# COMPARISON OF MULTIVARIATE DATA REPRESENTATIONS: THREE EYES ARE BETTER THAN ONE

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# MULTIVARIATE DATA REPRESENTATION

#### o Numerical data

- Biplot (Gabriel 1971)
- Scatter plot matrix (Cleveland 1984)
- GGobi (Cook, D. et.al 2007)
- Glyphs (Anderson 1957, Chernoff 1973, Fienberg 1979)
- Parallel coordinate plot (Inselberg 1985, Wegman 1990)
- Matrix visualization (Chen 2002)

### Categorical data

- Mosaic plot (Hartigan 1981)
- MANET (Unwin et.al. 1996)

#### • Numerical/Categorical data

- Trellis/Lattice (Chambers 1992, Cleveland 1993)
- Textile plot (Kumasaka and Shibata 2008)

#### • General

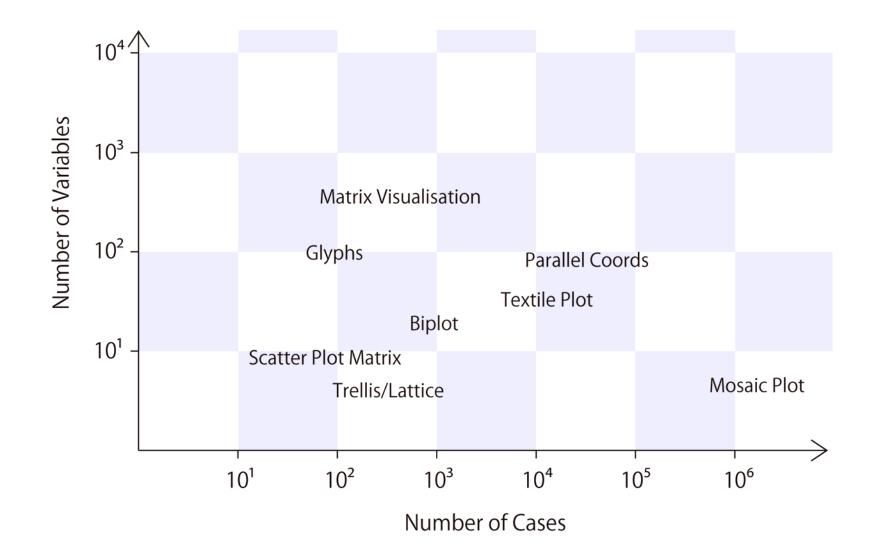
- Graphics of Large Datasets (Unwin et.al. 2006)
- Handbook of Data Visualization (Chen, et.al. 2008)

# CONTENT

# o3 multivariate data representations

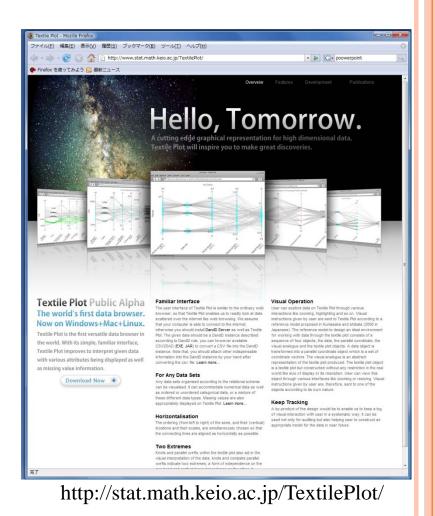
- Parallel coordinate plot
- Mosaic plot
- Textile plot
- Visual data analysis
  - Decathlon data
  - Wine data
  - Animal data
  - Titanic data

# CAPABILITY OF THE NUMBER OF CASES AND VARIABLES ON A DISPLAY



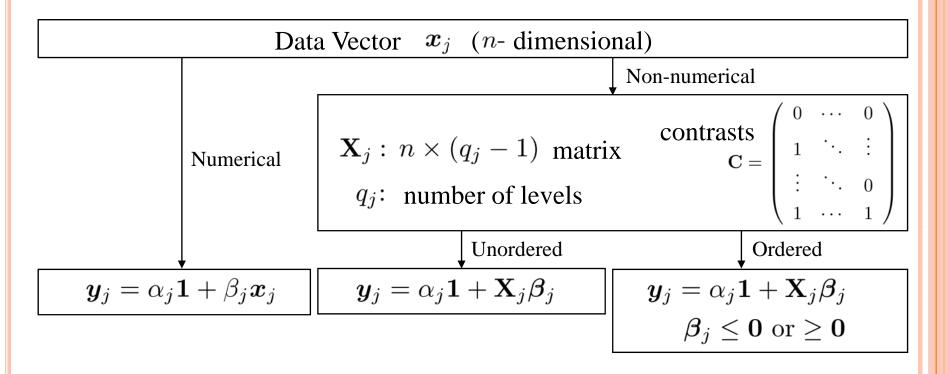
## TEXTILE PLOT (Kumaska and Shibata 2006, 2007, 2008)

- Parallel coordinate system
- Horizontalisation criterion
- Any type of data
- Order of Axes

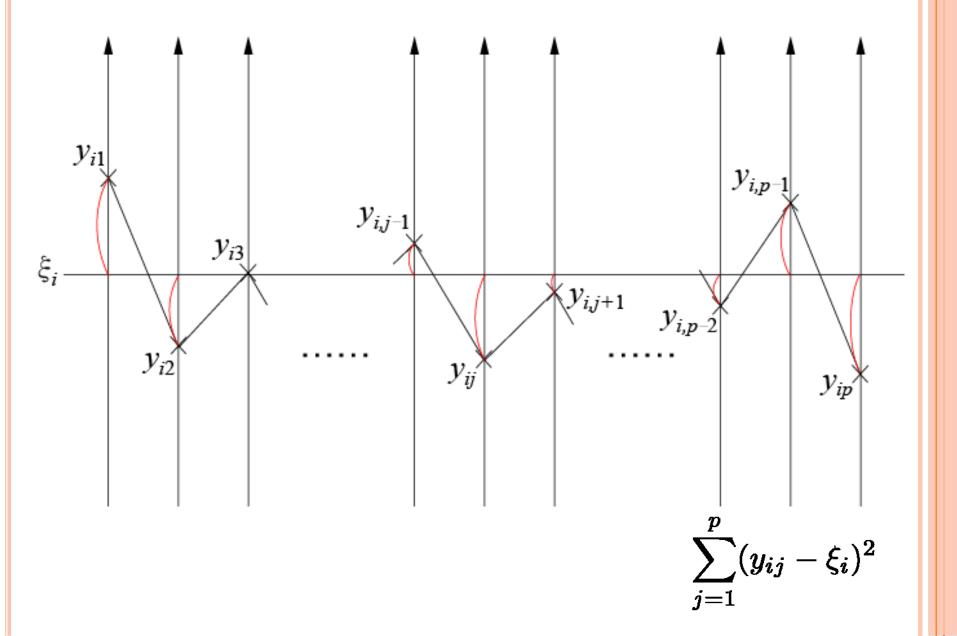


#### TRANSFORM DATAVECTOR INTO COORDINATE VECTOR

$$\left(\begin{array}{c} x_{ij} \\ n \times p \end{array}\right) = (\boldsymbol{x}_1, \dots, \boldsymbol{x}_p) \quad \Box \rangle \quad \left(\begin{array}{c} y_{ij} \\ n \times p \end{array}\right) = (\boldsymbol{y}_1, \dots, \boldsymbol{y}_p)$$



# HORIZONTALISATION CRITERION

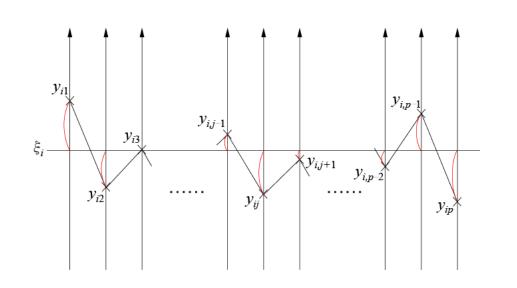


## **OPTIMISATION PROBLEM**

Minimise

$$\sum_{i=1}^{n} \sum_{j=1}^{p} (y_{ij} - \xi_i)^2 = \sum_{j=1}^{p} \left\| \boldsymbol{y}_j - \boldsymbol{\xi} \right\|^2 \underset{\boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\xi}}{\rightarrow} \min$$
$$\sum_{j=1}^{p} \left\| \boldsymbol{y}_j - \bar{y}_{\cdot j} \mathbf{1} \right\|^2 = np$$

Subject to



Location Parameter Vector  $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_p)^T$ Scale Parameter Vector  $\boldsymbol{\beta} = (\beta_1, \dots, \beta_p)^T$ Ideal Coordinate Vector

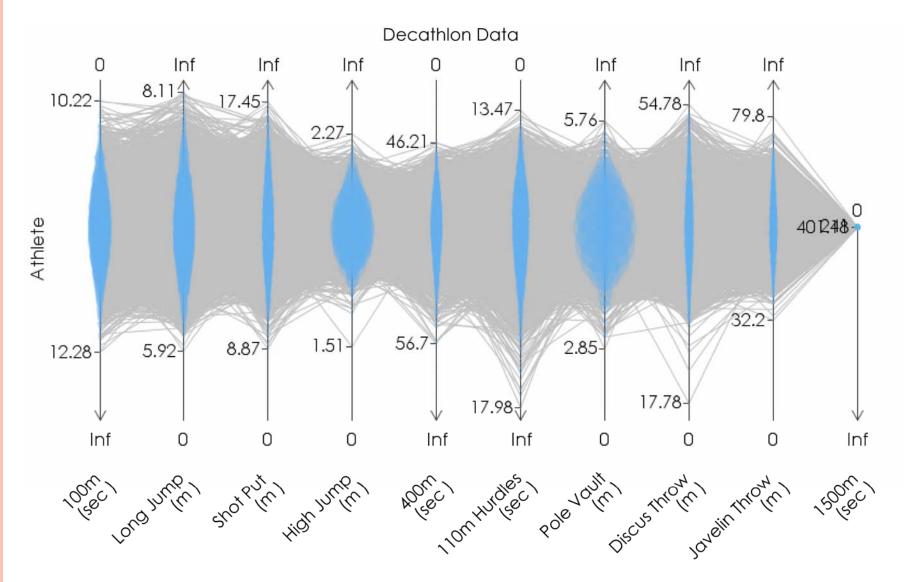
$$\boldsymbol{\xi} = (\xi_1, \dots, \xi_n)^T$$

**SOLUTION**  $(\mathbf{1}^T \boldsymbol{x}_j = 0 \text{ and } \|\boldsymbol{x}_j\| = 1; \ j = 1, ..., p)$ 

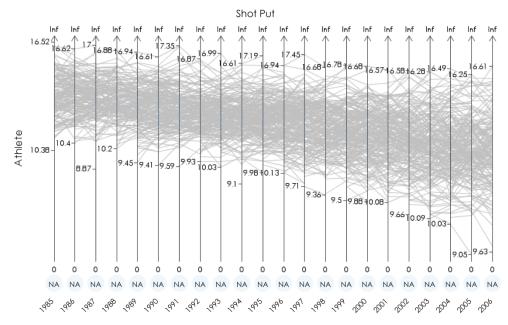
$$\sum_{j=1}^{p} \left\| \boldsymbol{y}_{j} - \boldsymbol{\xi} \right\|^{2} = \sum_{j=1}^{p} \left\| \boldsymbol{y}_{j} - \boldsymbol{m} \right\|^{2} + p \left\| \boldsymbol{m} - \boldsymbol{\xi} \right\|^{2}$$
$$\implies \hat{\boldsymbol{\xi}} = \boldsymbol{m} = \frac{1}{p} \sum_{j=1}^{p} \boldsymbol{y}_{j} \qquad (\boldsymbol{m}: \text{ mean vector})$$

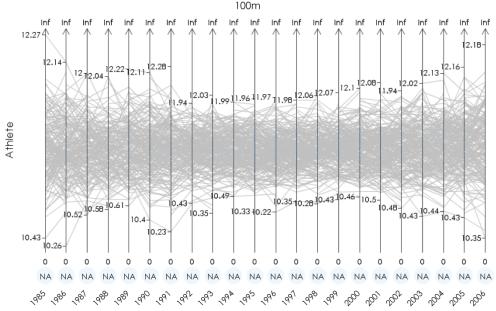
 $\sum_{j=1}^{p} \|\boldsymbol{y}_{j} - \bar{\boldsymbol{y}}_{\boldsymbol{\cdot}j} \mathbf{1}\|^{2} - p \|\boldsymbol{m} - \bar{\boldsymbol{y}}_{\boldsymbol{\cdot}} \mathbf{1}\|^{2} = \|\boldsymbol{\beta}\|^{2} - \frac{1}{p} \boldsymbol{\beta}^{T} \mathbf{R} \boldsymbol{\beta}$   $\implies \hat{\boldsymbol{\beta}}: \text{ Eigenvector of sample correlation matrix } \mathbf{R} \text{ with the largest eigenvalue, such that } \|\hat{\boldsymbol{\beta}}\|^{2} = np.$   $(\sum_{j=1}^{p} \|\boldsymbol{y}_{j} - \bar{\boldsymbol{y}}_{\boldsymbol{\cdot}j} \mathbf{1}\|^{2} = \|\boldsymbol{\beta}\|^{2} = np)$ 

## TEXTILE PLOT OF DECATHLON DATASET (PERFORMANCES NOT POINTS)



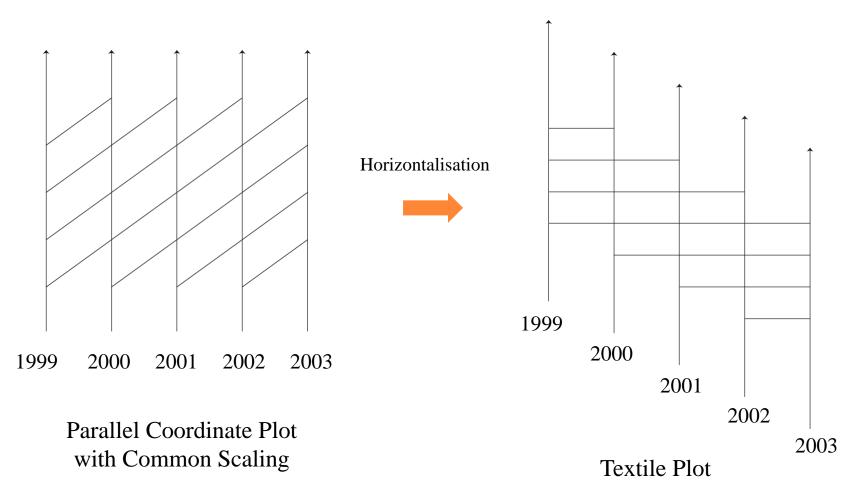
## **RE-ORGANISED DECATHLON DATASET**





# TREND ON TEXTILE PLOT

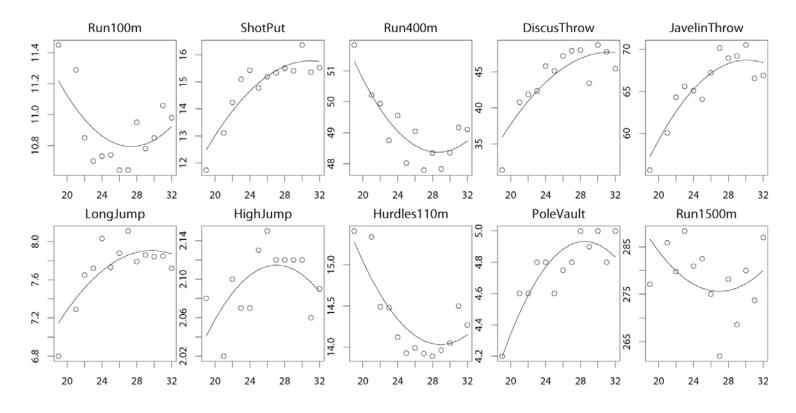
Assumption: All athletes improve their performances year by year, and stop their careers at their peak.



# FURTHER CONFIRMATORY DATA ANALYSIS



#### • Performances of Mr. Roman Sebrle (best record holder)



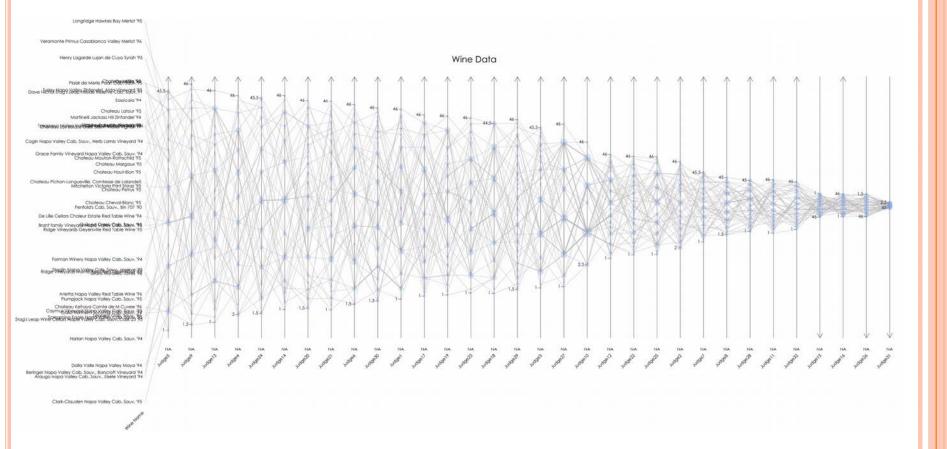
 $Performance_{ik} = \alpha_{ik} + \beta_k (Age_i - \gamma_{ik})^2 + \varepsilon_{ik},$ 

i: athlete, k: event

## WINE DATASET (LIQUID ASSETS: WWW.LIQUIDASSET.COM)

- Cabernet challenge 1999
- Case
  - 47 (only 46 rated) Cabernet Sauvignons: 34 US, 9 French, 2 Italian, 2 others
  - Vintages from 1994 to 1996
- Variable
  - 33 judges (Californian) ranked the wines
- Analysis goals:
  - Which wines were rated best?
  - Is the ranking of wines clear-cut?
  - Do the judges have similar opinions?
  - Are there clusters of judges?

# TEXTILE PLOT OF WINE DATASET

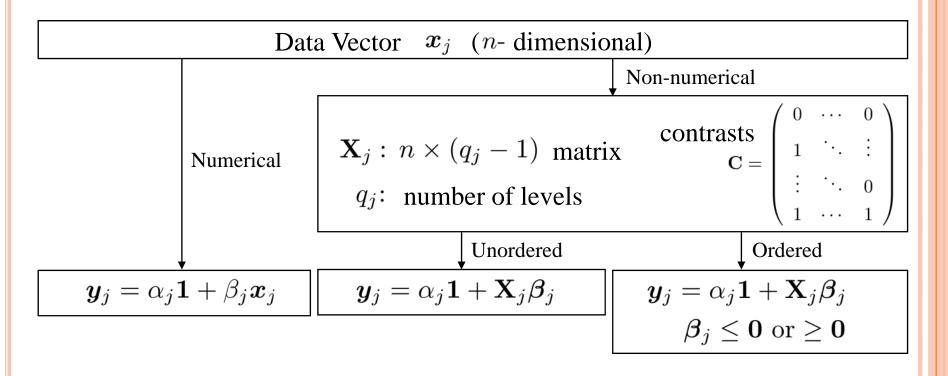


## GRAPHICS FOR MULTIVARIATE NUMERICAL DATA

- Textile plot or parallel coordinate plot gives an overview of the data
- Re-organisation of data is always useful to know another aspects of the data
- Textile plots suggest potential avenues for subsequent further confirmatory data analysis

#### TRANSFORM DATAVECTOR INTO COORDINATE VECTOR

$$\left(\begin{array}{c} x_{ij} \\ n \times p \end{array}\right) = (\boldsymbol{x}_1, \dots, \boldsymbol{x}_p) \quad \Box \rangle \quad \left(\begin{array}{c} y_{ij} \\ n \times p \end{array}\right) = (\boldsymbol{y}_1, \dots, \boldsymbol{y}_p)$$



# CATEGORICAL DATAVECTOR

• Coordinate vector transformation

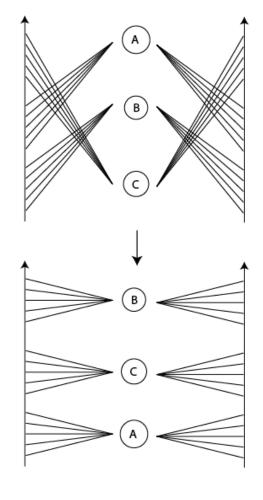
• Determine optimised default position for each level

 $\begin{array}{c} A \\ B \\ C \end{array} \left( \begin{array}{cc} 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{array} \right)$ 

• Introduction of a set of contrasts

Ex: Using a *treatment* contrast

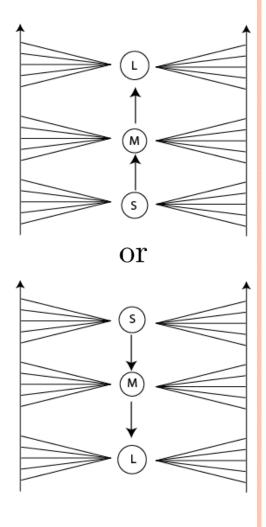
$$\boldsymbol{x} = \begin{pmatrix} A \\ A \\ B \\ C \\ C \end{pmatrix} \longrightarrow \mathbf{X} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{pmatrix}$$
  
Coordinate vector:  
$$\boldsymbol{y} = \alpha \mathbf{1} + \mathbf{X} \boldsymbol{\beta} = \begin{pmatrix} \alpha \\ \alpha \\ \alpha + \beta_1 \\ \alpha + \beta_2 \\ \alpha + \beta_2 \end{pmatrix}$$



# ORDERED CATEGORICAL DATAVECTOR

• Order of levels are retained on the axis

- Introduction of the specific contrasts
- Additional constraints



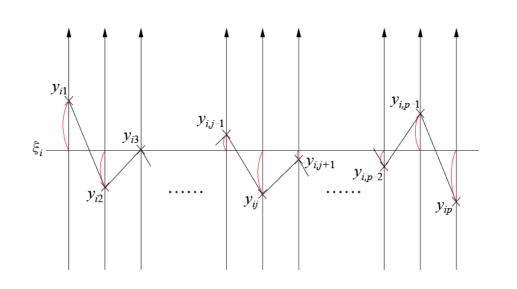
## **OPTIMISATION PROBLEM**

Minimise

$$\sum_{i=1}^{n} \sum_{j=1}^{p} (y_{ij} - \xi_i)^2 = \sum_{j=1}^{p} \left\| \boldsymbol{y}_j - \boldsymbol{\xi} \right\|^2 \xrightarrow[\boldsymbol{\alpha},\boldsymbol{\beta},\boldsymbol{\xi}]{\min}$$

$$\sum_{i=1}^{p} \left\| \boldsymbol{y}_j - \bar{y}_{\cdot j} \mathbf{1} \right\|^2 = np \quad (\boldsymbol{\beta}_j \ge \mathbf{0} \text{ or } \boldsymbol{\beta}_j \le \mathbf{0})$$

Subject to



Location Parameter Vector  $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_p)^T$ 

Scale Parameter Vector  $\boldsymbol{\beta} = (\boldsymbol{\beta}_1^T, \dots, \boldsymbol{\beta}_p^T)^T$ Ideal Coordinate Vector  $\boldsymbol{\xi} = (\xi_1, \dots, \xi_n)^T$ 

# ANIMAL DATA (UCI MACHINE LEARNING GROUP 2008)

## • Case

- 101 animals
- Invalid cases
  - Two frogs
  - Girl?

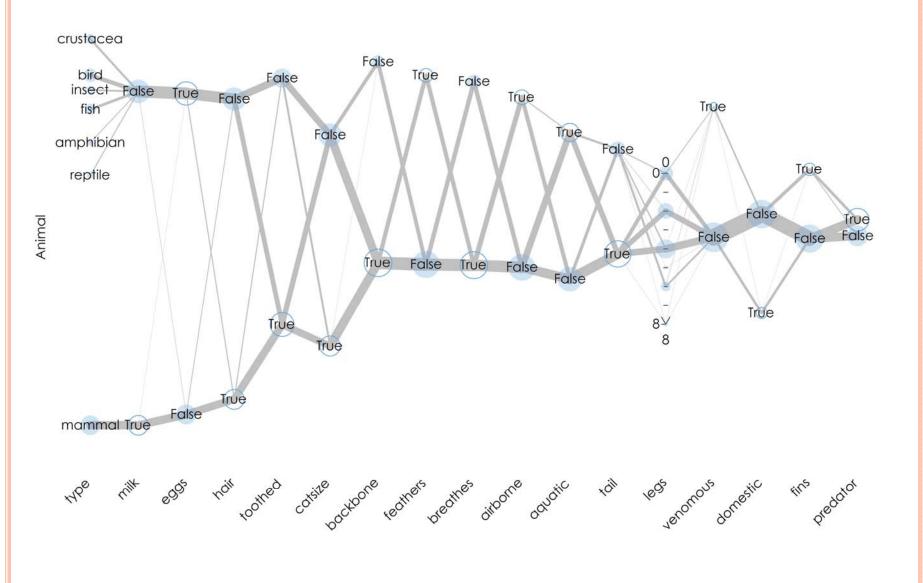
## • Response

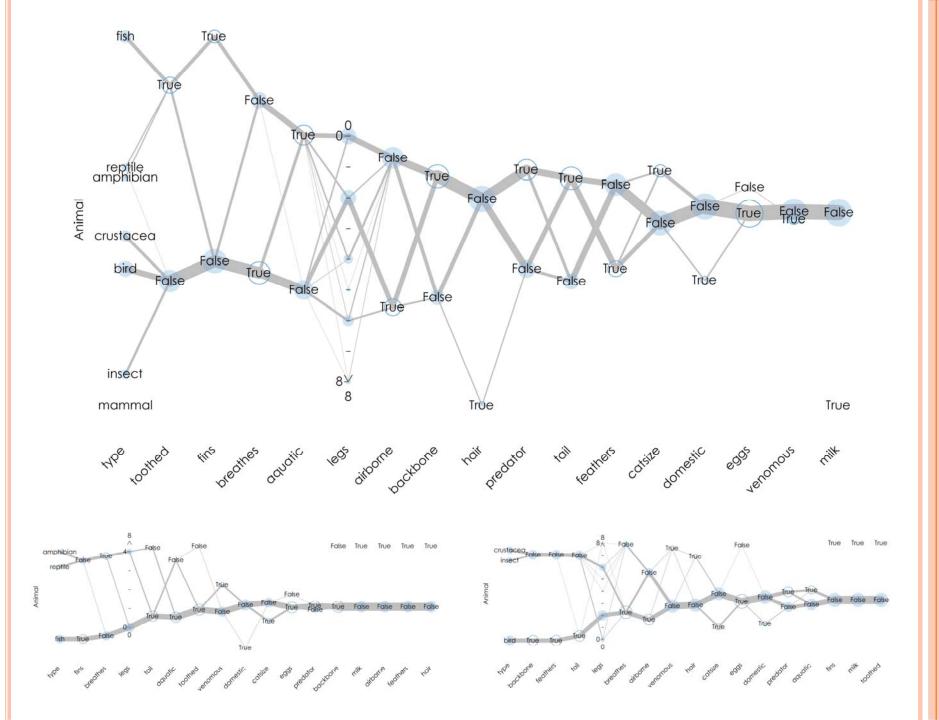
- Animal type
  - Mammal
  - o Reptile (爬虫類)
  - Amphibian (両生類)
  - Fish
  - Insect
  - Bird
  - o Invertebrate (無脊椎動物)

## • 16 Covariates (binary)

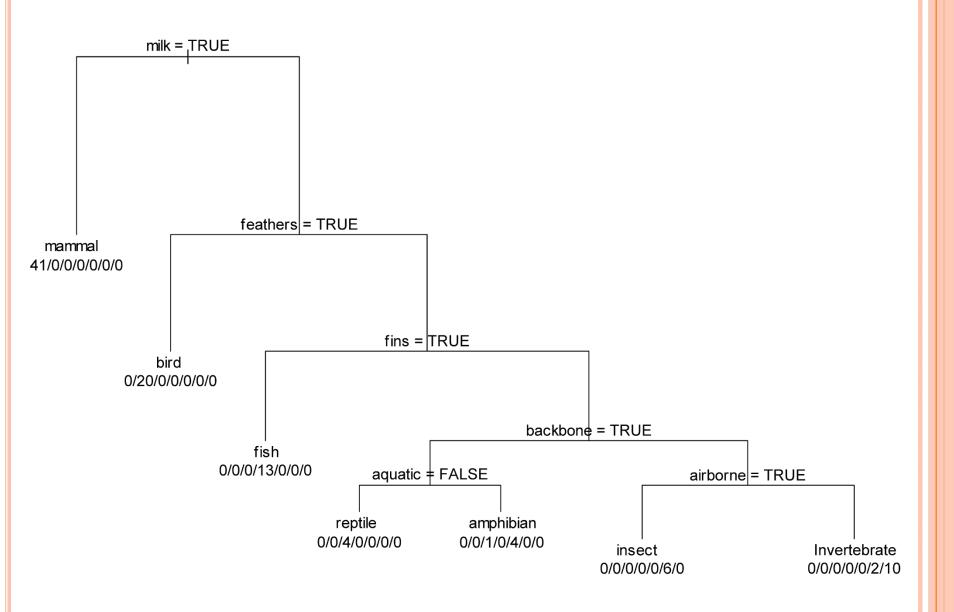
- Hair/Feathers/Eggs/Milk/Airborne /Aquatic/Predator/Toothed/Backb one/Breathes/Venomous/Fins/Leg s/Tail/Domestic/Cat-size
- Analysis goals:
  - What features best classify animals by type?
  - How are the features related?







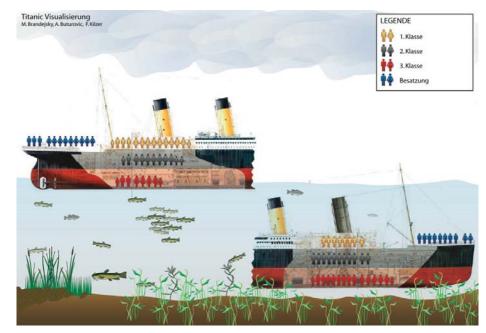
# **RELATION TO PARTITIONING TREE**



# TITANIC DATASET (BRITISH BOARD OF TRADE 1990)

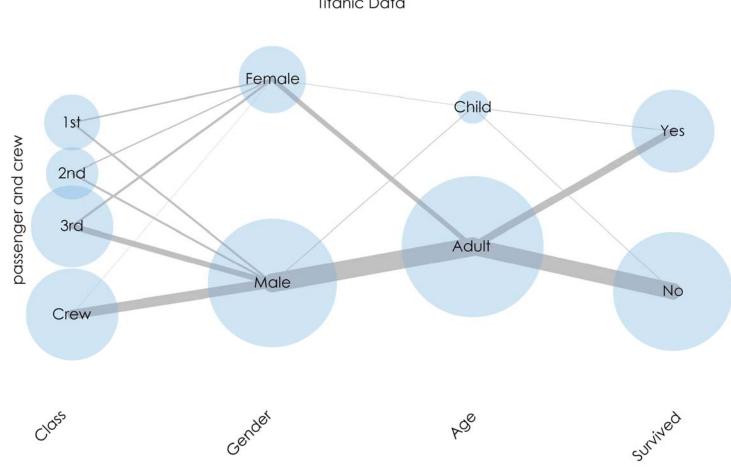
• Case

- 2201 passengers and crew
- Variable
  - Class (First, Second, Third, Crew)
  - Age (Young, Old)
  - Gender (Male, Female)
  - Survived (Yes, No)



http://eagereyes.org/

## **TEXTILE PLOT OF TITANIC DATASET**



Titanic Data

# SUMMARY: TEXTILE PLOT FOR MULTIVARIATE CATEGORICAL DATASETS

- Textile plots provide rough idea of classifying cases
- Textile plots of multivariate categorical data emphasise absolute numbers
- Detailed conditional probability is difficult to interpret

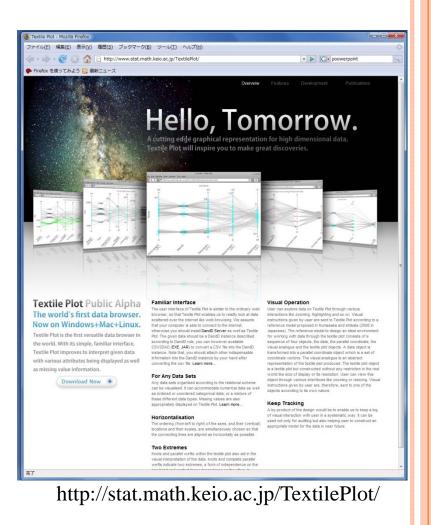
## SOFTWARE: TEXTILE PLOT ENVIRONMENT

#### • Network ready

• Based on DandD Client Server System (Yokouchi and Shibata 2004)

### • Cross-platform

- JAVA JRE 1.5
- Interactive user interfaces
  - Reference model (Kumasaka and Shibata, 2007)



# CONCLUSIONS

# • Textile plot

- Show an overview of the given data in an optimal way
- Accommodate numerical and categorical data
- Suggest several avenues for further exploratory or confirmatory data analysis
- Three eyes are better than one
  - Further investigations should be carried out with other graphical representations

## **BIBLIOGRAPHY**

- Anderson, E. (1957). A semigraphical method for the analysis of complex problems. *Proceedings of the National Academy of Sciences* **13** 923-927.
- British Board of Trade (1990), *Report on the Loss of the `Titanic' (S.S.)*. British Board of Trade Inquiry Report (reprint). Gloucester, UK: Allan Sutton Publishing.
- Chambers, J.M., and Hastie, T.J. (1992) Statistical Models in S, Wadsworth and Brooks/Cole, Pacific Grove CA.
- Chen, C. H. (2002) Generalized Association Plots: Information Visualization via Iteratively Generated Correlation Matrices. *Statistica Sinica* **12** pp. 7--29.
- Chen, C. H., haerdle, W. and Unwin, A.R. (2008) Handbook of Data Visualization, Springer, Berlin.
- Chernoff, H. (1973) The use of faces to represent points in k-dimensional space graphically, *Journal of American Statistical Association* **68** 361-368.
- Cleveland, W.S. and McGill, R. (1984). The Many Faces of a Scatterplot, *Journal of the American Statistical Association* **79** 807-822.
- Cook, D. and Swayne, D. Interactive and dynamic graphics for Data Analysis, Springer New York.

DandD Project (2007) Home Page, http://www.stat.math.keio.ac.jp/DandD/.

Decathlon 2000 (2008) Decathlon 2000 Home Page, www.decathlon2000.ee.

Fienberg, S.E. (1979) Graphical Methods in Statis-tics, The American Statistician 33 165-178.

- Gabriel, K. R. (1971). The biplot graphic display of matrices with application to principal components analysis. *Biometrics*, **58** (3) pp. 453-467.
- Hartigan, J. A. and Kleiner, B. (1981) Mosaics for Contingency Tables, *Computer Science and Statistics: Proceedings of the 13th Symposium on the Interface*, Springer-Verlag, pp.268-273.

## **BIBLIOGRAPHY**

Hurley, C. B. (2004) Clustering Visualizations of Multidimensional Data, *Journal of Computational and Graphical Statistics* **13** 788-806.

Inselberg, A. (1985) The plane with parallel coordinates, *The Visual Computer* **1** 69-91.

- Kumasaka, N., Shibata, R. (2007) Textile Plot Environment, 統計数理特集号「統計データの可視化」, **55**, 47-68.
- Kumasaka, N. and Shibata, R. (2008) High Dimesional Data Visualisation: the Textile Plot, *Computational Statistics & Data Analysis*, Submitted, **52**, 3616-3644.

Kumasaka, N. ANOVA on Textile Plot, Proceedings in COMPSTAT 2008, submitted.

Liquid Assets (2008) Liquid Assets Home Page, http://www.liquidasset.com/.

- Unwin, A.R., Hawkins, G., Hofmann, H., and Siegl, B. (1996) *Interactive Graphics for Data Sets with Missing Values* – MANET, Journal of Comp and graph Stat, 5 113-122.
- Wegman, E. (1990) Hyperdimensional data analysis using parallel coordinates. *Journal of The American Statistical Association* **85** 664-675.
- Yokouchi, D. and Shibata, R. (2004), DandD: Client Server System, *Proceedings in COMPSTAT 2004*, Physica-Verlag.