbf{x}^t - \mathbf{m}_1)^T\mathbf{w} r^t \\ &= \mathbf{w}^T\mathbf{S}_1\mathbf{w}\end{aligned}$$

$$\mathbf{S}_1 = \sum_t r^t (\mathbf{x}^t - \mathbf{m}_1)(\mathbf{x}^t - \mathbf{m}_1)^T$$

Within-class scatter matrix for C_1

$$s_2^2 = \mathbf{w}^T\mathbf{S}_2\mathbf{w}$$

$$\mathbf{S}_2 = \sum_t (1-r^t)(\mathbf{x}^t - \mathbf{m}_2)(\mathbf{x}^t - \mathbf{m}_2)^T$$

$$s_1^2 + s_2^2 = \mathbf{w}^T\mathbf{S}_W\mathbf{w}$$

$$\mathbf{S}_W = \mathbf{S}_1 + \mathbf{S}_2$$

Total within-class scatter matrix

LDA: Methodology (3/3)

$$J(\mathbf{w}) = \frac{(\mu_1 - \mu_2)^2}{s_1^2 + s_2^2} \rightarrow J(\mathbf{w}) = \frac{|\mathbf{w}^T(\mathbf{m}_1 - \mathbf{m}_2)|^2}{\mathbf{w}^T\mathbf{S}_W\mathbf{w}}$$

$$J(\mathbf{w}) = \frac{\mathbf{w}^T\mathbf{S}_B\mathbf{w}}{\mathbf{w}^T\mathbf{S}_W\mathbf{w}}$$

$$\frac{\partial J}{\partial \mathbf{w}} = \frac{\mathbf{w}^T(\mathbf{m}_1 - \mathbf{m}_2)}{\mathbf{w}^T\mathbf{S}_W\mathbf{w}}(2(\mathbf{m}_1 - \mathbf{m}_2) - \frac{\mathbf{w}^T(\mathbf{m}_1 - \mathbf{m}_2)}{\mathbf{w}^T\mathbf{S}_W\mathbf{w}}\mathbf{S}_W\mathbf{w}) = 0$$

$$\mathbf{w} = c\mathbf{S}_W^{-1}(\mathbf{m}_1 - \mathbf{m}_2)$$

- Because it is the direction that is important for us and not the magnitude, set ***c=1*** and find ***w***

NOTE: $p(\mathbf{x}|C_i) \sim N(\mu_i, \Sigma)$

Linear discriminant $\mathbf{w} = \Sigma^{-1}(\mu_1 - \mu_2)$

LDA: More Than 2 Classes

$$\mathbf{z} = \mathbf{W}^T\mathbf{x} \qquad \mathbf{z} \in \mathcal{R}^k \qquad \mathbf{W} = [d \times k]$$

The within-class scatter matrix for C_i

$$\mathbf{S}_i = \sum_t r_i^t (\mathbf{x}^t - \mathbf{m}_i)(\mathbf{x}^t - \mathbf{m}_i)^T$$

$r^t = 1$ if $\mathbf{x}^t \in C_i$ and 0 otherwise

The total within-class scatter

$\mathbf{S}_W = \sum_{i=1}^K \mathbf{S}_i$

The between-class scatter matrix

$$\mathbf{S}_B = \sum_{i=1}^K N_i (\mathbf{m}_i - \mathbf{m})(\mathbf{m}_i - \mathbf{m})^T$$

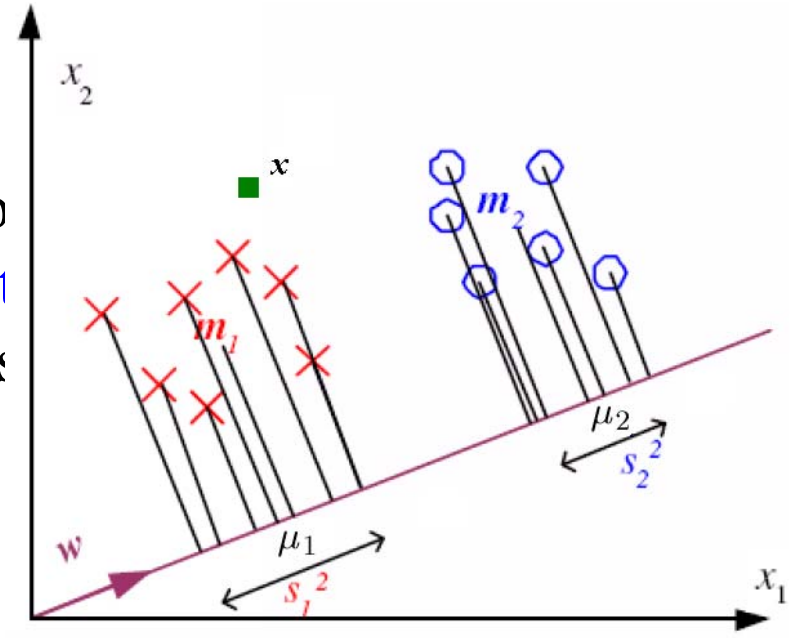
$$\mathbf{m} = \frac{1}{K}\sum_{i=1}^K \mathbf{m}_i \qquad N_i = \sum_t r_i^t$$

$$J(\mathbf{W}) = \frac{\mathbf{W}^T\mathbf{S}_B\mathbf{W}}{\mathbf{W}^T\mathbf{S}_W\mathbf{W}}$$

- The largest eigenvectors of $\mathbf{S}_W^{-1}\mathbf{S}_B$ are the solution.
- $\mathbf{S}_B$ is the sum of K matrices of rank 1, $(\mathbf{m}_i - \mathbf{m})(\mathbf{m}_i - \mathbf{m})^T$, and only $K-1$ of them are independent.
- $\mathbf{S}_B$ has a maximum rank of $K-1$ and we take $k = K-1$.
- define a new lower $(K-1)$ dimensional space, where the discriminant is then to be constructed.

LDA: Classification

- Fisher's linear discriminant is optimal normally distributed.
- After projection, for the two classes to would like the means to be as far apart examples of classes be scatteres in as s possible.



Classification Rules:

For an observation $\mathbf{x} = (x_1, \ldots, x_d)$

$d_k(\mathbf{x}) = ((\mathbf{x} - \bar{\mathbf{x}}_k)\mathbf{w})^2$

denote its (squared) Euclidean distance,
in terms of the discriminant variables,
from the $1 \times d$ vector of class k averages $\bar{\mathbf{x}}$ for the learning set $\mathcal{L}$.

The predicted class for observation $\mathbf{x}$ is

$\mathcal{C}(\mathbf{x}, \mathcal{L}) = \text{argmin}_k \, d_k(\mathbf{x})$,

the class whose mean vector is closest to $\mathbf{x}$ in the space of discriminant variables.

R: LDA

```
> library(MASS)

> help(lda)
```

```
data(iris3)
Iris <- data.frame(rbind(iris3[,,1], iris3[,,2], iris3[,,3]),
                   Species = rep(c("setosa","versicolor","virginica"), rep(50,3)))

## LDA
> library(MASS)
data <- Iris[,1:4]
class <- Iris[,5]
Iris.lda <- lda(x=data, grouping=class)
Iris.lda <- lda(Species ~ ., Iris)
lda.dim1 <- as.matrix(data)%*%iris.lda$scaling[,1]
lda.dim2 <- as.matrix(data)%*%iris.lda$scaling[,2]

## LDA for classification
trainingIndex <- sample(1:150, 75)
trainingSample <- Iris[trainingIndex, ]
testSample <- Iris[-trainingIndex, ]
table(Iris$Species[trainingIndex])

ldaRule <- lda(Species ~ ., Iris,
               subset = trainingIndex)
predict(ldaRule, testSample)$class
```

```
lda(Species ~ ., data = Iris)

Prior probabilities of groups:
    setosa versicolor  virginica
 0.3333333  0.3333333  0.3333333

Group means:
           Sepal.L. Sepal.W. Petal.L. Petal.W.
setosa        5.006    3.428    1.462    0.246
versicolor    5.936    2.770    4.260    1.326
virginica     6.588    2.974    5.552    2.026

Coefficients of linear discriminants:
                LD1         LD2
Sepal.L.  0.8293776  0.02410215
Sepal.W.  1.5344731  2.16452123
Petal.L. -2.2012117 -0.93192121
Petal.W. -2.8104603  2.83918785

Proportion of trace:
   LD1    LD2
0.9912 0.0088
```

(9) Sliced Inverse Regression (SIR)

K.C. Li, (1991),
Sliced inverse regression for dimension reduction, *JASA* **86**, 316 – 342.

y is a univariate variable.

f is an arbitrary function.

$$y = f(\beta'_1 \mathbf{x}, \cdots, \beta'_K \mathbf{x}, \epsilon)$$

ϵ is a random variable independent of $\mathbf{x}$.

The β's are referred to effective dimension reduction ($e.d.r.$) or projection directions.

$\mathbf{x}$ is a random vector with dimension $p \times 1$, $p \geq K$.

Sliced inverse regression (SIR) is a method for estimating the $e.d.r.$ directions based on y and $\mathbf{x}$.

SIR: Algorithm

$$\begin{array}{c|cccc} & y & X_1 & X_2 & \cdots & X_p \\ \mathbf{x}_1 & 10 & 1 & 4 & & 2 \\ \mathbf{x}_2 & 13 & 3 & 5 & & 3 \\ \mathbf{x}_3 & 9 & 0 & 3 & & 2 \\ & 17 & 5 & 5 & \cdots & 6 \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ & 12 & 2 & 4 & & 3 \\ \mathbf{x}_N & 11 & 2 & 5 & & 2 \end{array}$$

$$\begin{array}{c|cccc|c} & y & X_1 & X_2 & \cdots & X_p & \\ \bar{\mathbf{x}}_{(1)} & 9 & 0 & 3 & & 2 & 1 \\ \bar{\mathbf{x}}_{(2)} & 10 & 1 & 4 & & 2 & \\ \hline \bar{\mathbf{x}}_{(3)} & 11 & 2 & 5 & & 2 & 2 \\ & 12 & 2 & 4 & \cdots & 3 & \\ \hline \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\ & 13 & 3 & 5 & & 3 & \\ \bar{\mathbf{x}}_{(N)} & 17 & 5 & 5 & & 6 & H \end{array}$$

$$\begin{array}{c|cccc} & X_1 & X_2 & \cdots & X_p \\ \bar{\mathbf{x}}_1 & 0.5 & 3.5 & \cdots & 2.0 \\ \bar{\mathbf{x}}_2 & 2.0 & 4.5 & & 2.5 \\ \vdots & \vdots & \vdots & & \vdots \\ \bar{\mathbf{x}}_H & 4.0 & 5.0 & & 4.5 \end{array}$$

Sample Mean

$$\bar{\mathbf{x}} = \frac{\sum_{i=1}^{N} \mathbf{x}_i}{N}$$

Sample Covariance Matrix

$$\hat{\Sigma}_X = \sum_{i=1}^{N} N^{-1}(\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^T$$

Sliced Mean

$$\bar{\mathbf{x}}_h = n_h^{-1} \sum_{(i)\in \text{slice}_h} \mathbf{x}_{(i)}$$

Weighted Covariance Matrix for the Slice Means

$$\hat{\Sigma}_W = \sum_{h=1}^{H} \frac{n_h}{N}(\bar{\mathbf{x}}_h - \bar{\mathbf{x}})(\bar{\mathbf{x}}_h - \bar{\mathbf{x}})^T$$

$$\hat{\Sigma}_W \hat{\beta}_i = \hat{\lambda}_i \hat{\Sigma}_X \hat{\beta}_i$$

$$\hat{\lambda}_1 \geq \hat{\lambda}_1 \geq \cdots \geq \hat{\lambda}_p$$

$$\begin{array}{c|cccc} y & \text{SIR}_1 & \text{SIR}_2 & \cdots & \text{SIR}_K \\ 10 & \hat{\beta}_1 \mathbf{x}_1 & \hat{\beta}_2 \mathbf{x}_1 & \cdots & \hat{\beta}_K \mathbf{x}_1 \\ 13 & \hat{\beta}_1 \mathbf{x}_2 & \hat{\beta}_2 \mathbf{x}_2 & \cdots & \hat{\beta}_K \mathbf{x}_2 \\ 9 & & & & \\ 17 & & & & \\ 12 & & & & \\ 11 & \hat{\beta}_1 \mathbf{x}_N & \hat{\beta}_2 \mathbf{x}_N & \cdots & \hat{\beta}_K \mathbf{x}_N \end{array}$$

SIR: Theorem

Linear Design Condition (L.D.C.)

For any b in R^p,

the conditional expectation $E(b'\mathbf{x}|\beta_1'\mathbf{x}, \cdots, \beta_K'\mathbf{x})$ is linear in $\beta_1'\mathbf{x}, \cdots, \beta_K'\mathbf{x}$;

- that is, for some constants $c_0, c_1, \cdots, c_k$,
  $E(b'\mathbf{x}|\beta_1'\mathbf{x}, \cdots, \beta_K'\mathbf{x}) = c_0 + c_1\beta_1'\mathbf{x} + \cdots + c_k\beta_K'\mathbf{x}$.

THEOREM:
under regular conditions, the centered inverse regression curve $E[\mathbf{x}|y] - E[\mathbf{x}]$ is contained in the linear subspace spanned by $\beta_k\Sigma_{\mathbf{x}}$ $(k = 1, \cdots, K)$.

COROLLARY 3.1 (Li, 1991)

Assume that $\mathbf{x}$ has been standardized to $\mathbf{z}$. Then under the model and (3.1), the standardized inverse regression curve $E(\mathbf{z}|y)$ is contained in the linear space generated by the standardized *e.d.r.* directions θ_1 θ_2 $\cdots$ θ_K

SIR: Theorem

The SIR directions $\mathbf{v_i}$ falls into the $e.d.r$ space.

$$\text{Cov}(E[\mathbf{z}|y]) = E_y[E[\mathbf{z}|y]E[\mathbf{z}|y]^T]$$

$$E[\mathbf{z}|y] = c_1\theta_1 + \cdots + c_K\theta_K$$

$$= E_y[(c_1\theta_1 + \cdots + c_K\theta_K)(c_1\theta_1 + \cdots + c_K\theta_K)^T]$$

$$= (\theta_1\ \theta_2\ \cdots\ \theta_K) \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_K \end{pmatrix} (c_1\ c_2\ \cdots\ c_K) \begin{pmatrix} \theta_1^T \\ \theta_2^T \\ \vdots \\ \theta_K^T \end{pmatrix}$$

$$= (\theta_1\ \theta_2\ \cdots\ \theta_K) \begin{pmatrix} c_1^2 & c_1c_2 & \cdots & c_1c_K \\ c_2c_1 & c_2^2 & \cdots & \\ c_3c_1 & c_3c_2 & c_3^2\cdots & \\ \vdots & & & \\ c_Kc_1 & & & c_K^2 \end{pmatrix} \begin{pmatrix} \theta_1^T \\ \theta_2^T \\ \vdots \\ \theta_K^T \end{pmatrix}$$

$$= \mathbf{\Theta C \Theta}^T$$

$$= \mathbf{\Theta(UDU}^T)\mathbf{\Theta}^T$$

$$= (\mathbf{\Theta U})\mathbf{D}^T(\mathbf{\Theta U})^T$$

$$\text{Cov}(E[\mathbf{z}|y])\mathbf{v}_i = \lambda_i\mathbf{v}_i$$

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p$$

R: dr package

- dr: Methods for Dimension Reduction for Regression

```
dr(formula, data, subset, group=NULL, na.action = na.fail,
    weights,method = "sir", chi2approx="bx",...)
```

Table 1: Methods implemented in `dr`. "Multivariate" is yes if the response can be multivariate. "Partial" is yes if conditioning on categorical predictors is allowed using the `group` argument. "Coord" is yes if coordinate tests are available.

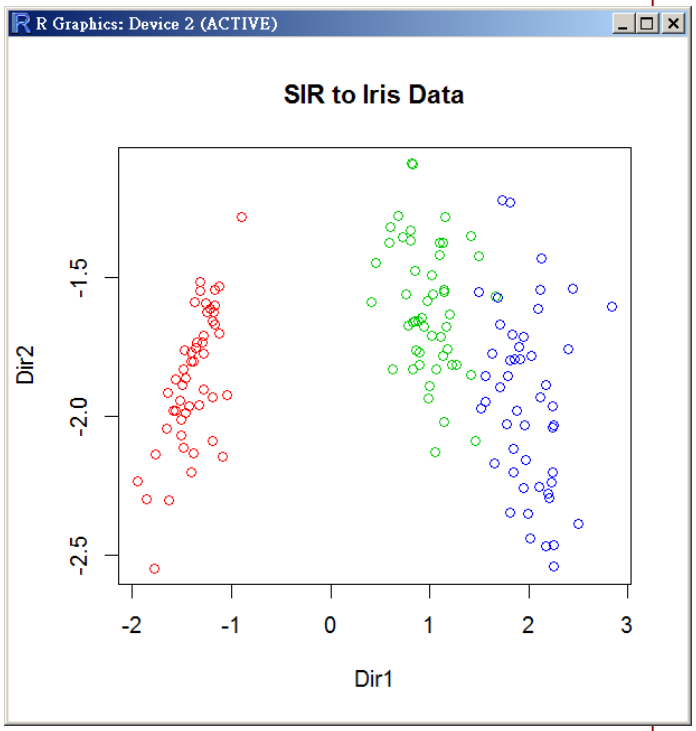
Name	Reference	Multivariate	Partial	Coord
sir	Li (1991), Chiaromonte, Cook and Li (2002)	Yes	Yes	Yes
save	Cook and Weisberg (1991); Shao, Cook and Weisberg (2007)	Yes	Yes	Yes
phdy	Li (1992), Cook (1998)	No	No	No
phdres	Cook (1998)	No	No	No
phdq	Li (1992)	No	No	No
ire	Cook and Ni (2006), Wen and Cook (2007)	No	Yes	Yes

Source: The dr package, Vignettes, Sanford Weisberg

SIR to Iris Data

```
> iris.sir <- dr(as.integer(Species) ~ Sepal.Length + Sepal.Width + Petal.Length +
Petal.Width , data=iris, nslices=3, chi2approx="wood", method="sir")
> summary(iris.sir)
Call:
dr(formula = as.integer(Species) ~ Sepal.Length + Sepal.Width +
    Petal.Length + Petal.Width, data = iris, nslices = 3, chi2approx = "wood",
    method = "sir")
Method:
sir with 3 slices, n = 150.

Slice Sizes:
50 50 50

Estimated Basis Vectors for Central Subspace:
                Dir1      Dir2
Sepal.Length -0.2087 -0.006532
Sepal.Width  -0.3862 -0.586611
Petal.Length  0.5540  0.252562
Petal.Width   0.7074 -0.769453

               Dir1  Dir2
Eigenvalues 0.9699 0.222
R^2(OLS|dr) 0.9874 1.000

Large-sample Marginal Dimension Tests:
             Stat df   p.value
0D vs >= 1D 178.8  8 0.000e+00
1D vs >= 2D  33.3  3 2.779e-07
> comp.sir <- as.matrix(iris[,1:4]) %*% as.matrix(iris.sir$evectors[,1:2])
> plot(comp.sir, col=as.integer(iris$Species)+1, main="SIR to Iris Data")
```

```
> install.packages("dr")
> library(dr)
```



模擬(1): SIR to the Simulated Data from the Linear Model


```
Li6.1 <- function(n){
    p <- 5
    x <- matrix(0, ncol=p, nrow=n)
    for(i in 1:p){
        x[,i] <- rnorm(n, mean=0, sd=1)
    }

    epsilon <- rnorm(n, mean=0, sd=1)
    y <- x[,1] +  x[,2] +  x[,3]+  x[,4] + ep
    colnames(x) <- c("x1","x2","x3","x4","x5"

    as.data.frame(cbind(y, x))
}

mydata <- Li6.1(200)
attach(mydata)
library(dr)
my.sir <- dr(y~x1+x2+x3+x4+x5, method="sir",
nslices=10)
my.sir
```

1 Linear Model (6.1)

- $y = x_1 + x_2 + x_3 + x_4 + 0x_5 + \epsilon$
- $x_1, x_2, \cdots, x_5 \sim N(0,1), \epsilon \sim N(0,1),\ x_i\text{'s} \perp \epsilon$
- $X_{[100\times 5]}$
- $\beta = (1,1,1,1,0)$

```
> my.sir

 dr(formula = y ~ x1 + x2 + x3 + x4 + x5, method =
"sir",
     nslices = 10)
Estimated Basis Vectors for Central Subspace:
          Dir1       Dir2       Dir3        Dir4
x1 -0.52809049 -0.4830910  0.2286112 -0.03295919
x2 -0.47623158  0.6938396  0.3784483  0.32234068
x3 -0.49866200 -0.3134047 -0.4832488  0.62730069
x4 -0.49551956  0.1774727 -0.3674617 -0.68542820
x5 -0.01097735 -0.3943230  0.6602699 -0.17802302
Eigenvalues:
[1] 0.81108317 0.07944489 0.03748905 0.01976887
```

模擬(2): SIR to the Simulated Data from the Quadratic Function Model

2 Quadratic Model (6.2)

- $y = x_1(x_1 + x_2 + 1) + \sigma \cdot \epsilon$
- $X_{[400\times 10]}$
- $x_1, x_2, \cdots, x_{10} \sim N(0,1), \epsilon \sim N(0,1)$, x_i's $\perp \epsilon$
- $\sigma = 0.5$, $\sigma = 1$
- $\beta_1 = (1, 0, \cdots, 0)$, $\beta_2 = (0, 1, 0, \cdots, 0)$

$$R^2(b) = \max_{\beta \in B} \frac{(b\Sigma_{xx}\beta')^2}{b\Sigma_{xx}b \cdot \beta\Sigma_{xx}\beta'}, \qquad (2.2)$$

the squared multiple correlation coefficient between the projected variable $b\mathbf{x}$ and the ideally reduced variables $\beta_1\mathbf{x}$, ..., $\beta_K\mathbf{x}$.

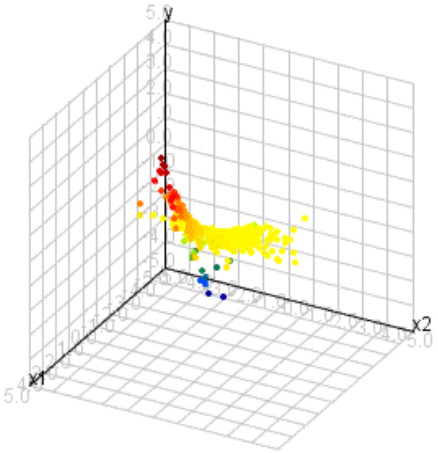
$\Delta(\hat{\beta}) =$ canonical correlations between $(\beta_1, \beta_2; \hat{\beta}_1, \hat{\beta}_2)$.

Table 2. Mean and Standard Deviation of $R^2(\hat{\beta}_1)$ and $R^2(\hat{\beta}_2)$ for the Quadratic Model (6.2), $p = 10$, $n = 400$

	$\sigma = 0.5$		$\sigma = 1$	
H	$R^2(\hat{\beta}_1)$	$R^2(\hat{\beta}_2)$	$R^2(\hat{\beta}_1)$	$R^2(\hat{\beta}_2)$
5	.91	.75	.88	.52
	(.05)	(.15)	(.07)	(.21)
10	.92	.80	.89	.55
	(.04)	(.13)	(.08)	(.24)
20	.93	.77	.88	.49
	(.04)	(.15)	(.08)	(.26)

模擬(3): SIR to the Simulated Data from the Rational Function Model

http://www.hmwu.idv.tw/KSIR/Data/Li-DataIII/index.htm



3 Rational Function Model (6.3)

- $y = x_1/(0.5 + (x_2 + 1.5)^2) + \sigma \cdot \epsilon$
- $x_1, x_2, \cdots, x_{10} \sim N(0,1), \epsilon \sim N(0,1)$, x_i's $\perp \epsilon$
- $X_{[400\times 10]}$, $\sigma = 0.5$, $\sigma = 1$
- $\beta_1 = (1, 0, \cdots, 0)$, $\beta_2 = (0, 1, 0, \cdots, 0)$

best view of the data

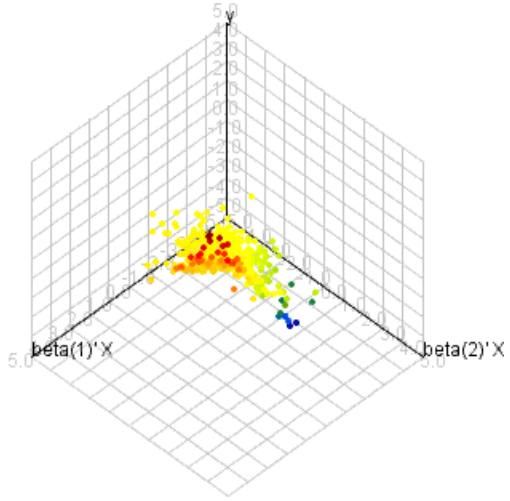
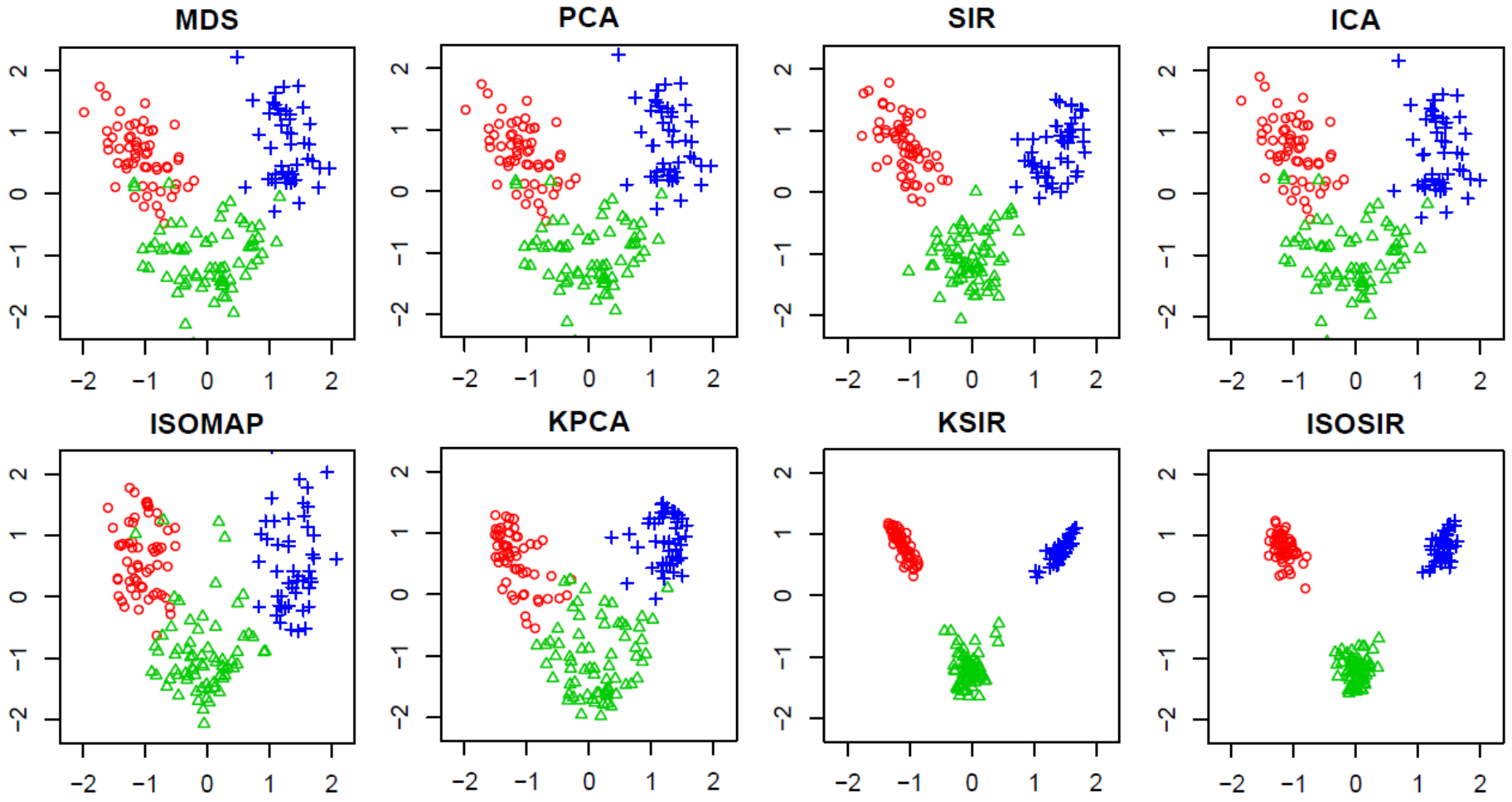


Table 3. Mean and Standard Deviation of $R^2(\hat{\beta}_1)$ and $R^2(\hat{\beta}_2)$ for the Rational Function Model (6.3), p = 10, n = 400

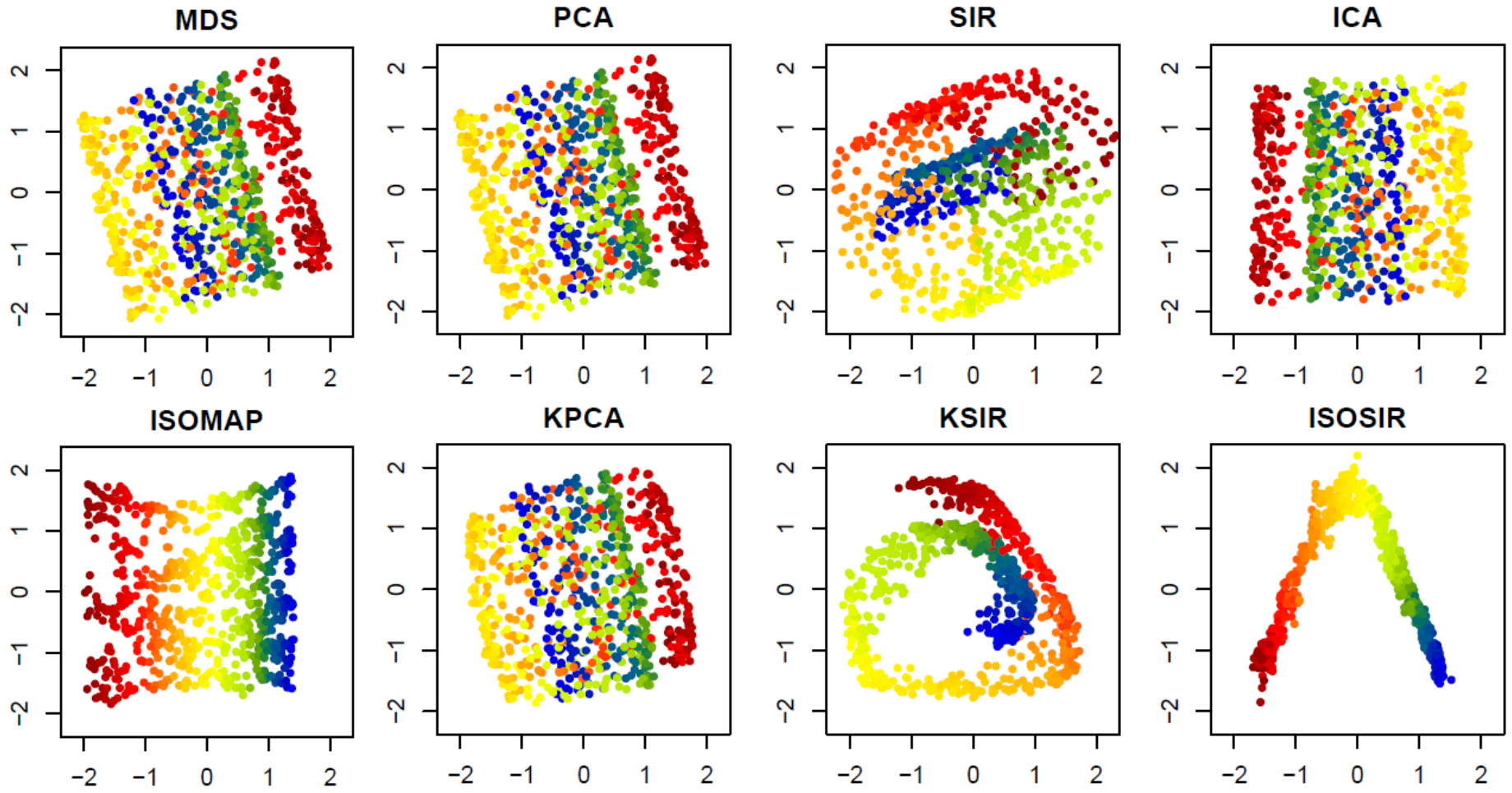
	σ = 0.5		σ = 1	
H	$R^2(\hat{\beta}_1)$	$R^2(\hat{\beta}_2)$	$R^2(\hat{\beta}_1)$	$R^2(\hat{\beta}_2)$
5	.96	.83	.89	.51
	(.02)	(.08)	(.06)	(.23)
10	.96	.88	.90	.56
	(.02)	(.06)	(.06)	(.23)
20	.96	.89	.90	.53
	(.02)	(.06)	(.06)	(.24)

ISOSIR for Nonlinear Dimension Reduction and Data Visualization: Wine Data (178x13)

https://archive.ics.uci.edu/ml/datasets/Wine



ISOSIR for Nonlinear Dimension Reduction and Data Visualization: Swissroll Data (800x3)

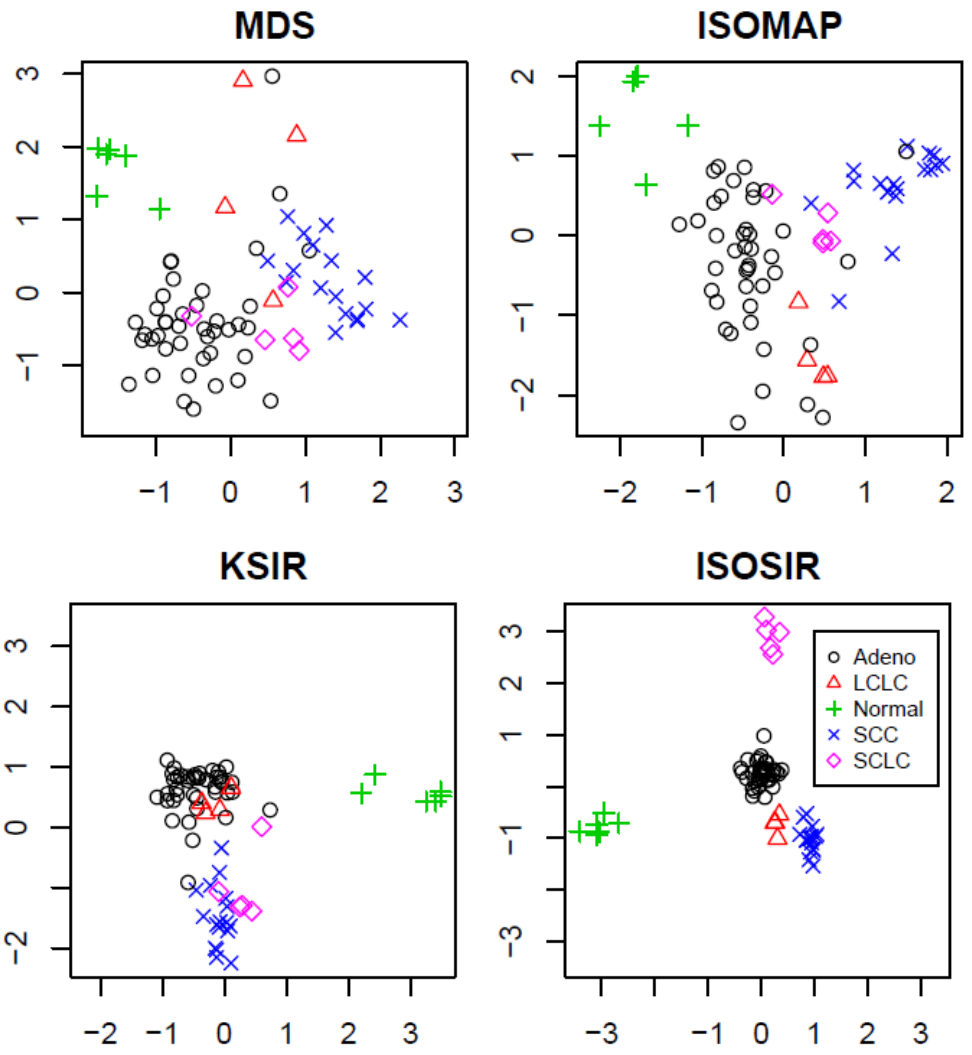


ISOSIR for Nonlinear Dimension Reduction and Data Visualization: Lung Cancer Microarray Data (73x831)

Aim: find differentially expressed genes that can provide a basis for the classification of lung cancer subtypes (Garber et al. 2001).

Samples: 73 samples were divided into five diagnostic classes: adenocarcinoma (Adeno, 41), large-cell lung cancer (LCLC, 4), Normal (6), small-cell lung cancer (SCLC, 5), and squamous cell carcinoma (SCC, 17).

Genes: Nilsson et al. (2004) selected a subset of 831 genes and performed MDS and ISOMAP to visualize these samples.



小細胞肺癌 (SCLC) | 非小細胞肺癌(NSCLC): 包括腺癌(adenocarcinoma)、鱗狀細胞癌(SCC)、大細胞癌(LCLC)。

High-dimensional data (HDD)

- Three different groups of HDD:
  - d is large but smaller than n;
  - d is large and larger than n: **the high-dimension low sample size data (HDLSS)**; and
  - the data are functions of a continuous variable d: the **functional data**.
- In high dimension, the space becomes emptier as the dimension increases
  - when p > n, the rank r of the covariance matrix S satisfies $r \leq \min\{p, n\}$.
  - For HDLSS data, one cannot obtain more than n principal components.
  - Either PCA needs to be adjusted, or other methods such as ICA or Projection Pursuit could be used.

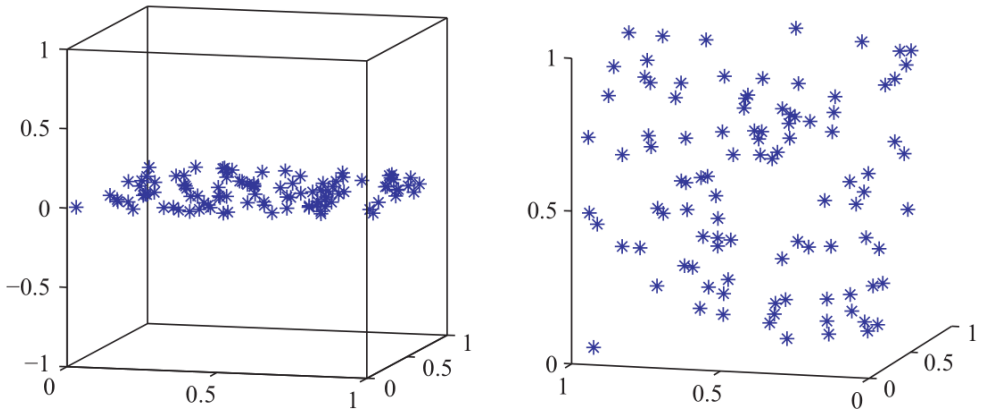
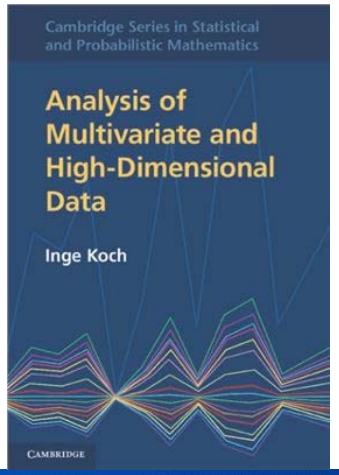


Figure 2.12 Distribution of 100 points in 2D and 3D unit space.



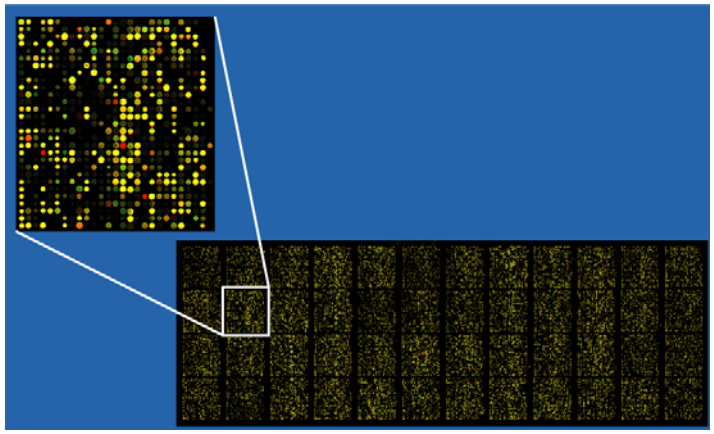
HDLSS examples

Sungkyu Jung and J. S. Marro, 2009, Pca Consistency In High Dimension, Low Sample Size Context, The Annals of Statistics 37(6B), 4104–4130.

- Examples:
  - in face recognition (**images**) we have many thousands of variables (pixels), the number of training samples defining a class (person) is usually small (usually less than 10).
  - **Microarray** experiments is unusual for there to be more than 50 repeats (data points) for several thousand variables (genes).
- The covariance matrix will be singular, and therefore cannot be inverted. In these cases we need to find some method of estimating a full rank covariance matrix to calculate an inverse.

Face recognition using PCA

https://www.mathworks.com/matlabcentral/fileexchange/45750-face-recognition-using-pca



https://zh.wikipedia.org/wiki/DNA微陣列

eigen/cov/PCA of a data set when n<<p

```
> x <- matrix(rnorm(100), ncol=20)
> dim(x)
[1]  5 20
> princomp(x)
Error in princomp.default(x) :
  'princomp' can only be used with more units than variables
```

```
> princomp
function (x, ...)
UseMethod("princomp")
<bytecode: 0x000000000aa0a3e8>
<environment: namespace:stats>
> methods(princomp)
[1] princomp.default* princomp.formula*
see '?methods' for accessing help and source code
> getAnywhere('princomp.default') # or stats:::princomp.default
A single object matching  ‘princomp.default’  was found
...
function (x, cor = FALSE, scores = TRUE, covmat = NULL, subset = rep_len(TRUE,
    nrow(as.matrix(x))), ...)
{
...
        dn <- dim(z)
        if (dn[1L] < dn[2L])
            stop("'princomp' can only be used with more units than variables")
        covmat <- cov.wt(z)
...
<environment: namespace:stats>
>
> ?cov.wt
```

eigen/cov/PCA of a data set when n<<p

```
> e.cor <- eigen(cor(x, use="pairwise.complete.obs"))
> e.cor$values
 [1]  6.263117e+00  5.443693e+00  4.702980e+00  3.590210e+00
 [5]  3.644515e-15  1.258361e-15  3.437109e-16  2.431887e-16
 [9]  1.508096e-16  6.521571e-17  4.539563e-17  2.806356e-17
[13]  1.782844e-17  2.135321e-18 -9.004648e-18 -1.546332e-17
[17] -5.765008e-17 -6.563774e-17 -9.621985e-17 -5.282082e-16
> # e.cor$vectors
```

```
> pca.pkg <- c("FactoMineR", "factoextra", "corrplot")
> lapply(pca.pkg, library, character.only=TRUE)
> x.pca <- PCA(x, graph = FALSE) # works, why?
> PCA # check the code
function (X, scale.unit = TRUE, ncp = 5, ind.sup = NULL, quanti.sup = NULL,
...
    tmp <- svd.triplet(X, row.w = row.w, col.w = col.w, ncp = ncp)
    ...
<environment: namespace:FactoMineR>
> str(x.pca)
List of 5
 $ eig :'data.frame':   4 obs. of  3 variables:
...
 $ svd :List of 3
  ..$ vs: num [1:4] 2.5 2.33 2.17 1.89
  ..$ U : num [1:5, 1:4] 1 -1.256 -0.129 1.272 -0.888 ...
  ..$ V : num [1:20, 1:4] 0.1651 0.3414 -0.0531 -0.1638 0.2618 ...
...
 - attr(*, "class")= chr [1:2] "PCA" "list "
```

```
> get_eigenvalue(x.pca)
> x.pca$svd$V
```

The breast tumour (gene expression) data of van't Veer et al

- The breast tumour (gene expression) data of van't Veer et al. (2002): 78 observations and 4,751 gene expressions, log 10 transformations.
- Typically, gene expression data contain intensity levels or expression indices of genes which are measured for a large number of genes
- In gene microarray experiments, the chips are the observations, and the genes are the variables.
- The data contain survival times in months as well as binary responses regarding survival.
- Patients who left the study or metastasised before the end of five years were grouped into the first class (DM), and those who survived five years formed the second class. Of the 78 patients, 44 survived the critical five years (NODM).

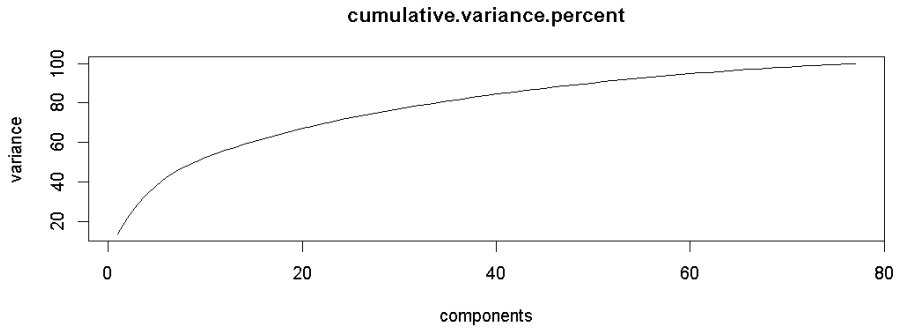
PCA for The breast tumour data

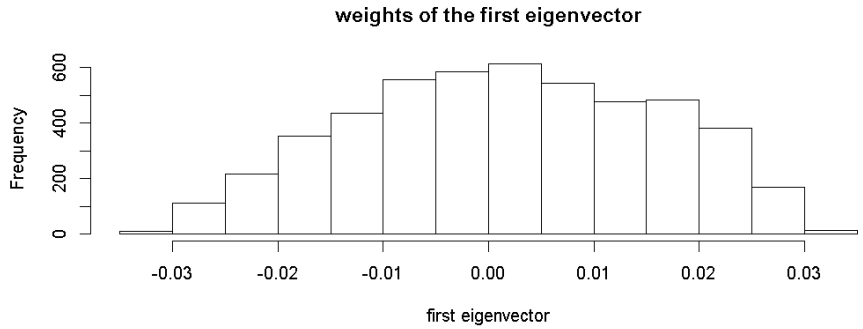
```
> library(cancerdata)
> data(VEER1) # Breast cancer gene expression data (van't Veer)
> # load("VEER1.RData")
> VEER1
ExpressionSet (storageMode: lockedEnvironment)
assayData: 4948 features, 78 samples
  element names: exprs
protocolData: none
phenoData
  sampleNames: X1 X2 ... X79 (78 total)
  varLabels: info class
  varMetadata: labelDescription
featureData
  featureNames: J00129 Contig29982_RC ... AF067420 (4948 total)
  fvarLabels: symbol
  fvarMetadata: labelDescription
experimentData: use 'experimentData(object)'
Annotation: Hu25K
> dim(exprs(VEER1))
[1] 4948   78
> str(VEER1)
Formal class 'ExpressionSet' [package "Biobase"] with 7 slots
  ..@ experimentData   :Formal class 'MIAME' [package "Biobase"] with 13 slots
  ...
  ..@ featureData      :Formal class 'AnnotatedDataFrame' [package "Biobase"] with 4 slots
  ...
> exprs(VEER1)[1:3, 1:5] X1     X2     X3     X4     X5
J00129         -0.448 -0.480 -0.568 -0.819 -0.112
Contig29982_RC -0.296 -0.512 -0.411 -0.267 -0.670
Contig42854    -0.100 -0.031 -0.398  0.023  0.421
```

```
> VEER1@phenoData@data$info
 [1] Sample.1..5.yr.survival.150...
...
97 Levels: Sample.1..5.yr.survival...
> table(VEER1@phenoData@data$class)
  DM NODM
  34   44
```

PCA for The breast tumour data

```
> library(FactoMineR); library(factoextra); library(corrplot)
> x <- t(exprs(VEER1))
> x.pca <- PCA(x, graph = FALSE)
> x.pca
**Results for the Principal Component Analysis (PCA)**
The analysis was performed on 78 individuals, described by 4948 variables
*The results are available in the following objects:

   name               description
1  "$eig"             "eigenvalues"
2  "$var"             "results for the variables"
...
15 "$call$col.w"      "weights for the variables"
> eig.val <- get_eigenvalue(x.pca)
> plot(eig.val[,3], type="l", xlab="components", ylab="variance",
+      main="cumulative.variance.percent")
> hist(x.pca$svd$V[,1], xlab="first eigenvector", main="weights of the first eigenvector")
```

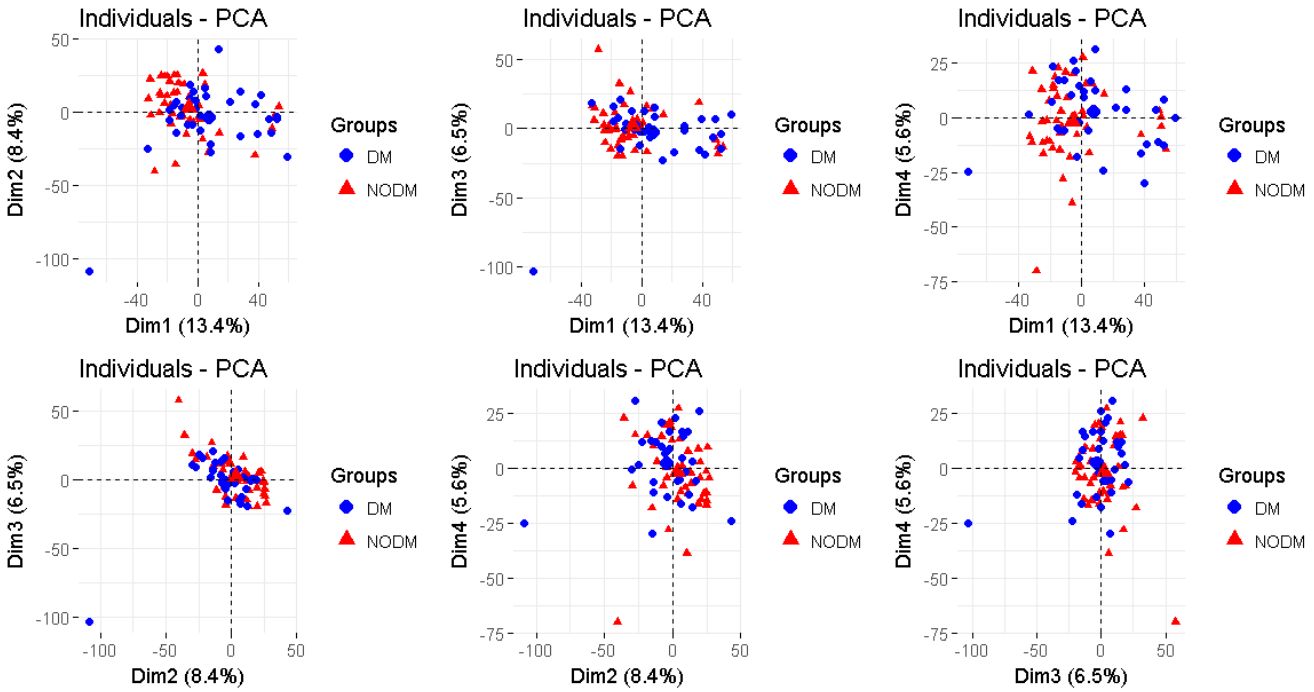




PCA for The Breast Tumour Data

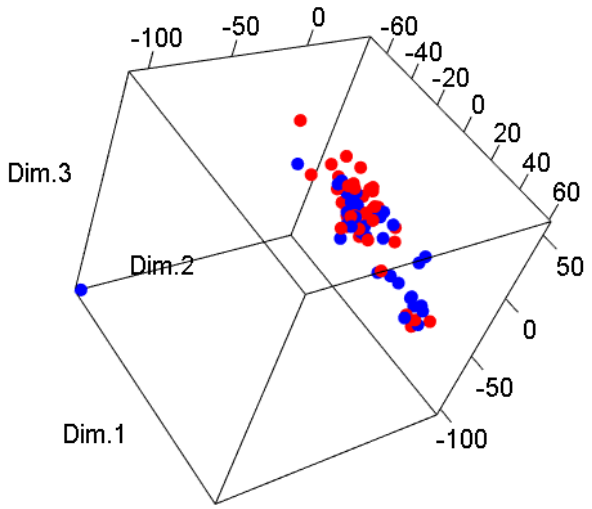
```
> x.pc <- rep(1:3, 3:1)
> y.pc <- unlist(lapply(2:4, function(x) seq(x, 4)))
>
> mypca.plot <- function(used.pc){
+     fviz_pca_ind(x.pca, axes = used.pc,
                   geom.ind = "point",
+                  col.ind = VEER1@phenoData@data$class,
+                  palette = c("blue", "red"),
+                  legend.title = "Groups")
+ }
> plot.list <- apply(cbind(x.pc, y.pc), 1, mypca.plot)
```

```
> library(gridGraphics)
> library(grid)
> grid.newpage()
> library(gridExtra)
> grid.arrange(grobs=plot.list,
                nrow=2,
                ncol=3)
```



PCA for The Breast Tumour Data

```
> x.pca.scores <- get_pca_ind(x.pca)
> dim(x.pca.scores$coord)
[1] 78  5
> group.col <- c("blue", "red")[as.integer(VEER1@phenoData@data$class)]
> library("rgl")
> open3d()
> plot3d(x.pca.scores$coord[,1:3],
+        col=group.col,
+        type ="p", size=10)
> play3d(spin3d(), duration=10)
```



Efficient Estimation of Covariance: a Shrinkage Approach

$$s_{ij} = \frac{1}{n-1}\sum_{k=1}^{n}(x_{ki} - \bar{x}_i)(x_{kj} - \bar{x}_j),$$

a shrinkage estimator

$$\hat{\mathbf{\Sigma}}_{\mathrm{LW}} = \alpha_1 \mathbf{I} + \alpha_2 \mathbf{S}.$$

"Small *n*, Large *p*"

Covariance and Correlation Estimators $S^\star$ and $R^\star$:

$$s^\star_{ij} = \begin{cases} s_{ii} & \text{if } i = j \\ r^\star_{ij}\sqrt{s_{ii}s_{jj}} & \text{if } i \neq j \end{cases}$$

$$r^\star_{ij} = \begin{cases} 1 & \text{if } i = j \\ r_{ij}\min(1, \max(0, 1 - \hat{\lambda}^\star)) & \text{if } i \neq j \end{cases}$$

with $$\hat{\lambda}^\star = \frac{\sum_{i\neq j}\widehat{\mathrm{Var}}(r_{ij})}{\sum_{i\neq j} r^2_{ij}}$$

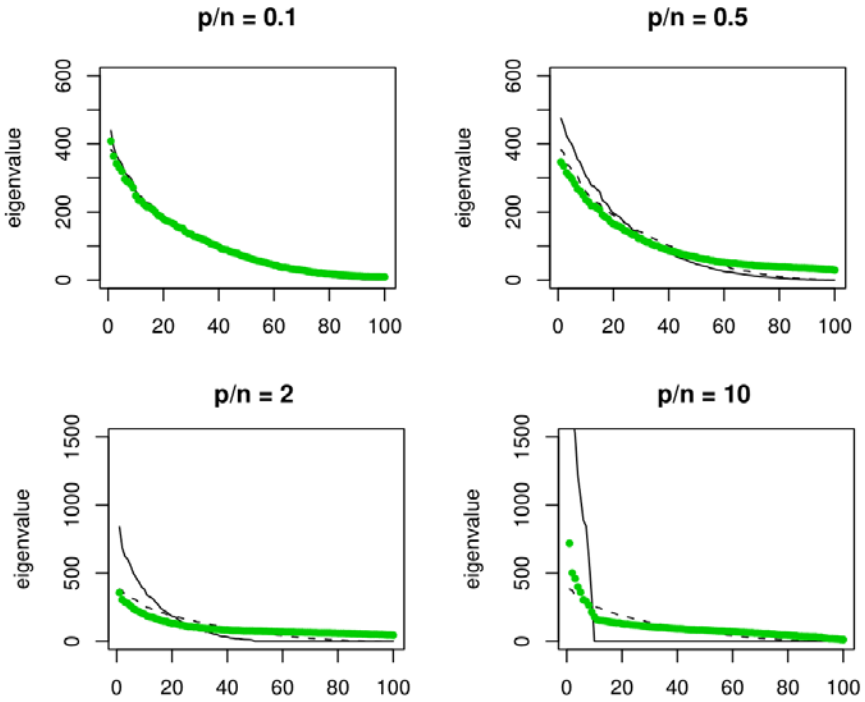


Figure 1: Ordered eigenvalues of the sample covariance matrix $\boldsymbol{S}$ (thin black line) and that of an alternative estimator $\boldsymbol{S}^\star$ (fat green line, for definition see Tab. 1), calculated from simulated data with underlying p-variate normal distribution, for $p = 100$ and various ratios p/n. The true eigenvalues are indicated by a thin black dashed line.

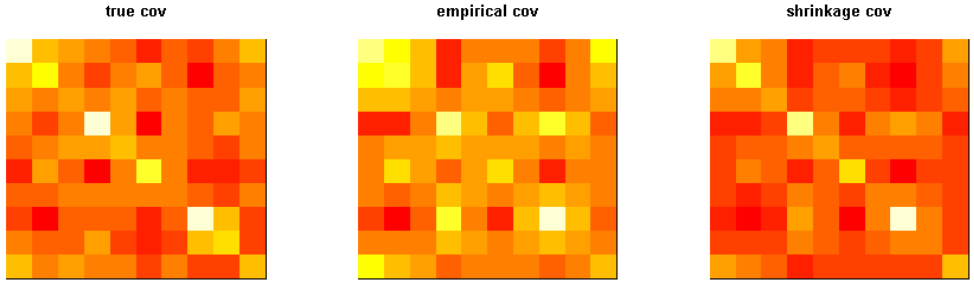
Schäfer, J., and K. Strimmer. 2005. A shrinkage approach to large-scale covariance matrix estimation and implications for functional genomics. Statistical Applications in Genetics and Molecular Biology . 4: 32.

Example Script from corpcor Package

corpcor: Efficient Estimation of Covariance and (Partial) Correlation

```
> library("corpcor")
>
> n <- 6 # try 20, 500
> p <- 10 # try 100, 10
> set.seed(123456)
> # generate random pxp covariance matrix
> sigma <- matrix(rnorm(p * p), ncol = p)
> sigma <- crossprod(sigma) + diag(rep(0.1, p)) #  t(x) %*% x
>
> # simulate multinormal data of sample size n
> sigsvd <- svd(sigma)
> y <- t(sigsvd$v %*% (t(sigsvd$u) * sqrt(sigsvd$d)))
> x <- matrix(rnorm(n * ncol(sigma)), nrow = n) %*% y # problem here! use mvrnorm {MASS}
> # x <- mvrnorm(n, mu=rep(0, p), Sigma=sigma)
> # estimate covariance matrix
> s1 <- cov(x)
> s2 <- cov.shrink(x)
Estimating optimal shrinkage intensity lambda.var (variance vector): 0.4378
Estimating optimal shrinkage intensity lambda (correlation matrix): 0.6494
> par(mfrow=c(1,3))
> image(t(sigma)[,p:1], main="true cov", xaxt="n", yaxt="n")
> image(t(s1)[,p:1], main="empirical cov", xaxt="n", yaxt="n")
> image(t(s2)[,p:1], main="shrinkage cov", xaxt="n", yaxt="n")
>
> # squared error
> sum((s1 - sigma) ^ 2)
[1] 4427.215
> sum((s2 - sigma) ^ 2)
[1] 850.2443
```

mvrnorm {MASS}:
Simulate from a Multivariate Normal Distribution
`mvrnorm(n = 1, mu, Sigma, ...)`



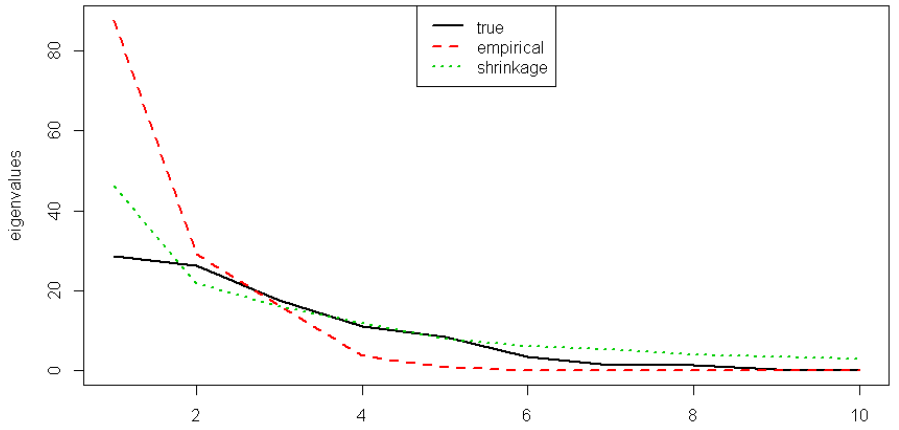
Compare Eigenvalues

```
> # compare positive definiteness
> is.positive.definite(sigma)
[1] TRUE
> is.positive.definite(s1)
[1] FALSE
> is.positive.definite(s2)
[1] TRUE
>
> # compare ranks and condition
> rc <- rbind(
+   data.frame(rank.condition(sigma)),
+   data.frame(rank.condition(s1)),
+   data.frame(rank.condition(s2)))
> rownames(rc) <- c("true", "empirical", "shrinkage")
> rc
          rank condition          tol
true        10 256.35819 6.376444e-14
empirical    5       Inf 1.947290e-13
shrinkage   10  15.31643 1.022819e-13
>
>
>
> # compare eigenvalues
> e0 <- eigen(sigma, symmetric = TRUE)$values
> e1 <- eigen(s1, symmetric = TRUE)$values
> e2 <- eigen(s2, symmetric = TRUE)$values
>
> matplot(data.frame(e0, e1, e2), type = "l", ylab="eigenvalues", lwd=2)
> legend("top", legend=c("true", "empirical", "shrinkage"), lwd=2, lty=1:3, col=1:3)
```

Shrinkage estimation of covariance matrix:

- `cov.shrink {corpcor}`
- `shrinkcovmat.identity {ShrinkCovMat}`
- `covEstimation {RiskPortfolios}`

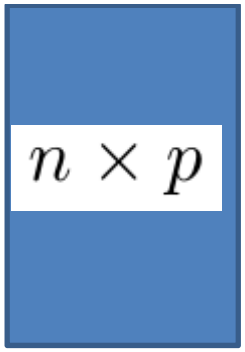
Re-analyze "The breast tumour of van't Veer et al" data by a shrinkage method

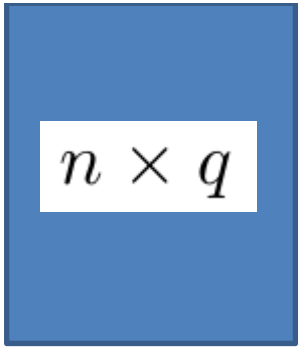


Canonical Correlation Analysis (CCA)

- The main purpose of CCA (Hotelling, 1936) is the exploration of sample correlations between two sets of quantitative variables observed on the same experimental units.

$$X = [X_1, X_2, \cdots, X_p]^T \qquad Y = [Y_1, Y_2, \cdots, Y_q]^T$$





assumed that $p \leq q$

assumed that the columns of X and Y are standardized

Classical CCA assumes first $p \leq n$ and $q \leq n$

$$\begin{aligned}
U_1 = \mathbf{a}_1^T X &= a_{11}X_1 + a_{12}X_2 + \cdots + a_{1p}X_p & V_1 = \mathbf{b}_1^T Y &= b_{11}Y_1 + b_{12}Y_2 + \cdots + b_{1q}Y_q \\
U_2 = \mathbf{a}_2^T X &= a_{21}X_1 + a_{22}X_2 + \cdots + a_{2p}X_p & V_2 = \mathbf{b}_2^T Y &= b_{21}Y_1 + b_{22}Y_2 + \cdots + b_{2q}Y_q \\
&\vdots \quad \vdots & &\vdots \quad \vdots \\
U_p = \mathbf{a}_p^T X &= a_{p1}X_1 + a_{p2}X_2 + \cdots + a_{pp}X_p & V_q = \mathbf{b}_q^T Y &= b_{q1}Y_1 + b_{q2}Y_2 + \cdots + b_{qq}Y_q
\end{aligned}$$

$$\rho_1 = corr(U_1, V_1) = \max corr(\mathbf{a}_1^T X, \mathbf{b}_1^T Y) \text{ subject to } Var(\mathbf{a}_1^T X) = Var(\mathbf{b}_1^T Y) = 1.$$

Mathematical Aspects

$$Corr(U_i, V_i) = \frac{Cov(U_i, V_i)}{\sqrt{Var(U_i)}\sqrt{VarV_i}}, \quad i = 1, 2, \cdots, r = \min(p, q).$$

The first pair canonical variables is defined by $Corr(U_1, V_1) = \rho_1$.

- $\rho_1^2 \geq \rho_2^2 \geq \cdots \geq \rho_r^2$: the eigenvalues of the matrix $\Sigma_{XX}^{-1/2}\Sigma_{XY}\Sigma_{YY}^{-1}\Sigma_{XY}^T\Sigma_{XX}^{-1/2}$.
- Σ_{XX}: the variance-covariance of X.
- Σ_{YY}: the variance-covariance of Y.
- Σ_{XY}: the covariance matrix of the random vector X and Y.
- ρ_1: the first canonical correlation (the square root of the largest eigenvalue).

$$\frac{\mathbf{a}'\mathbf{\Sigma}_{XY}\mathbf{b}}{\sqrt{\mathbf{a}'\mathbf{\Sigma}_X\mathbf{a}}\sqrt{\mathbf{b}'\mathbf{\Sigma}_Y\mathbf{b}}}$$

The second pair canonical variable is $Corr(U_2, V_2) = \rho_2$ and so on.

$$\rho_1 = corr(U_1, V_1) = \max corr(\mathbf{a}_1^T X, \mathbf{b}_1^T Y) \text{ subject to } Var(\mathbf{a}_1^T X) = Var(\mathbf{b}_1^T Y) = 1.$$

Mathematical Aspects

$$\Sigma_{XX} = \operatorname{cov}(X, X) \qquad \Sigma_{YY} = \operatorname{cov}(Y, Y)$$

maximize $$\rho = \frac{a' \Sigma_{XY} b}{\sqrt{a' \Sigma_{XX} a} \sqrt{b' \Sigma_{YY} b}}.$$

define $$c = \Sigma_{XX}^{1/2} a,$$

$$d = \Sigma_{YY}^{1/2} b.$$

$$\rho = \frac{c' \Sigma_{XX}^{-1/2} \Sigma_{XY} \Sigma_{YY}^{-1/2} d}{\sqrt{c'c} \sqrt{d'd}}.$$

By the Cauchy–Schwarz inequality, $\left|\langle \mathbf{u}, \mathbf{v} \rangle\right|^2 \le \langle \mathbf{u}, \mathbf{u} \rangle \cdot \langle \mathbf{v}, \mathbf{v} \rangle,$

$$\left(c' \Sigma_{XX}^{-1/2} \Sigma_{XY} \Sigma_{YY}^{-1/2}\right) d \le \left(c' \Sigma_{XX}^{-1/2} \Sigma_{XY} \Sigma_{YY}^{-1/2} \Sigma_{YY}^{-1/2} \Sigma_{YX} \Sigma_{XX}^{-1/2} c\right)^{1/2} (d'd)^{1/2},$$

$$\rho \le \frac{\left(c' \Sigma_{XX}^{-1/2} \Sigma_{XY} \Sigma_{YY}^{-1} \Sigma_{YX} \Sigma_{XX}^{-1/2} c\right)^{1/2}}{(c'c)^{1/2}}.$$

https://en.wikipedia.org/wiki/Canonical_correlation

Mathematical Aspects

$$\rho \leq \frac{\left(c' \Sigma_{XX}^{-1/2} \Sigma_{XY} \Sigma_{YY}^{-1} \Sigma_{YX} \Sigma_{XX}^{-1/2} c\right)^{1/2}}{(c'c)^{1/2}}.$$

There is equality if the vectors d and $\Sigma_{YY}^{-1/2} \Sigma_{YX} \Sigma_{XX}^{-1/2} c$ are collinear.

c is an eigenvector of $\Sigma_{XX}^{-1/2} \Sigma_{XY} \Sigma_{YY}^{-1} \Sigma_{YX} \Sigma_{XX}^{-1/2}$

d is an eigenvector of $\Sigma_{YY}^{-1/2} \Sigma_{YX} \Sigma_{XX}^{-1} \Sigma_{XY} \Sigma_{YY}^{-1/2}$

- a is an eigenvector of $\Sigma_{XX}^{-1} \Sigma_{XY} \Sigma_{YY}^{-1} \Sigma_{YX}$
- b is an eigenvector of $\Sigma_{YY}^{-1} \Sigma_{YX} \Sigma_{XX}^{-1} \Sigma_{XY}$

$$c = \Sigma_{XX}^{1/2} a,$$

$$d = \Sigma_{YY}^{1/2} b.$$

The canonical variables are defined by:

$$U = c' \Sigma_{XX}^{-1/2} X = a' X$$

$$V = d' \Sigma_{YY}^{-1/2} Y = b' Y$$

https://en.wikipedia.org/wiki/Canonical_correlation

LifeCycleSavings {datasets}: Intercountry Life-Cycle Savings Ratio Data

- Under the life-cycle savings hypothesis as developed by Franco Modigliani, the savings ratio (aggregate personal saving divided by disposable income (可支配收入)) is explained by per-capita disposable income (平均每人可支配所得), the percentage rate of change in per-capita disposable income, and two demographic variables: the percentage of population less than 15 years old and the percentage of the population over 75 years old. The data are averaged over the decade 1960–1970 to remove the business cycle or other short-term fluctuations.

A data frame with 50 observations on 5 variables.
[,1] sr : aggregate personal savings
[,2] pop15: % of population under 15
[,3] pop75: % of population over 75
[,4] dpi: real per-capita disposable income
[,5] ddpi: % growth rate of dpi

```
> head(LifeCycleSavings)
             sr pop15 pop75     dpi ddpi
Australia 11.43 29.35  2.87 2329.68 2.87
Austria   12.07 23.32  4.41 1507.99 3.93
Belgium   13.17 23.80  4.43 2108.47 3.82
Bolivia    5.75 41.89  1.67  189.13 0.22
Brazil    12.88 42.19  0.83  728.47 4.56
Canada     8.79 31.72  2.85 2982.88 2.43
> pop <- LifeCycleSavings[, 2:3]
> oec <- LifeCycleSavings[, -(2:3)]
```

```
> cancor(pop, oec)
$cor
[1] 0.8247966112 0.3652761515

$xcoef
                 [,1]           [,2]
pop15 -0.009110856229 -0.03622206049
pop75  0.048647513750 -0.26031158157

$ycoef
            [,1]           [,2]           [,3]
sr   0.00847102  0.0333793558 -0.00515712977
dpi  0.00013073 -0.0000758823  0.00000454370
ddpi 0.00417059 -0.0122678964  0.05188323606

$xcenter
  pop15   pop75
35.0896  2.2930

$ycenter
       sr       dpi      ddpi
   9.6710 1106.7584    3.7576
```

Regularized CCA

- CCA cannot be performed when the $n \leq \max(p, q)$).
- When the number of variables increases, greatest canonical correlations are nearly 1 because of recovering of canonical subspaces that do not provide any meaningful information.
- A standard condition usually advocated for CCA (Eaton and Perlman 1973) is $n \geq p + q + 1$.
- A regularization step in the data processing (Bickel and Li 2006) to perform a regularized canonical correlation analysis (RCCA).

S_{XX} and S_{YY} are replaced respectively by $\Sigma_{XX}(\lambda_1)$ and $\Sigma_{YY}(\lambda_2)$ defined by

$$\Sigma_{XX}(\lambda_1) = S_{XX} + \lambda_1 I_p \quad \text{and} \quad \Sigma_{YY}(\lambda_2) = S_{YY} + \lambda_2 I_q.$$

How to get the "good" values for the regularization parameters?

Bickel PJ, Li B (2006). "Regularization in Statistics." Sociedad de Estadistica e Investigacion Operativa, Test, 15(2), 271–344.

Cross-validation for tuning regularization parameters

- Denote $\alpha = (\alpha_1, \alpha_2)$. For a given value of α, do $i = 1, \cdots, n$:
  - $\rho_\alpha^{(-i)}$: the first canonical correlation computed from the units with rows X^i and Y^i removed.
  - $\mathbf{a}_\alpha^{(-i)}$ and $\mathbf{b}_\alpha^{(-i)}$: the first canonical variates vectors.

$$\Sigma_{XX}(\alpha_1) = S_{XX} + \alpha_1 \mathbf{I}_p$$

$$\Sigma_{YY}(\alpha_2) = S_{YY} + \alpha_2 \mathbf{I}_q$$

- Obtain n pairs of vectors

$$(\mathbf{a}_\alpha^{(-1)}, \mathbf{b}_\alpha^{(-1)}), \cdots, (\mathbf{a}_\alpha^{(-n)}, \mathbf{b}_\alpha^{(-n)}).$$

- The leave-one-out cross validation score for $\alpha = (\alpha_1, \alpha_2)$ is then defined by Leurgans et al. (1993):

$$CV(\alpha_1, \alpha_2) = corr(\{(\mathbf{a}_\alpha^{(-i)})^T X^i\}_{i=1}^n, \{(\mathbf{b}_\alpha^{(-i)})^T Y^i\}_{i=1}^n).$$

- Choose the value of α_1 and α_2 that maximizes this correlation:

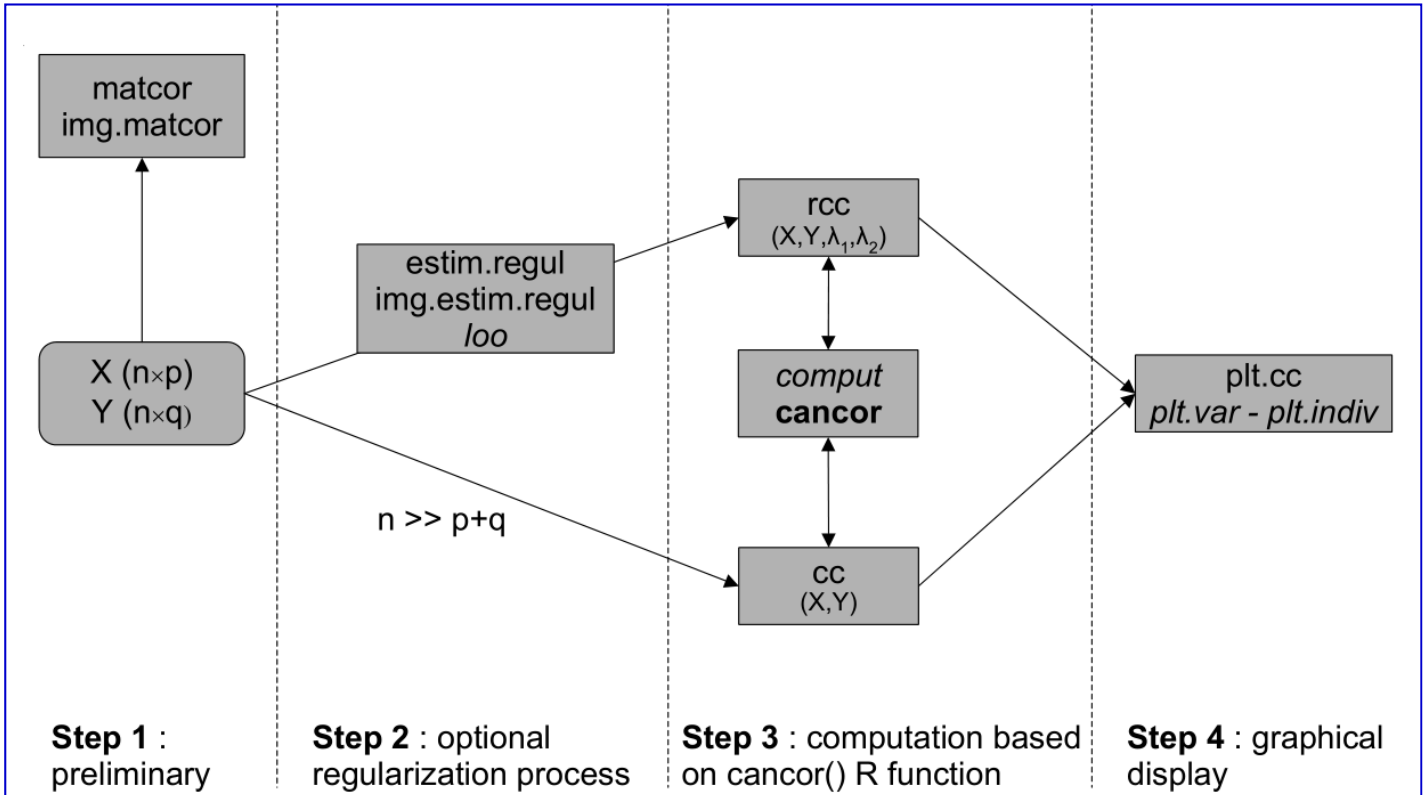
$$\hat{\alpha} = (\hat{\alpha_1}, \hat{\alpha_2}) = \arg\max_{\alpha_1, \alpha_2} CV(\alpha_1, \alpha_2).$$

Ignacio González, Sébastien Déjean, Pascal G. P. Martin, Alain Baccini, 2008, CCA: An R Package to Extend Canonical Correlation Analysis, Journal of Statistical Software, Vol 23, Issue 12.

- Note that $\hat{\alpha_1}$ and $\hat{\alpha_2}$ are chosen with respect to the first canonical variates and are then fixed for higher order canonical variates.

Two tuning parameters in the regularized CCA,
so the CV is performed on a 2D surface.
(1) Directly searching for a maximum on the 2D parameter surface. or
(2) A relatively small grid of reasonable values for α_1 and α_2.

CCA: An R Package to Extend Canonical Correlation Analysis



Schematic view of the canonical correlation analysis process using **CCA**.

Ignacio González, Sébastien Déjean, Pascal G. P. Martin, Alain Baccini, 2008, CCA: An R Package to Extend Canonical Correlation Analysis, Journal of Statistical Software, Vol 23, Issue 12.

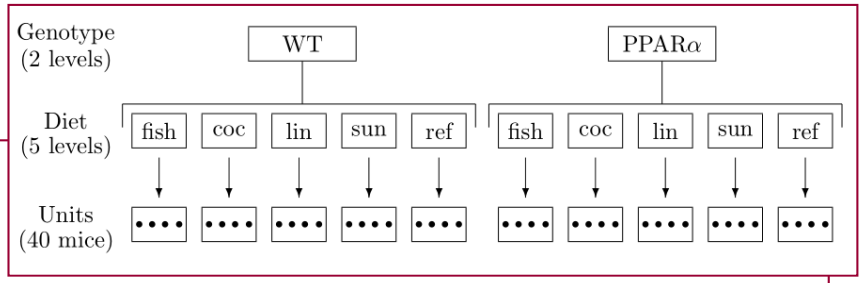
nutrimouse {CCA}: a Nutrition Study in the Mouse

Two sets of variables were measured on 40 mice:

- gene (40 x 120): expressions of 120 genes measured in liver cells potentially involved in nutritional problems.
- lipid (40 x 21): concentrations of 21 hepatic fatty acids (肝脂肪酸).

The 40 mice were distributed in a 2-factors experimental design (4 replicates):

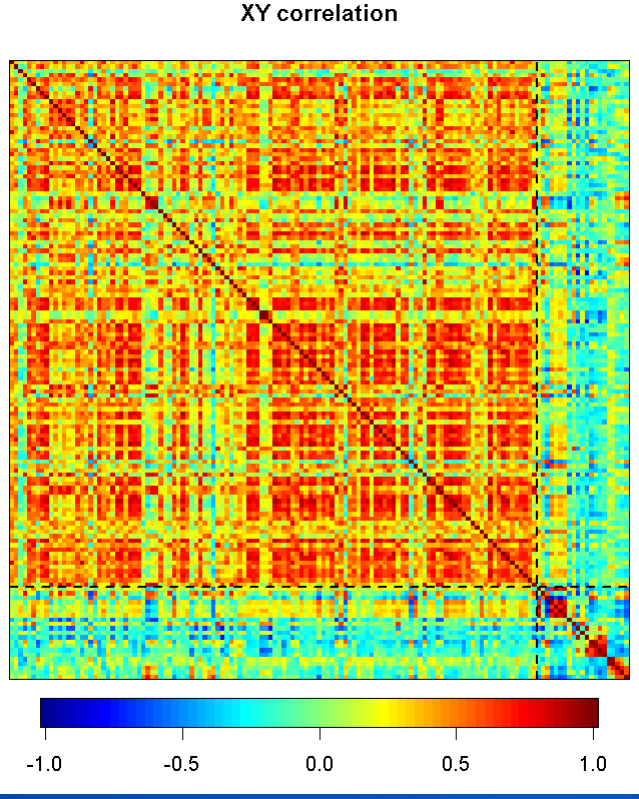
- genotype (2-levels factor): wild-type and PPARalpha -/-
- diet (5-levels factor): Oils used

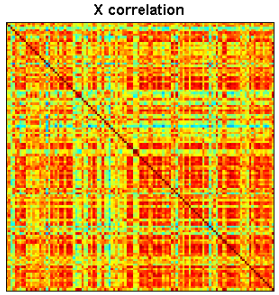


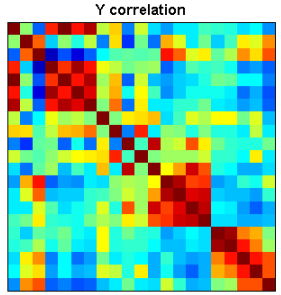

```
> library(CCA)
> data(nutrimouse)
> str(nutrimouse)
List of 4
 $ gene    :'data.frame':        40 obs. of  120 variables:
  ..$ X36b4    : num [1:40] -0.42 -0.44 -0.48 -0.45 -0.42 -0.43 -0.53 -0.49 -0.36 -0.5 ...
...
  ..$ Tpbeta   : num [1:40] -1.11 -1.09 -1.14 -1.04 -1.2 -1.05 -1 -1.16 -0.91 -1.07 ...
  .. [list output truncated]
 $ lipid   :'data.frame':        40 obs. of  21 variables:
  ..$ C14.0    : num [1:40] 0.34 0.38 0.36 0.22 0.37 1.7 0.35 0.34 0.22 1.38 ...
...
  ..$ C22.6n.3: num [1:40] 10.39 2.61 2.51 14.99 6.69 ...
 $ diet    : Factor w/ 5 levels "coc","fish","lin",..: 3 5 5 2 4 1 3 3 2 1 ...
 $ genotype: Factor w/ 2 levels "wt","ppar": 1 1 1 1 1 1 1 1 1 1 ...
>
> table(nutrimouse$genotype, nutrimouse$diet)

      coc fish lin ref sun
  wt    4    4   4   4   4
  ppar  4    4   4   4   4
```

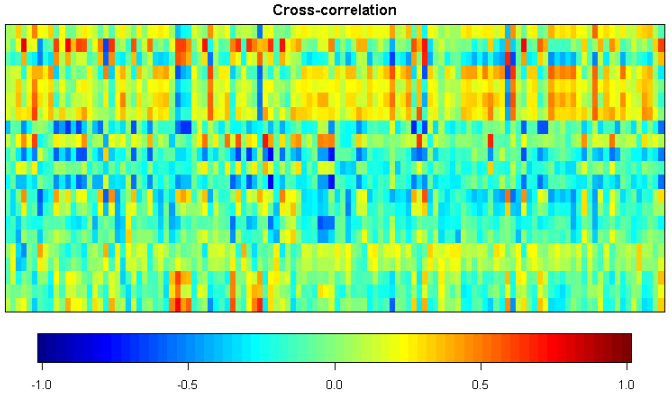
Visualizing the Correlation Matrices

```
> # convert the data into the matrix format before performing CCA.
> X <- as.matrix(nutrimouse$gene)
> Y <- as.matrix(nutrimouse$lipid)
> correl <- matcor(X, Y)
> img.matcor(correl)
> img.matcor(correl, type = 2)
> str(correl)
List of 3
 $ Xcor : num [1:120, 1:120] 1 0.328 0.107 0.262 0.491 ...
  ..- attr(*, "dimnames")=List of 2
  .. ..$ : chr [1:120] "X36b4" "ACAT1" "ACAT2" "ACBP" ...
  .. ..$ : chr [1:120]                                  .
 $ Ycor : num [1:21, 1                                 97
  ..- attr(*, "dimname                                  .
  .. ..$ : chr [1:21]                                   .
  .. ..$ : chr [1:21]                                   ..
 $ XYcor: num [1:141,                                   .
  ..- attr(*, "dimname                                  .
  .. ..$ : chr [1:141]
  .. ..$ : chr [1:141]
```



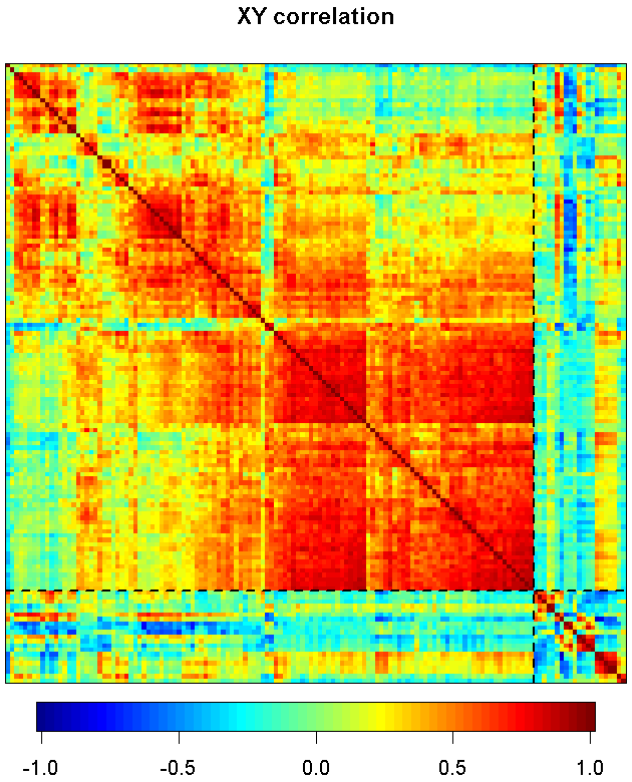


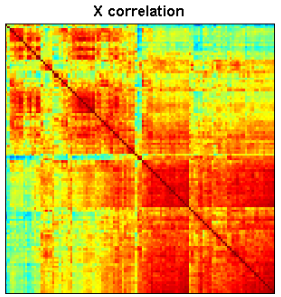


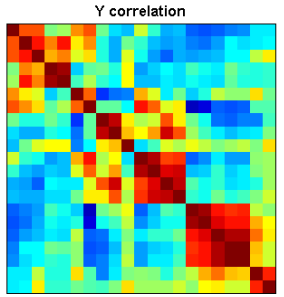


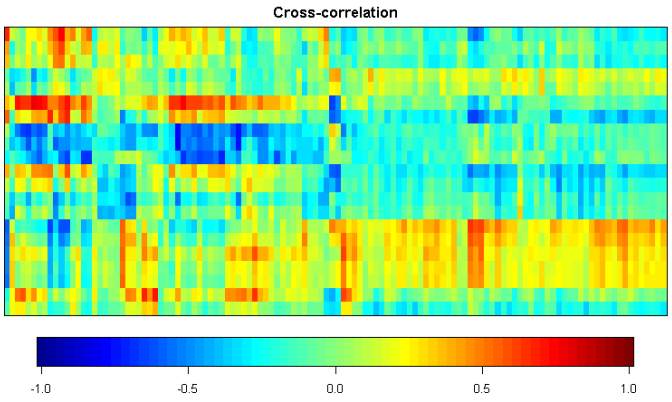
Visualizing the Correlation Matrices

```
> x.hm <- heatmap(correl$Xcor)
> y.hm <- heatmap(correl$Ycor)
> ordering <- c(x.hm$rowInd, y.hm$rowInd + 120)
> correl.2 <- list(Xcor=correl$Xcor[x.hm$rowInd, x.hm$rowInd],
+                  Ycor=correl$Ycor[y.hm$rowInd, y.hm$rowInd],
+                  XYcor=correl$XYcor[ordering, ordering])
> img.matcor(correl.2)
> img.matcor(correl.2, type = 2)
```



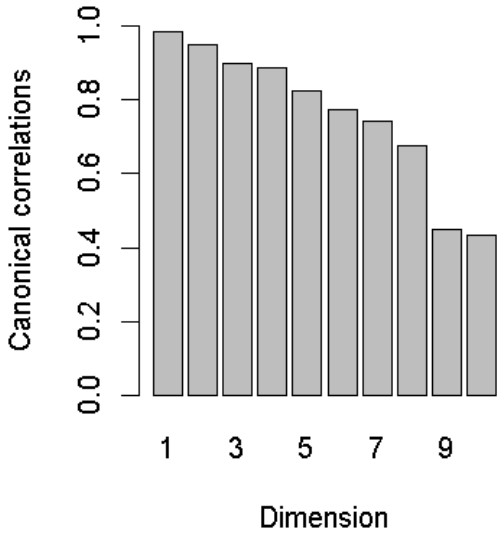


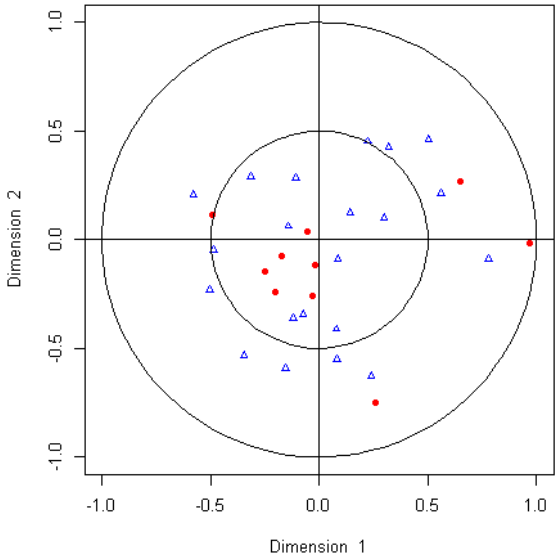


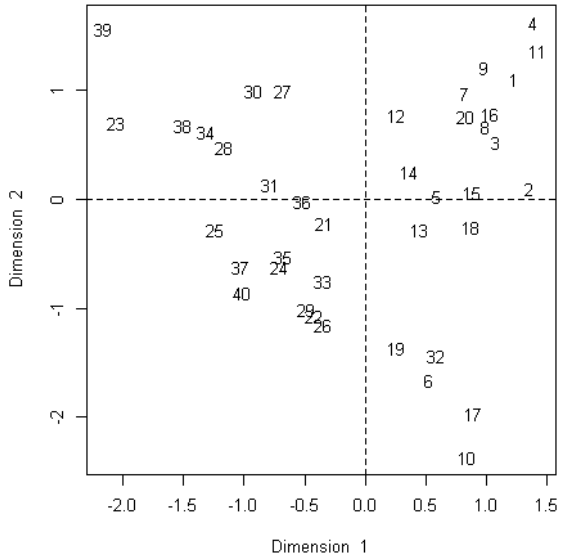


Classical CCA

```
> X.subset <- as.matrix(nutrimouse$gene[, sample(1:120, size = 10)])
> my.cca <- cc(X.subset, Y)
> barplot(my.cca$cor, xlab="Dimension",
+         ylab="Canonical correlations",
+         names.arg=1:10, ylim=c(0,1))
> plt.cc(my.cca)
> names(my.cca)
[1] "cor"    "names"  "xcoef"  "ycoef"  "scores"
> my.cca$cor
 [1] 0.9851407 0.9494411 0.8996597 0.8882256 0.8228657 0.7720856 0.7430616 0.6739105 0.4497435
[10] 0.4339681
```





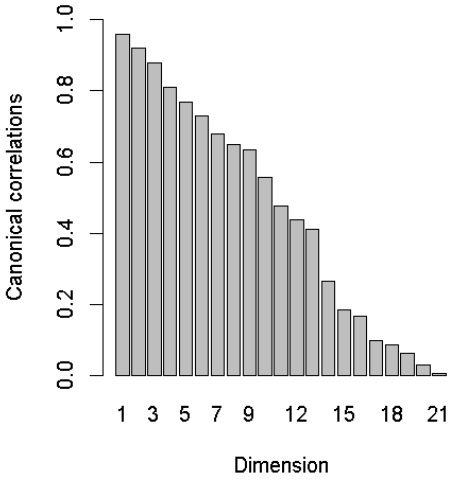


Regularized CCA

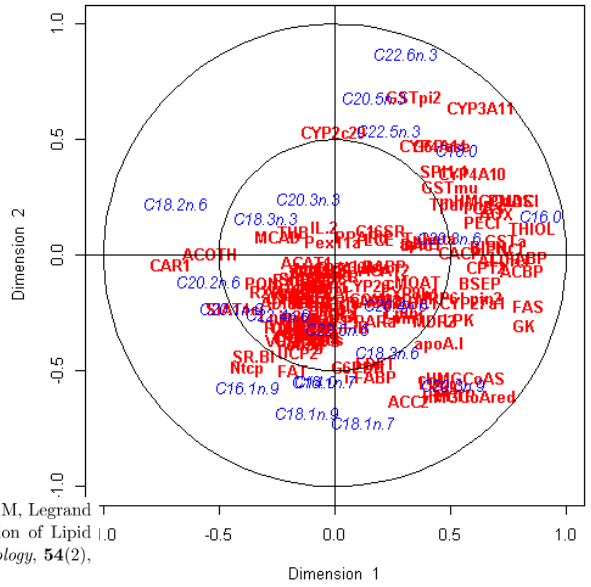
```
> regul.par <- estim.regul(X, Y, plt = TRUE,
+                          grid1 = seq(0.0001, 0.01, l=5), # l=50
+                          grid2 = seq(0, 0.1, l=5)) # l=50
  lambda1 =  0.01
  lambda2 =  0.075
 CV-score =  0.884716
> my.rcca <- rcc(X, Y, regul.par$lambda1, regul.par$lambda2)
> names(my.rcca)
[1] "cor"    "names"  "xcoef"  "ycoef"  "scores"
> barplot(my.rcca$cor, xlab = "Dimension",
+         ylab = "Canonical correlations", names.arg = 1:21, ylim = c(0,1))
> plt.cc(my.rcca, var.label = TRUE,
+        ind.names = paste(nutrimouse$genotype, nutrimouse$diet, sep = "."))
```

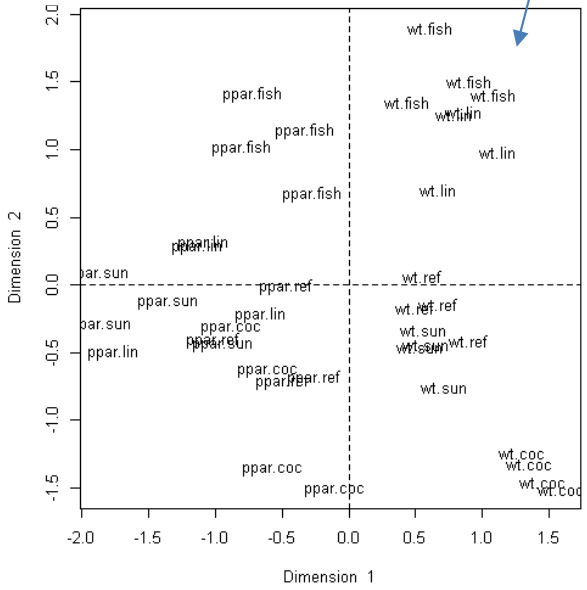
```
> names(my.rcca$scores)
[1] "xscores"       "yscores"       "corr.X.xscores"
[4] "corr.Y.xscores" "corr.X.yscores" "corr.Y.yscores"
```

```
my.rcca$scores$xscores[,1:2]
```



Variables (on the left) and units (on the right) representations on the plane defined by the first two canonical variates.





Martin PG, Guillou H, Lasserre F, Déjean S, Lan A, Pascussi JM, SanCristobal M, Legrand P, Besse P, Pineau T (2007). "Novel Aspects of PPARα-mediated Regulation of Lipid and Xenobiotic Metabolism Revealed through a Nutrigenomic Study." *Hepatology*, **54**(2), 767–777.

plt.cc

```
> plt.cc
function (res, d1 = 1, d2 = 2, int = 0.5, type = "b", ind.names = NULL,
    var.label = FALSE, Xnames = NULL, Ynames = NULL)
{
    par(mfrow = c(1, 1), pty = "s")
    if (type == "v")
        plt.var(res, d1, d2, int, var.label, Xnames, Ynames)
    if (type == "i")
        plt.indiv(res, d1, d2, ind.names)
    if (type == "b") {
        def.par <- par(no.readonly = TRUE)
        layout(matrix(c(0, 0, 1, 2, 0, 0), ncol = 2, nrow = 3,
            byrow = TRUE), widths = 1, heights = c(0.1, 1, 0.1))
        par(pty = "s", mar = c(4, 4.5, 0, 1))
        plt.var(res, d1, d2, int, var.label, Xnames, Ynames)
        plt.indiv(res, d1, d2, ind.names)
        par(def.par)
    }
}
<environment: namespace:CCA>
```

```
> plt.var
function (res, d1, d2, int = 0.5, var.label = FALSE, Xnames = NULL,
    Ynames = NULL)
{
    if (!var.label) {
        plot(0, type = "n", xlim = c(-1, 1), ylim = c(-1, 1),
            xlab = paste("Dimension ", d1), ylab = paste("Dimension ",
                d2))
        points(res$scores$corr.X.xscores[, d1], res$scores$corr.X.xscores[,
            d2], pch = 20, cex = 1.2, col = "red")
        points(res$scores$corr.Y.xscores[, d1], res$scores$corr.Y.xscores[,
            d2], pch = 24, cex = 0.7, col = "blue")
    }
    else {
        if (is.null(Xnames))
            Xnames = res$names$Xnames
        if (is.null(Ynames))
            Ynames = res$names$Ynames
        plot(0, type = "n", xlim = c(-1, 1), ylim = c(-1, 1),
            xlab = paste("Dimension ", d1), ylab = paste("Dimension ",
                d2))
        text(res$scores$corr.X.xscores[, d1], res$scores$corr.X.xscores[,
            d2], Xnames, col = "red", font = 2)
        text(res$scores$corr.Y.xscores[, d1], res$scores$corr.Y.xscores[,
            d2], Ynames, col = "blue", font = 3)
    }
    abline(v = 0, h = 0)
    lines(cos(seq(0, 2 * pi, l = 100)), sin(seq(0, 2 * pi, l = 100)))
    lines(int * cos(seq(0, 2 * pi, l = 100)), int * sin(seq(0,
        2 * pi, l = 100)))
}
<environment: namespace:CCA>
```

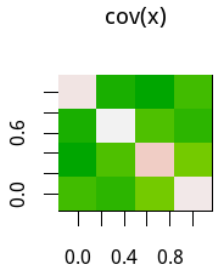
```
> plt.indiv
function (res, d1, d2, ind.names = NULL)
{
    if (is.null(ind.names))
        ind.names = res$names$ind.names
    if (is.null(ind.names))
        ind.names = 1:nrow(res$scores$xscores)
    plot(res$scores$xscores[, d1], res$scores$xscores[, d2],
        type = "n", main = "", xlab = paste("Dimension ", d1),
        ylab = paste("Dimension ", d2))
    text(res$scores$xscores[, d1], res$scores$xscores[, d2],
        ind.names)
    abline(v = 0, h = 0, lty = 2)
}
<environment: namespace:CCA>
```

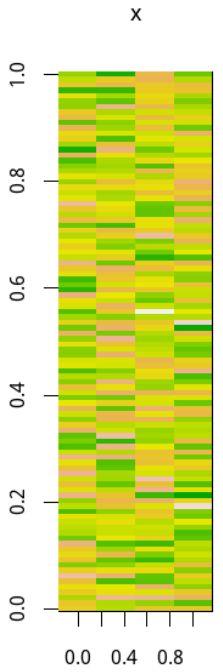
Check Data and its Covariance

```
> library("corpcor")
> options(digits=4)
>
> test <- function(x, s){
+   image(t(s)[,nrow(s):1], main="cov(x)", col=terrain.colors(100))
+   image(t(x)[,nrow(x):1], main="x", col=terrain.colors(100))
+   cat("is.positive.definite:", is.positive.definite(s), "\n")
+   cat("eigen:\n")
+   print(eigen(s))
+   cat("inverse:\n")
+   print(solve(s))
+ }
>
> layout(matrix(1:2, ncol=1), height=c(1,2))
> # set 1: regular data
> n <- 100
> p <- 4
> x1 <- matrix(rnorm(n*p), ncol=p)
> summary(x1)
       V1                 V2                 V3                 V4
 Min.   :-2.4964   Min.   :-2.5184   Min.   :-2.182   Min.   :-2.9044
 1st Qu.:-0.7516   1st Qu.:-0.5753   1st Qu.:-0.393   1st Qu.:-0.7751
 Median : 0.0941   Median : 0.0726   Median : 0.221   Median :-0.0412
 Mean   : 0.0382   Mean   : 0.1075   Mean   : 0.167   Mean   : 0.0181
 3rd Qu.: 0.6850   3rd Qu.: 0.9046   3rd Qu.: 0.770   3rd Qu.: 0.7272
 Max.   : 2.3993   Max.   : 2.3687   Max.   : 3.369   Max.   : 3.0475
```

Check Data and its Covariance

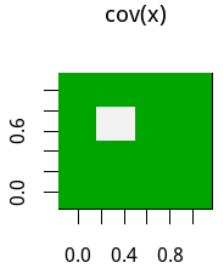
```
> s1 <- cov(x1)
> test(x1, s1)
is.positive.definite: TRUE
eigen:
$values
[1] 1.4157 1.2531 1.0118 0.7773

$vectors
        [,1]    [,2]    [,3]     [,4]
[1,]  0.6637  0.1010  0.4884  0.55746
[2,] -0.4384 -0.5896  0.6775  0.03517
[3,] -0.5707  0.3055 -0.1423  0.74879
[4,] -0.2040  0.7408  0.5313 -0.35681

inverse:
         [,1]     [,2]     [,3]     [,4]
[1,]  0.95483  0.09922  0.22535 -0.03536
[2,]  0.09922  0.86835 -0.02841  0.05419
[3,]  0.22535 -0.02841  1.04587 -0.15555
[4,] -0.03536  0.05419 -0.15555  0.91009
```

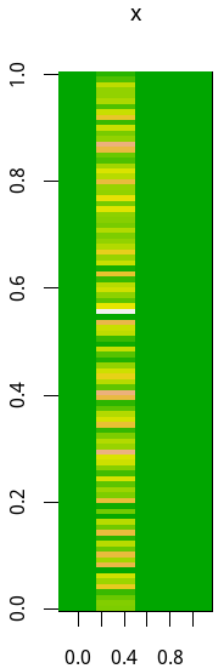




Check Data and its Covariance

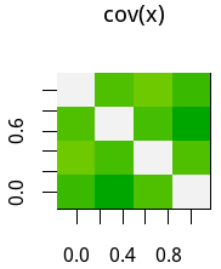
```
> # set 2: add some outlier variables
> x2 <- matrix(rnorm(n*p, sd=0.0001), ncol=p)
> id <- sample(1:p, floor(p/3))
> x2[, id] <- x2[, id] + abs(rnorm(n*length(id), m=10000, sd=5000))
> summary(x2)
       V1                    V2             V3                    V4
 Min.   :-0.00019325   Min.   :  318   Min.   :-0.0002198   Min.   :-0.00026808
 1st Qu.:-0.00004618   1st Qu.: 7273   1st Qu.:-0.0000667   1st Qu.:-0.00007213
 Median :-0.00000283   Median : 9900   Median : 0.0000107   Median : 0.00000007
 Mean   : 0.00000367   Mean   :10201   Mean   : 0.0000103   Mean   : 0.00000063
 3rd Qu.: 0.00005736   3rd Qu.:12617   3rd Qu.: 0.0000998   3rd Qu.: 0.00007487
 Max.   : 0.00021909   Max.   :27439   Max.   : 0.0003177   Max.   : 0.00027794
> s2 <- cov(x2)
> test(x2, s2)
is.positive.definite: FALSE
eigen:
$values
[1] 25301262.378715548664        0.000000012360        0.000000010255        0.000000007

$vectors
                 [,1]             [,2]            [,3]             [,4]
[1,] -0.0000000006300 -0.2198484423160 -0.123788454460  0.9676482216971
[2,] -1.0000000000000 -0.0000000004066  0.000000004536 -0.0000000001631
[3,] -0.0000000002447 -0.9600601615329 -0.148515578779 -0.2371236156468
[4,]  0.0000000045072 -0.1730640015964  0.981131765566  0.0861934449310

inverse:
                [,1]           [,2]            [,3]          [,4]
[1,] 133713761.94777 -0.06915255563 -12572701.82036  2664291.0791
[2,]        -0.06915  0.00000004155        -0.02882        0.4378
[3,] -12572701.82036 -0.02881648352  84429162.38724 -3566776.2275
[4,]   2664291.07907  0.43778259944  -3566776.22748 97309029.4158
```

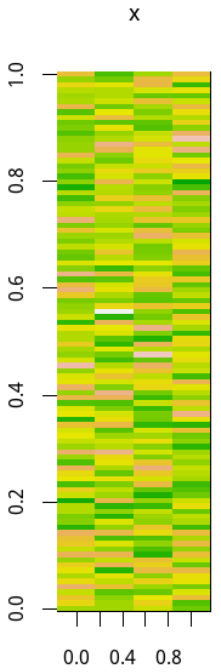




Check Data and its Covariance

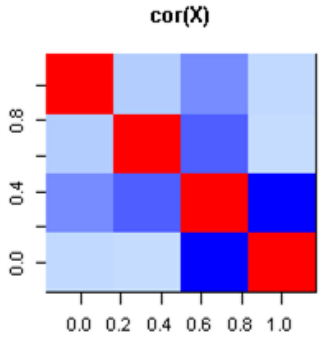
```
> # set 3: do the scaling
> x3 <- scale(x2)
> s3 <- cov(x3)
> test(x3, s3)
is.positive.definite: TRUE
eigen:
$values
[1] 1.2270 1.1165 0.8797 0.7768

$vectors
         [,1]     [,2]     [,3]     [,4]
[1,]  0.21350  0.66557  0.71239  0.06273
[2,]  0.69471 -0.06814 -0.20495  0.68610
[3,]  0.04397  0.71997 -0.67057 -0.17333
[4,] -0.68547  0.18442 -0.02884  0.70377

inverse:
         [,1]     [,2]     [,3]     [,4]
[1,]  1.01590 -0.03032 -0.12020  0.02415
[2,] -0.03032  1.05120 -0.01590  0.22895
[3,] -0.12020 -0.01590  1.01571 -0.04068
[4,]  0.02415  0.22895 -0.04068  1.05192
```

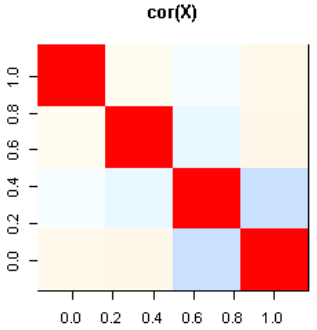


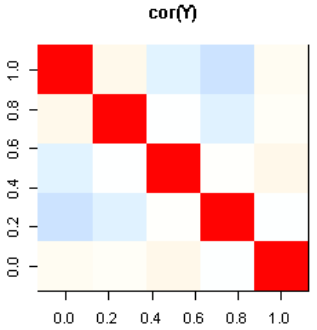


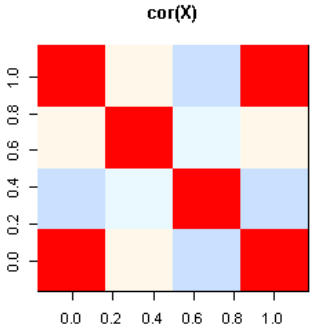
Some Columns are Linear Dependent

```
> library(fields); library("corpcor"); library(CCA)
> cor.col <- two.colors(start="blue", middle="white",
                        end="red") # length=255
> par(mfrow=c(3,1))
> n <- 100
> p <- 4
> q <- 5
> set.seed(12345)
> X <- matrix(rnorm(n*p), ncol=p); rX <- cor(X)
> range.col <- floor((1+range(rX))*127+1)
> # wrong: image(t(cor(Y))[,q:1], main="cor(Y)", col=cor.col)
> image(t(rX)[,p:1], main="cor(X)", col=cor.col[range.col[1]: range.col[2]])
> is.positive.definite(cov(X))
[1] TRUE
> Y <- matrix(rnorm(n*q), ncol=q); rY <- cor(Y)
> range.col <- floor((1+range(rY))*127+1)
> image(t(rY)[,q:1], main="cor(Y)", col=cor.col[range.col[1]: range.col[2]])
> is.positive.definite(cov(Y))
[1] TRUE
> xy.cca <- cc(X, Y)
>
> X[,1] <- 3*X[,4] + 1; rX <- cor(X)
> range.col <- floor((1+range(rX))*127+1)
> image(t(rX)[,p:1], main="cor(X)", col=cor.col[range.col[1]: range.col[2]])
> xy.cca <- cc(X, Y)
Error in chol.default(Bmat) :
  the leading minor of order 4 is not positive definite
> is.positive.definite(cov(X))
[1] FALSE
```









DR Quality Assessment: local continuity meta-criterion

$$\mathcal{N}^D_{K'}(i) = \{j_1, \ldots, j_{K'}\} \qquad K'\text{-NNs with regard to } D_{i,j}$$

$$\mathcal{N}^X_{K'}(i) = \{k_1, \ldots, k_{K'}\} \qquad K'\text{-NNs with regard to } \|\mathbf{x}_i - \mathbf{x}_k\| \text{ (excluding } i\text{)}.$$

$$N_{K'}(i) = \left|\mathcal{N}^D_{K'}(i) \cap \mathcal{N}^X_{K'}(i)\right|, \quad N_{K'} = \frac{1}{N}\sum_{i=1}^{N} N_{K'}(i).$$

normalize overlap to the [0, 1] interval: $M_{K'} = \frac{1}{K'} N_{K'}$

adjusted LC meta-criteria (Chen 2006) $M^{\text{adj}}_{K'} = M_{K'} - \frac{K'}{N-1}$.

Lee, J.A., Lee, J.A., Verleysen, M., 2009. Quality assessment of dimensionality reduction: Rank-based criteria. Neurocomputing 72.
Chen, L., Buja, A., 2009. Local Multidimensional Scaling for Nonlinear Dimension Reduction, Graph Layout and Proximity Analysis，JASA 104(485), 209-219.

Co-ranking Matrix and LCMC

```
my.coranking <- function(X.high, X.low){
  # X.high <- iris[1:10,1:4]
  # X.low <- princomp(X.high)$score[,1:2]

  D.high <- as.matrix(dist(X.high))
  D.low <- as.matrix(dist(X.low))
  f <- function(x){
     rank(x, ties.method = 'first', na.last = FALSE)
  }
  diag(D.high) <- NA # NA is rank 1
  diag(D.low) <- NA
  R.high <- apply(D.high, 1, f)
  R.low <- apply(D.low, 1, f)
  table(R.high, R.low)[-1, -1]

}
```

```
> LCMC
function (Q, K = 1:nrow(Q))
{
...
    nQ <- nrow(Q)
    nK <- length(K)
    N <- nQ + 1
    if (nK < 0.2 * nQ) {
        lcmc <- numeric(nK)
        for (i in 1:nK) {
            k <- K[i]
            lcmc[i] <- k/(1 - N) + sum(Q[cm.UL_K(k, nQ)])/N/k
        }
    }
    else {
        lcmc_ <- diag(apply(apply(Q, 2, cumsum), 1, cumsum))/(1:nQ)/N - (1:nQ)/nQ
        lcmc <- lcmc_[K]
    }
    lcmc
}
<environment: namespace:coRanking>
```

The *co-ranking matrix* [23] can then be defined as

$$\mathbf{Q} = [q_{kl}]_{1 \leqslant k,l \leqslant N-1} \quad \text{with} \quad q_{kl} = |\{(i,j) : \rho_{ij} = k \text{ and } r_{ij} = l\}|.$$

coRanking: Co-Ranking Matrix

Calculate the co-ranking matrix to assess the quality of a diminsionality reduction.

```
coranking(Xi, X, input = c("data", "dist", "rank"), use = "C")
```

Arguments

`Xi`: high dimensional data

`X`: low dimensional data

`input`: type of input

Plots the co-ranking matrix nicely

```
imageplot(Q, lwd = 2, bty = "n", main = "co-ranking matrix",
xlab = expression(R), ylab = expression(Ro),
col = colorRampPalette(colors = c("gray85", "red", "yellow",
"green", "blue"))(100), axes = FALSE, legend = TRUE, ...)
```

Calculate the local continuity meta-criterion from a co-ranking matrix.

```
LCMC(Q, K = 1:nrow(Q))
```

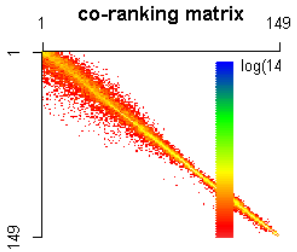
Arguments

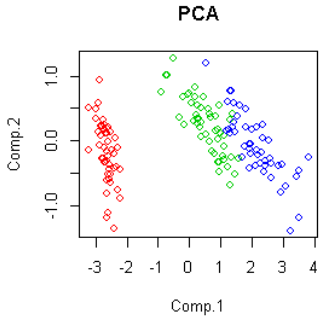
`Q`: a co-ranking matrix

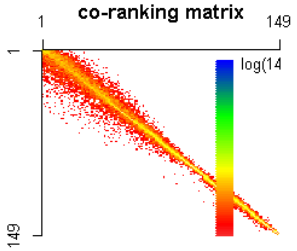
`K`: vector of integers describing neighborhood size

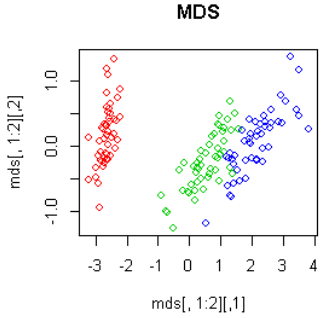
Example

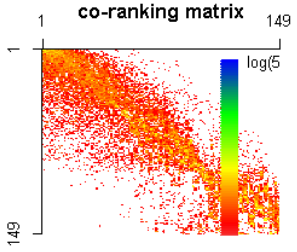
```
> library(coRanking) # install.packages("coRanking")
> library(MASS)
> par(mfrow=c(2, 3))
> x <- iris[,1:4]
> y <- iris[,5]
> pca <- princomp(x)
> Q.pca <- coranking(x, pca$score[,1:2], input = "data")
> imageplot(Q.pca)
> lcmc.pca <- LCMC(Q.pca, K = 5:10)
>
> mds <- cmdscale(dist(x))
> Q.mds <- coranking(x, mds[,1:2], input = "data")
> imageplot(Q.mds)
> lcmc.mds <- LCMC(Q.pca, K = 5:10)
>
> mylda <- lda(x, grouping=y)
> lda.dim <- as.matrix(x)%*%mylda$scaling[,1:2]
> Q.lda <- coranking(x, lda.dim, input = "data")
> imageplot(Q.lda)
> lcmc.lda <- LCMC(Q.lda, K = 5:10)
>
> names(lcmc.pca) <- paste0("K=", 5:10)
> rbind(lcmc.pca, lcmc.mds, lcmc.lda)
              K=5       K=6       K=7       K=8       K=9
lcmc.pca 0.6077763 0.6108427 0.6292106 0.6521421 0.6581158
lcmc.mds 0.6077763 0.6108427 0.6292106 0.6521421 0.6581158
lcmc.lda 0.3171096 0.3286204 0.3396868 0.3638087 0.3781158
> plot(pca$score[,1:2], col=as.integer(y)+1, main="PCA")
> plot(mds[,1:2], col=as.integer(y)+1, main="MDS")
> plot(lda.dim[,1:2], col=as.integer(y)+1, main="LDA")
```

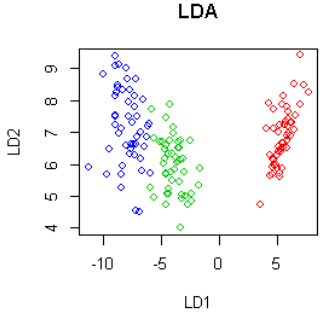












Evaluate DR by Classification (n>>p) UCI Datasets

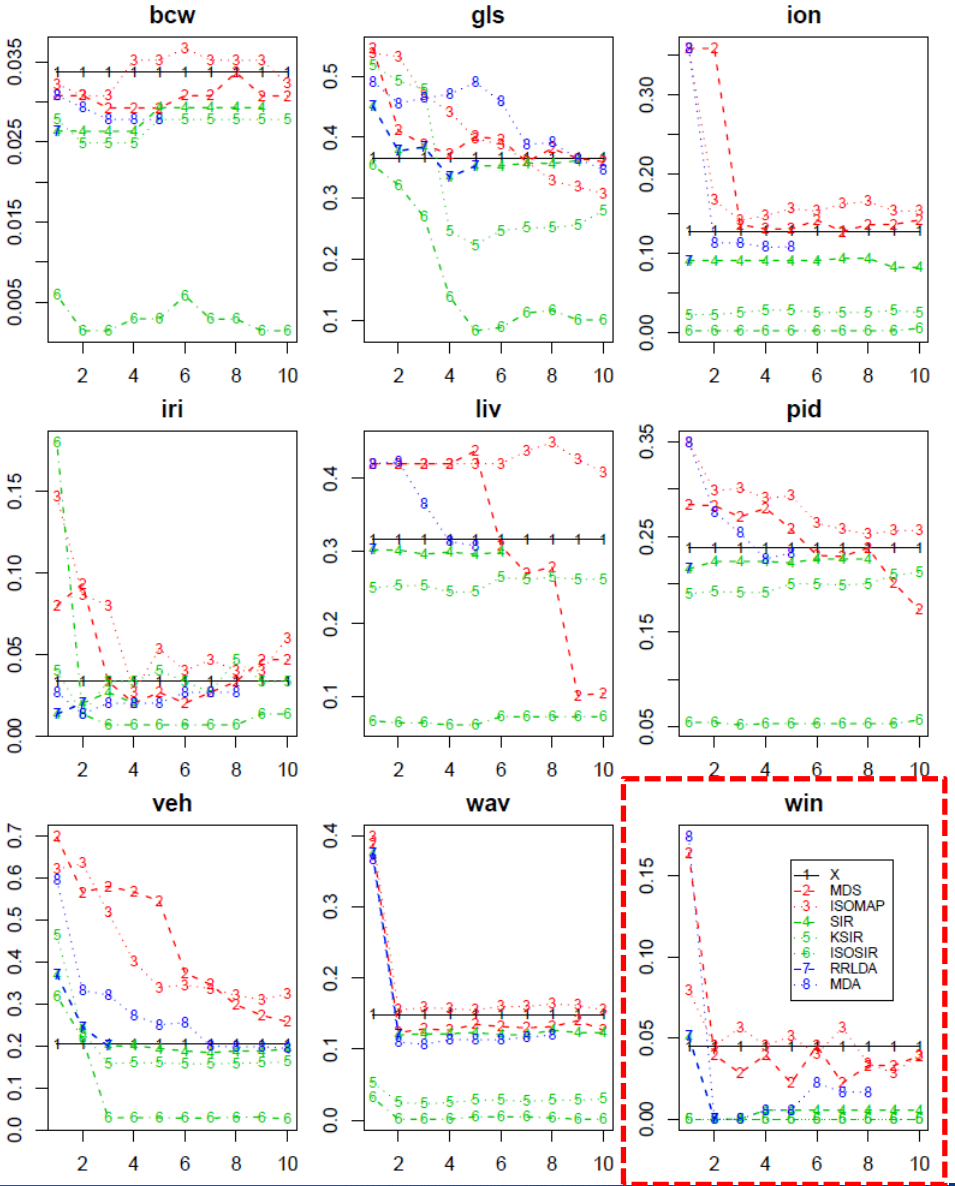
DR as a tool of feature extraction.

UCI machine learning repository datasets

Data set	n	p	$G(n_h)$
Wisconsin breast cancer (bcw)	683	9	2 (444, 239)
Glass identification (gls)	214	9	6 (70, 76, 17, 13, 9, 29)
Ionosphere (ion)	351	33	2 (225, 126)
Iris plants (iri)	150	4	3 (50×3)
BUPA liver disorders (liv)	345	6	2 (145, 200)
Pima Indians diabetes (pid)	768	8	2 (500, 268)
StatLog vehicle silhouettes (veh)	846	18	4 (212, 217, 218, 199)
Waveform database generator (wav)	600	21	3 (200×3)
Wine recognition data (win)	178	13	3 (59, 71, 48)

- Classifier : linear SVM
- 10-fold cross-validation error rate
- Gaussion kernel with scale 0.05

***See* 105/138**, 106/138, 107/138



Evaluate DR by Classification (n<<p) Microarray Datasets

Datasets	Publication	n	p	$G(n_h)$	Response
Brain	Pomeroy et al. 2002	42	5597	5(10, 10, 10, 4, 8)	Different tumor types
Colon	Alon et al. 1999	62	2000	2(22, 40)	Tumor/normal tissue
Leukemia	Golub et al. 1999	72	3571	2(47, 25)	Subtypes of leukemia
Lymphoma	Alizadeh et al. 2000	62	4026	3(42, 9, 11)	Subtypes of lymphoma
Prostate	Singh et al. 2002	102	6033	2(50, 52)	Tumor/normal tissue
SRBCT	Khan et al. 2001	63	2308	4(23, 20, 12, 8)	Different tumor types

n x p; n << p

$$\Sigma_{XX} \rightarrow p \times p$$

$$\text{IsoDistance} \rightarrow n \times n$$

- Classifier : linear SVM
- leave-one-out cross-validation error rate
- Gaussion kernel with scale 0.05