Advanced Applied Multivariate Analysis

STAT 2221, Spring 2015

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General Information

- Course Webpage:
  http://www.stat.pitt.edu/sungkyu/course/2221Spring15/
- Prerequisite: None (officially), but
  - probability and inference theory
  - linear algebra
  - R, SAS or Matlab programing.

What is multivariate analysis?

1. First course of statistics: numbers–random variables
2. **Second course of statistics: vectors of numbers–random vectors**
   - Basis for analysis of more complex objects, e.g. functions, matrices, tensors, images, networks.
3. Data Exploration: visualization of relationships between observations.
4. Discovering and modeling patterns from dataset: Visualization, Clustering, Multivariate distributions.
5. Confirming patterns: Inference.
6. Dimension Reduction: PCA, CCA, SVD.
7. Predictions: Regression, Classification.

What is a multivariate dataset?

Multivariate statistical analysis concerns multivariate data where each observation consisting of many measurements on the same subject. We suppose the dataset $\mathbf{X} = \{\mathbf{X}_1, \ldots, \mathbf{X}_n\}$ has n observations (Here, n is called the sample size), and each observation $\mathbf{X}_i = (x_{i1}, \ldots, x_{ip})$ is a vector in $\mathbb{R}^p$ (Here, p is called the dimension). These are often recorded in a $p \times n$ matrix:

$$\mathbf{X} = \left(\mathbf{X}_1, \cdots, \mathbf{X}_n\right) = \begin{pmatrix} x_{11} & \cdots & x_{n1} \\ \vdots & \ddots & \vdots \\ x_{1p} & \cdots & x_{np} \end{pmatrix}$$

Data Exploration - Visualization

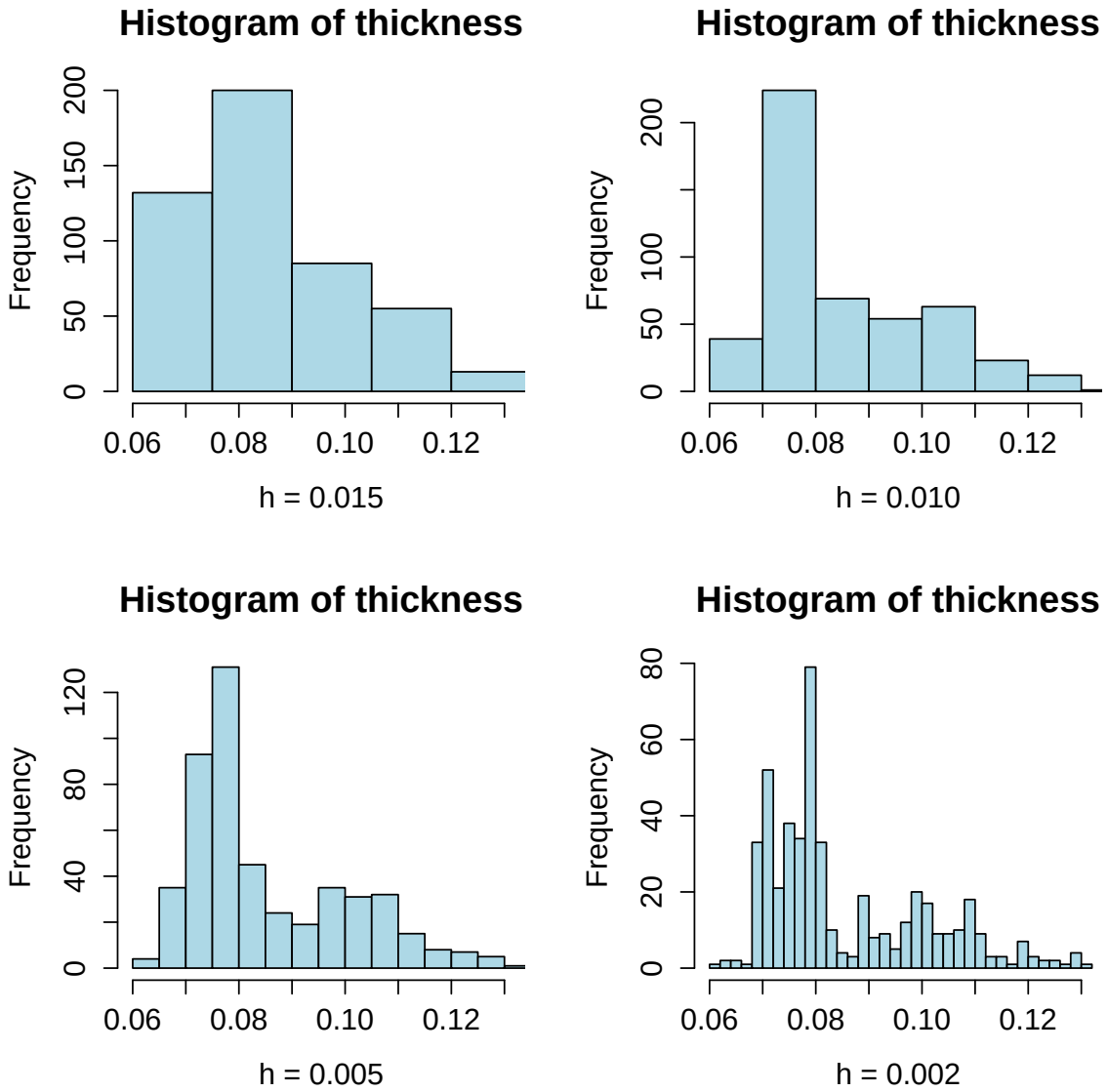
1D example – Hidalgo Stamp Data

- $n = 485$ observed values of thickness for Mexico stamps
- over > 70 years
- During 1980s
- Stamp papers produced in several factories?
- No records. Can we guess by looking at the data?

Izenman and Sommer (1988), here we use data "stamp" in R package BSDA.

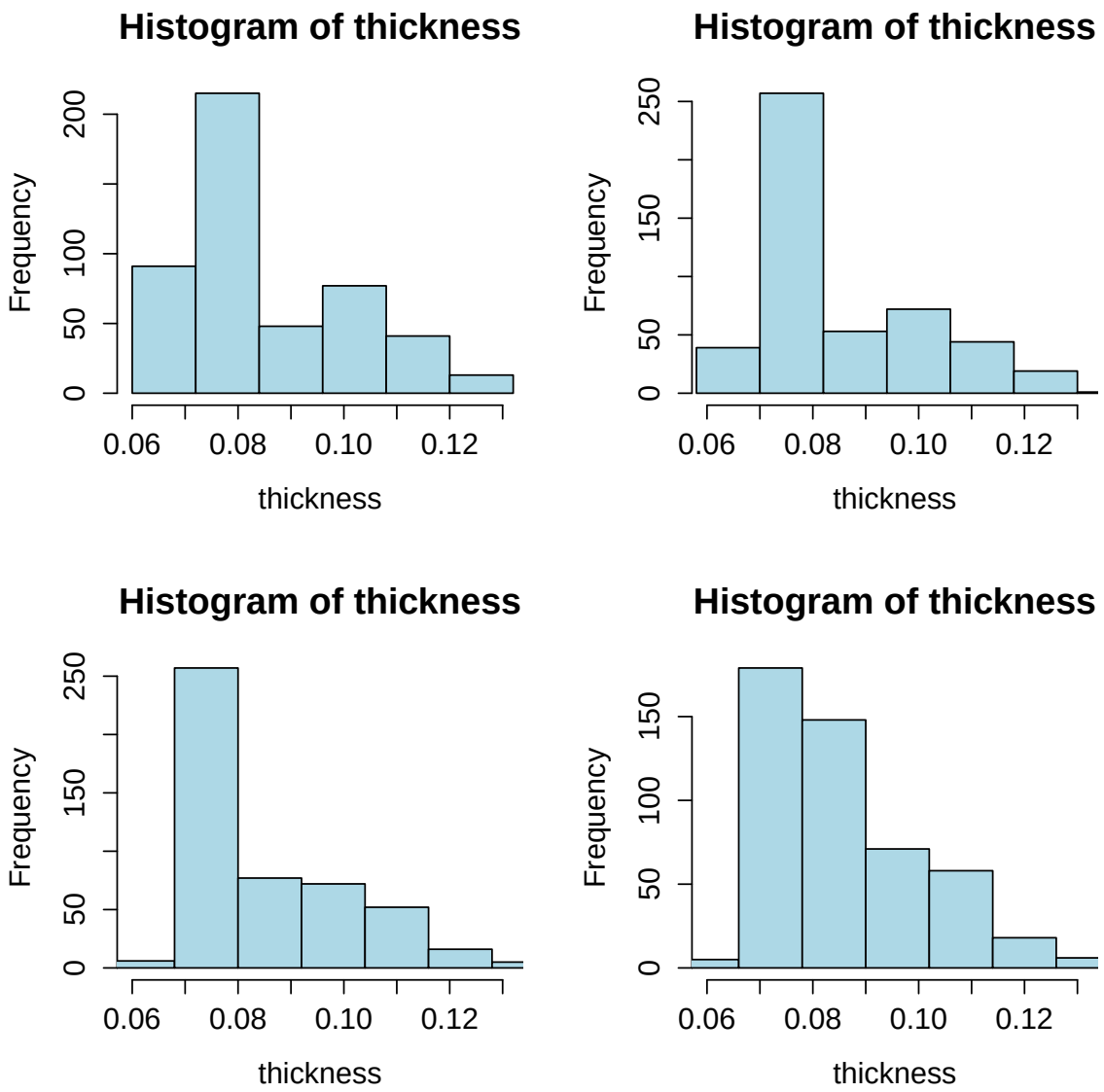
Data Exploration - 1D Hidalgo Stamp

Histograms with different bin widths. How many factories?



Data Exploration - 1D Hidalgo Stamp

Histograms with different bin locations. (Fixed bin width 0.012)



Data Exploration - Kernel density estimate

- Histograms are dependent on binwidth and bin location.
- Smaller binwidth preferred for exploration.
- Different bin locations can obscure important underlying patterns; A solution is to average out the effect on different bin location "Averaged histogram"
- A more elegant solution is kernel density estimate.
- For $X_1, \ldots, X_n \sim$ i.i.d. $f(x)$ (continuous pdf), a kernel density estimator of f is obtained as

$$\hat{f}_h(x) = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{h} K\left(\frac{x - X_i}{h}\right),$$

where the kernel $K(\cdot)$ is a function satisfying $\int K(x)dx = 1$.

Kernel density estimate - illustration

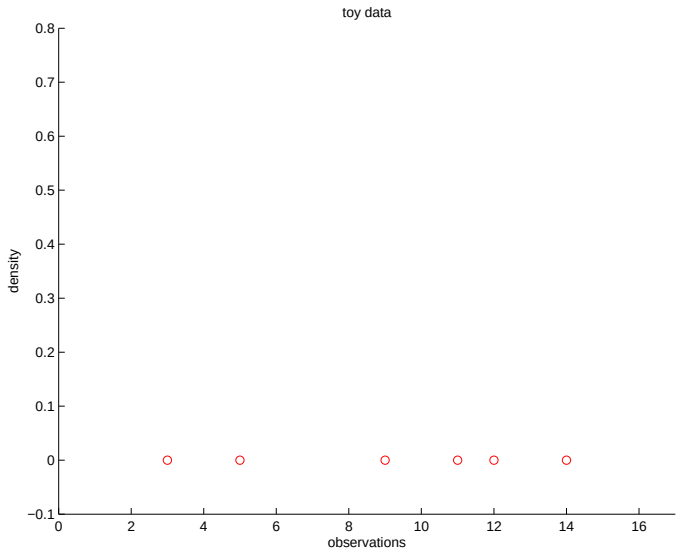
- Toy data: $x_i = 3, 5, 9, 11, 12, 14$.
- Consider a kernel density estimate with Gaussian kernel

$$K(t) = \frac{1}{\sqrt{2\pi}} e^{-t^2/2},$$

  with bandwidth $h = 1$.
- For each i,

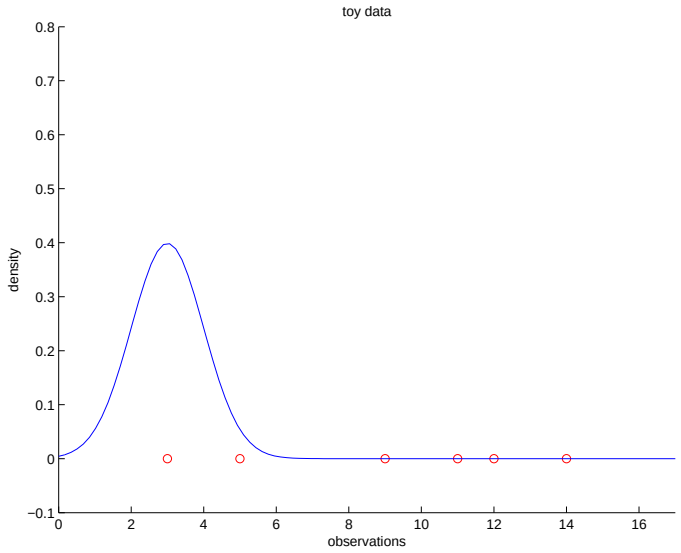
$$\frac{1}{h} K\left(\frac{x - x_i}{h}\right) = \frac{1}{\sqrt{2\pi h^2}} e^{-\frac{(x-x_i)^2}{2h^2}}.$$

Kernel density estimate - illustration



- Toy data: $x_i = 3, 5, 9, 11, 12, 14$.

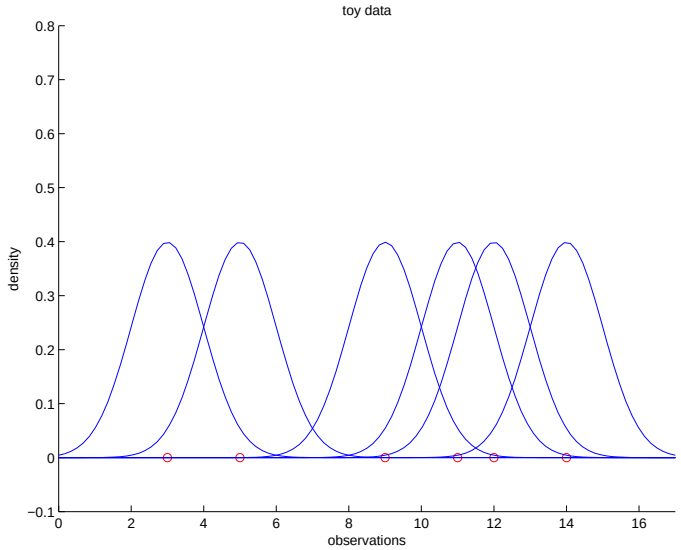
Kernel density estimate - illustration



- overlaid is, for $h = 1$,

$$\frac{1}{h} K\left(\frac{x - x_1}{h}\right) = \frac{1}{\sqrt{2\pi h^2}} e^{-\frac{(x-x_1)^2}{2h^2}}.$$

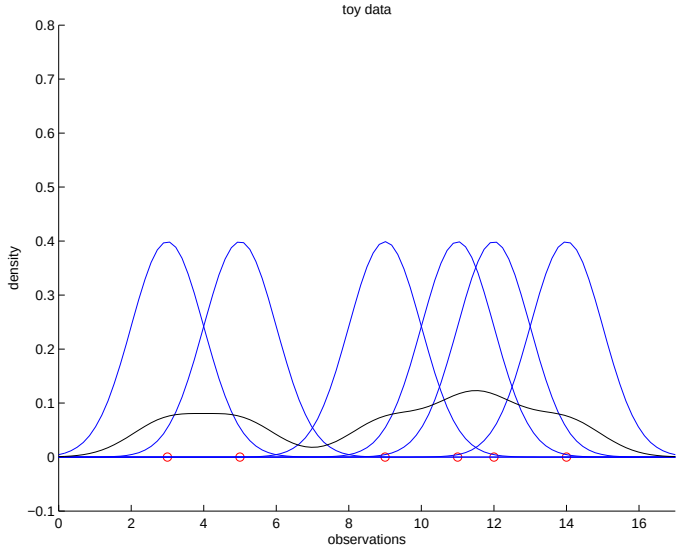
Kernel density estimate - illustration



- For all $i = 1, \ldots, 6$,

$$\frac{1}{h} K\left(\frac{x - x_i}{h}\right) = \frac{1}{\sqrt{2\pi h^2}} e^{-\frac{(x-x_i)^2}{2h^2}}.$$

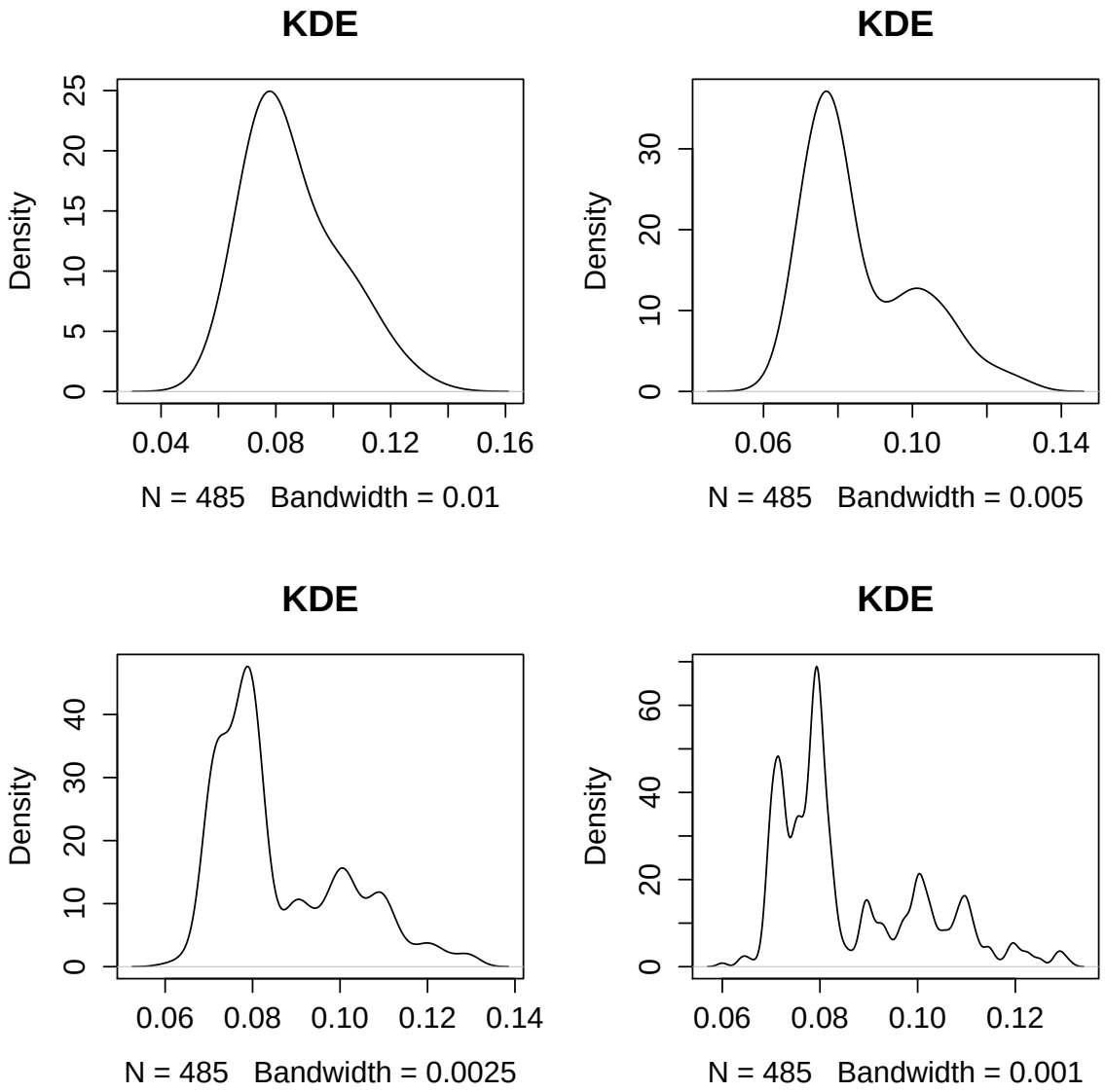
Kernel density estimate - illustration



- Kernel Density Estimate (KDE) of the pdf:

$$\hat{f}_h(x) = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{h} K\left(\frac{x - X_i}{h}\right),$$

KDE for Hidalgo Stamp

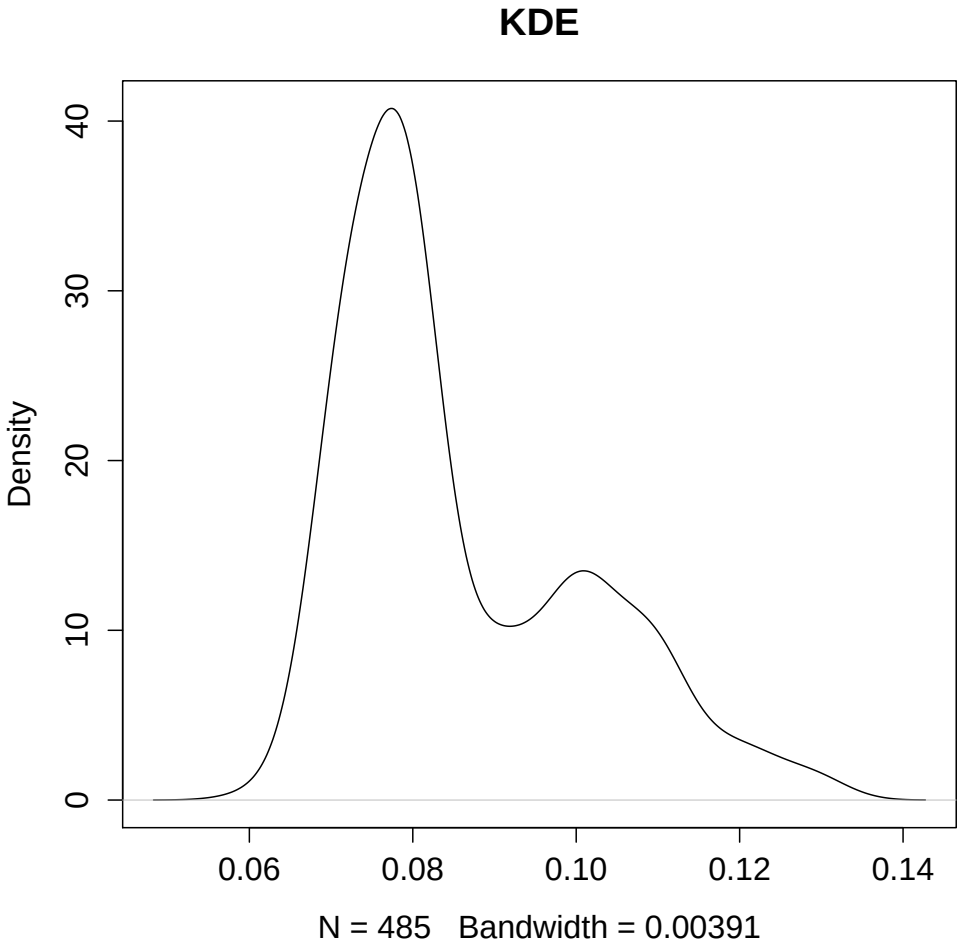


KDE for Hidalgo Stamp

- Small bandwidth leads undersmooth; Large bandwidth leads oversmooth
- Is it unimodal? Bi-modal? Or several modes? Which modes are really there?
- Choice of bandwidth
  - Important in practice.
  - Controversial issue.
  - Many recommendations (Silverman's rule of thumb, Sheather-Jones Plug-In.)
  - The consensus is that there is never a consensus.

KDE for Hidalgo Stamp

Bandwidth, by Silverman's rule-of-thumb, is (sample size)$^{-1/5}\times$ 90% of minimum of two population standard deviation estimates: i) the sample standard deviation, ii) $IQR/1.34$



Data Exploration - Multivariate data

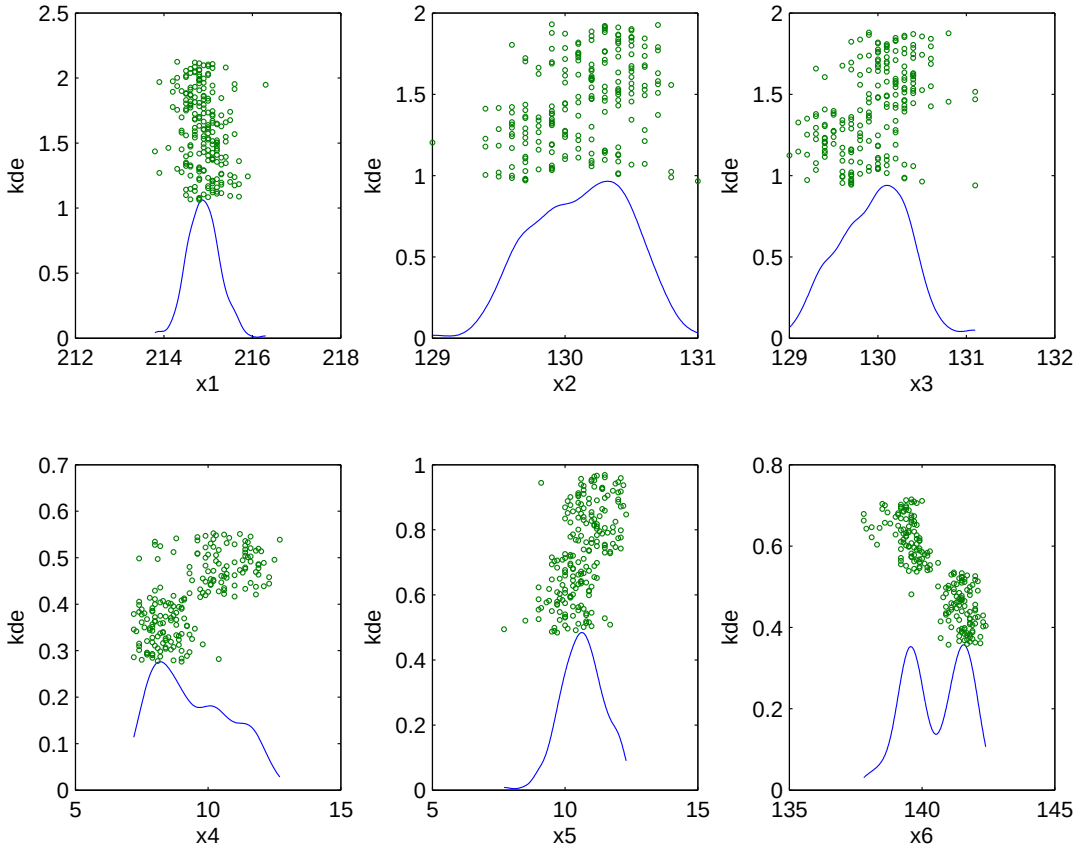
Dimension $p = 6$ example – Swiss bank notes

- $n = 200$ Swiss bank notes (See Fig. 1.1, Härdle and Simar)
- Each note (obs.) has $p = 6$ measurements (variables).
- Additional information: first half are genuine; the other half are counterfeit.
- Visualization of 6-dim'l data?
- Can use 6 KDEs overlaided with jitterplot for each measurements (variables)

Swiss bank notes - Marginal KDEs

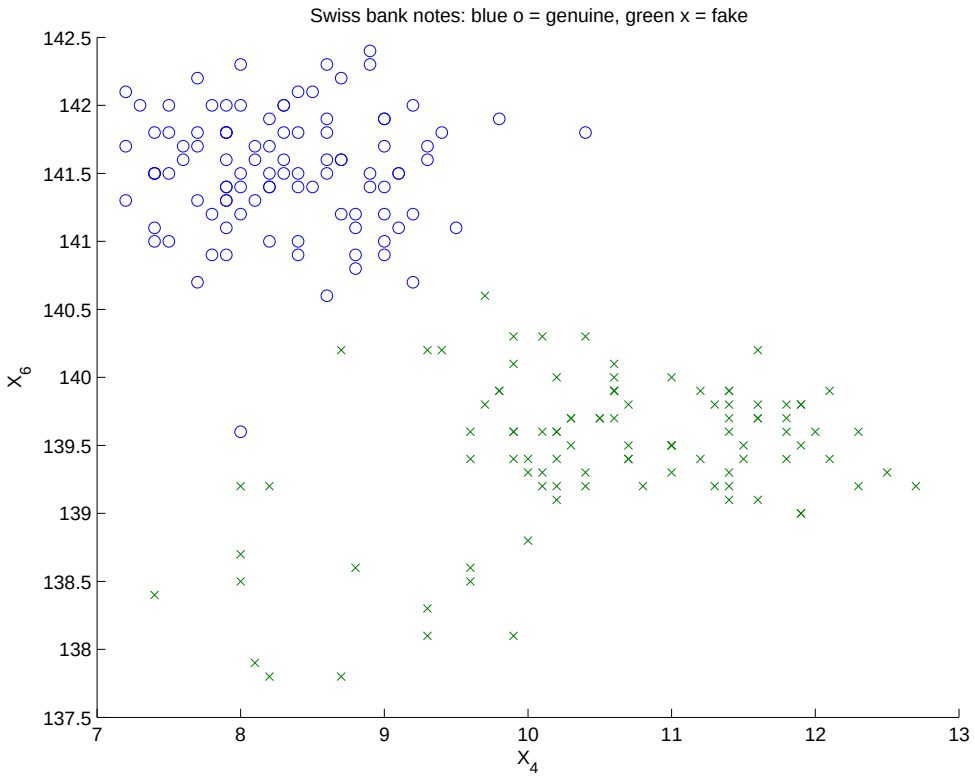
Marginal KDEs overlaided with jitterplot for each of 6 variables.

- Informative, realistic when p is small
- No information about association between variables.



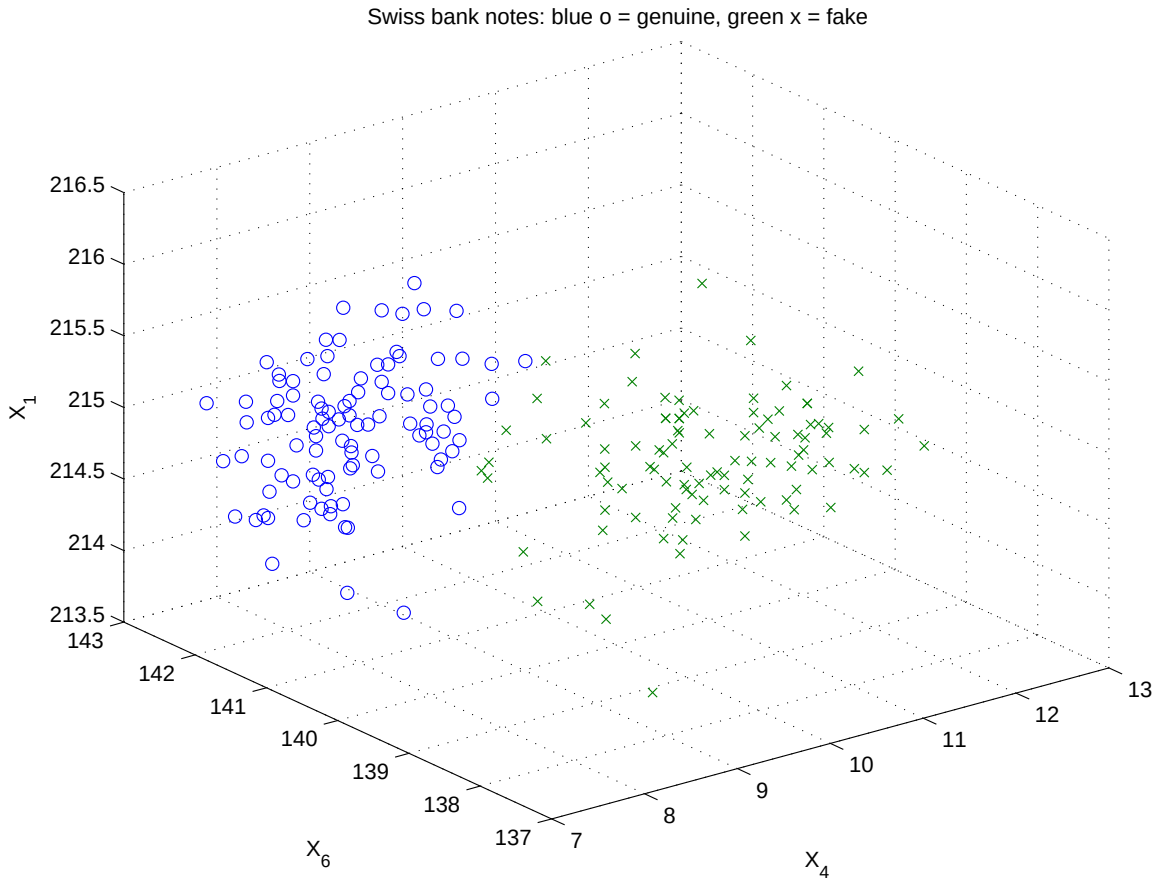
Swiss bank notes - Scatterplot

- Pairs of variables are best visualized by scatterplot, e.g. X_4 vs X_6 below.
- Understood as point clouds (representing the empirical distributions)
- $\binom{6}{2}$ many pairs to choose from.



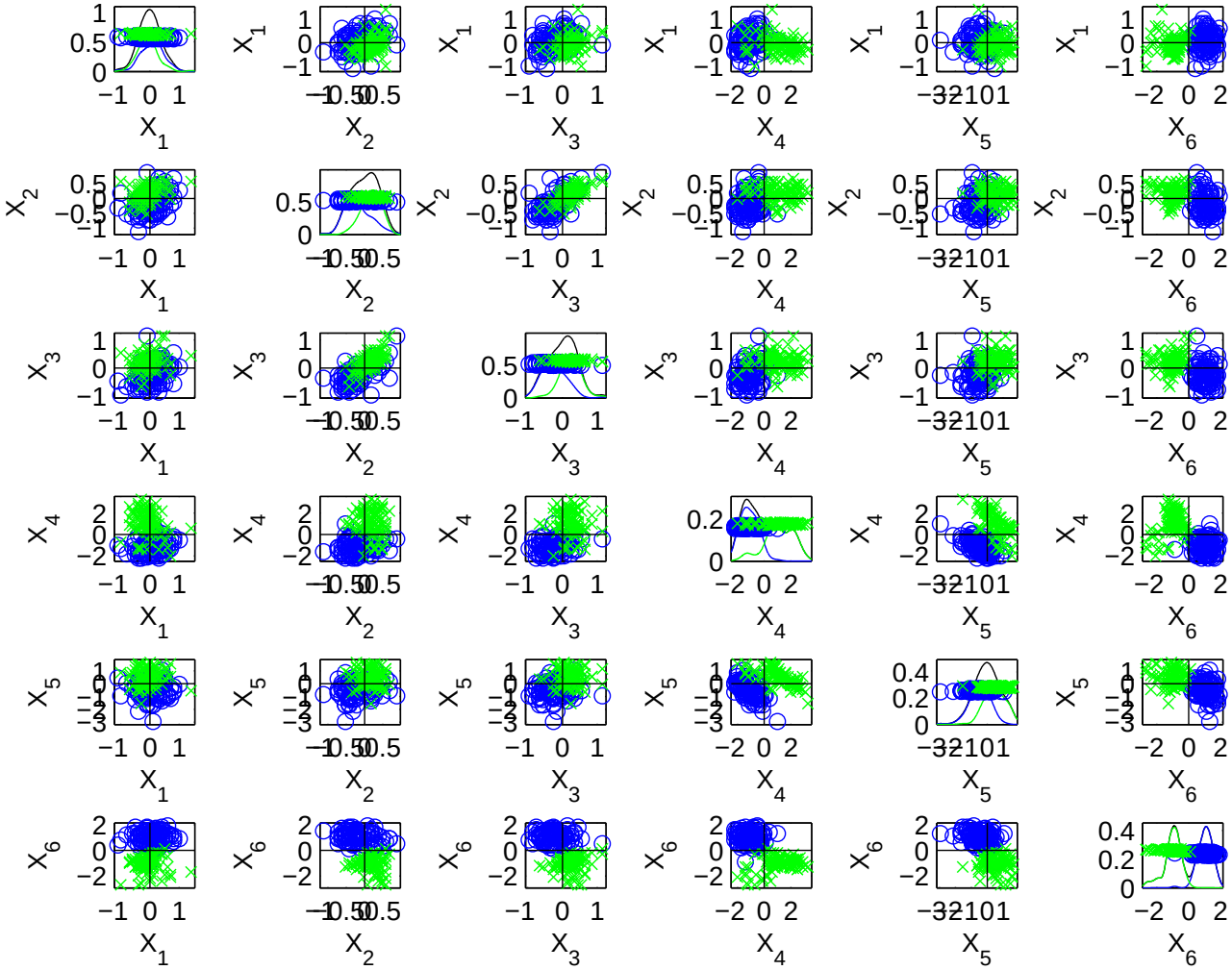
Swiss bank notes - Scatterplot

- Scatters of three variables can also be informative, if software allows to rotate the axes.
- Otherwise, the 3D scatterplot is a scatterplot of linear combinations of the three variables.



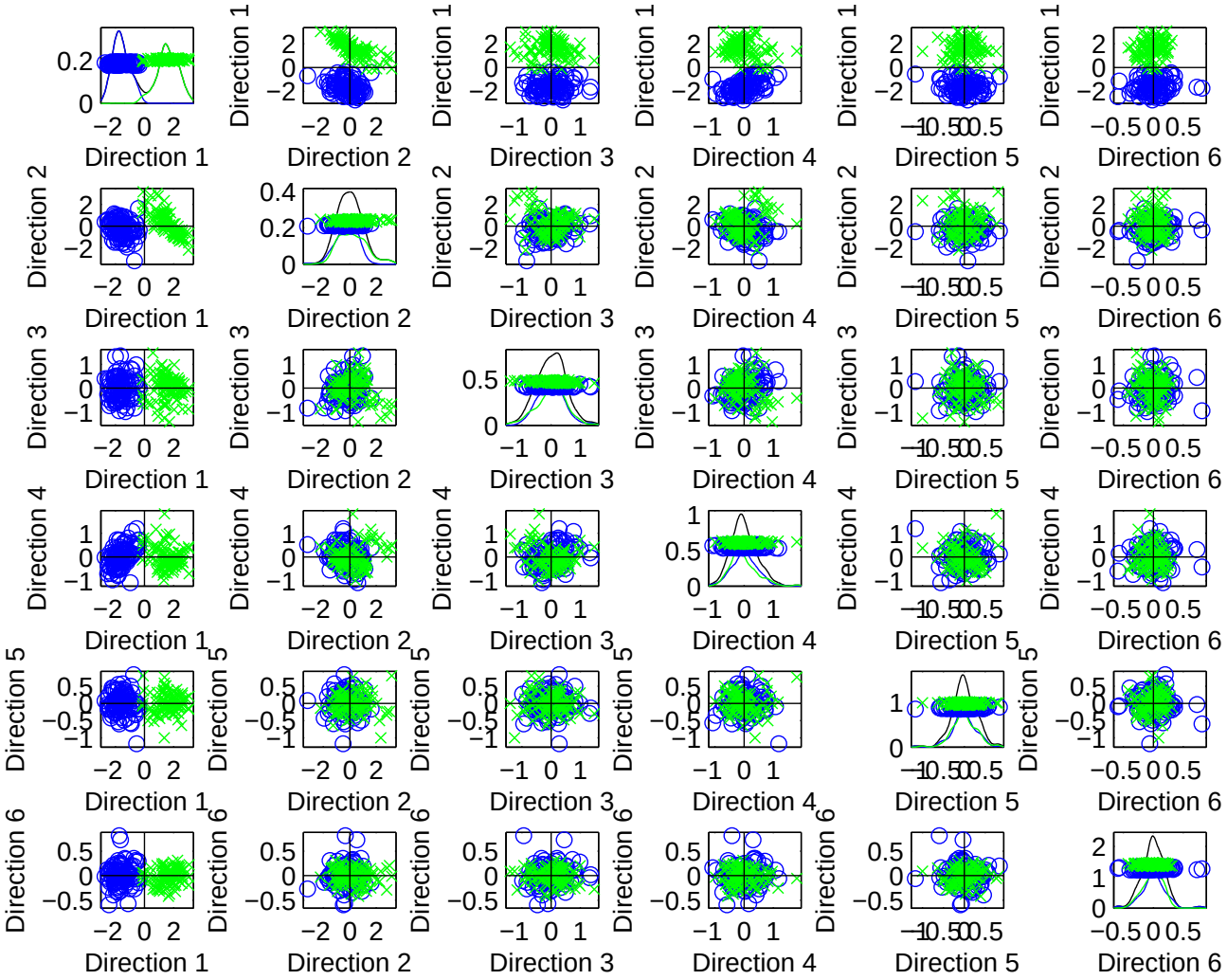
Swiss bank notes - scatterplot matrix

- A traditional, yet powerful, tool is to construct a matrix of scatterplots. - Too busy with $p = 6$.



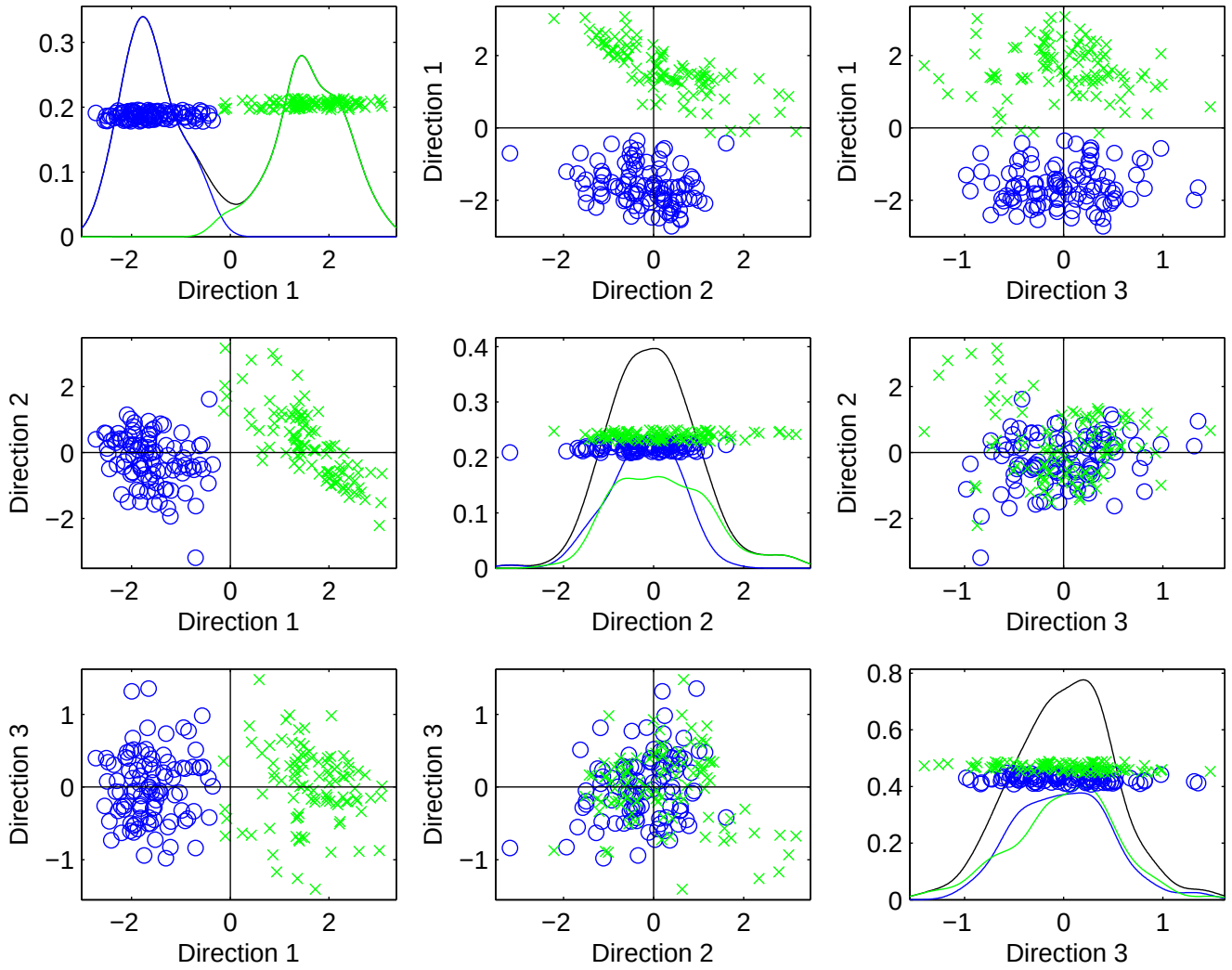
Swiss bank notes - scatterplot matrix

- Better to visualize with principal component scores.



Swiss bank notes - scatterplot matrix

- With principal component scores, we can focus on fewer combinations; Dimension Reduction



Swiss bank notes - related methods

1. If obtaining succint representation of data is of interest, then using the first two principal component scores appeared in the first 2×2 block of the scatterplot matrix would do the job (Principal Component Analysis)
2. Parametric modeling: Are distributions of Swiss bank note measurements normal (Gaussian)? (Multivariate Normal Distribution)
3. Without the information on genuine and counterfeit notes, can we classify $n = 200$ notes into two distinct groups? (Clustering)
4. With the information on genuine and counterfeit notes,
   - Are the means and covariances of genuine and counterfeit notes different? (Statistical inference)
   - When there is a new bank note, how to predict whether the new note is genuine? (Classification)

High dimensional data

1. Gene expression data in Golub et al. (1999)
2. $p = 7129$ gene expression levels (numeric) for $n_1 = 47$ subjects with acute lymphoblastic leukemia (ALL) and $n_2 = 25$ subjects with acute myeloid leukemia (AML).
3. Scientific task is to identify new cancer class and/or to assign tumors to known classes (ALL or AML).

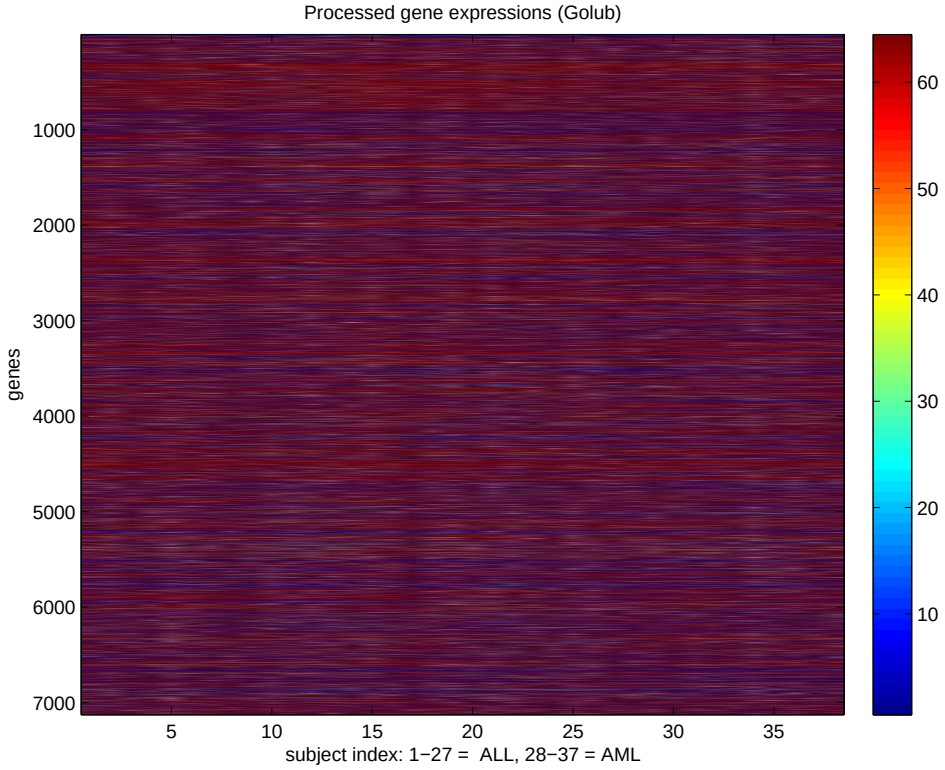
REPORTS

Molecular Classification of Cancer: Class Discovery and Class Prediction by Gene Expression Monitoring

T. R. Golub,[1,2*†] D. K. Slonim,[1†] P. Tamayo,[1] C. Huard,[1] M. Gaasenbeek,[1] J. P. Mesirov,[1] H. Coller,[1] M. L. Loh,[2] J. R. Downing,[3] M. A. Caligiuri,[4] C. D. Bloomfield,[4] E. S. Lander[1,5*]

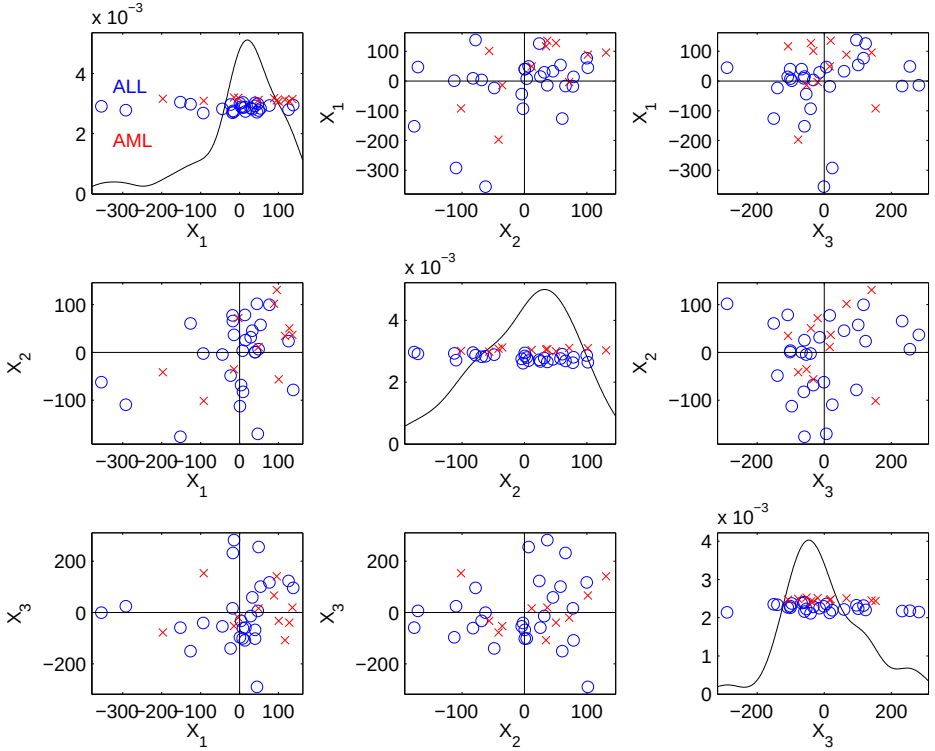
Golub data

Taking a subgroup of data with 27 ALLs and 11 AMLs.
A visualization of the matrix $X_{p \times n}$. Is it helpful?



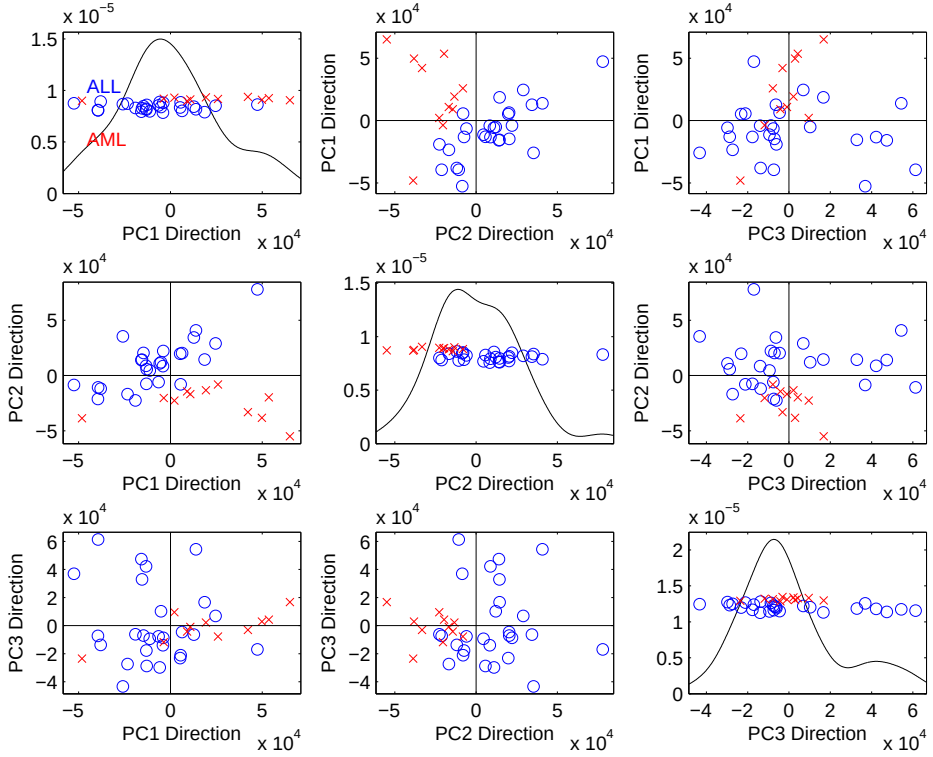
Golub data

Scatterplot matrix for the first three genes (variables).



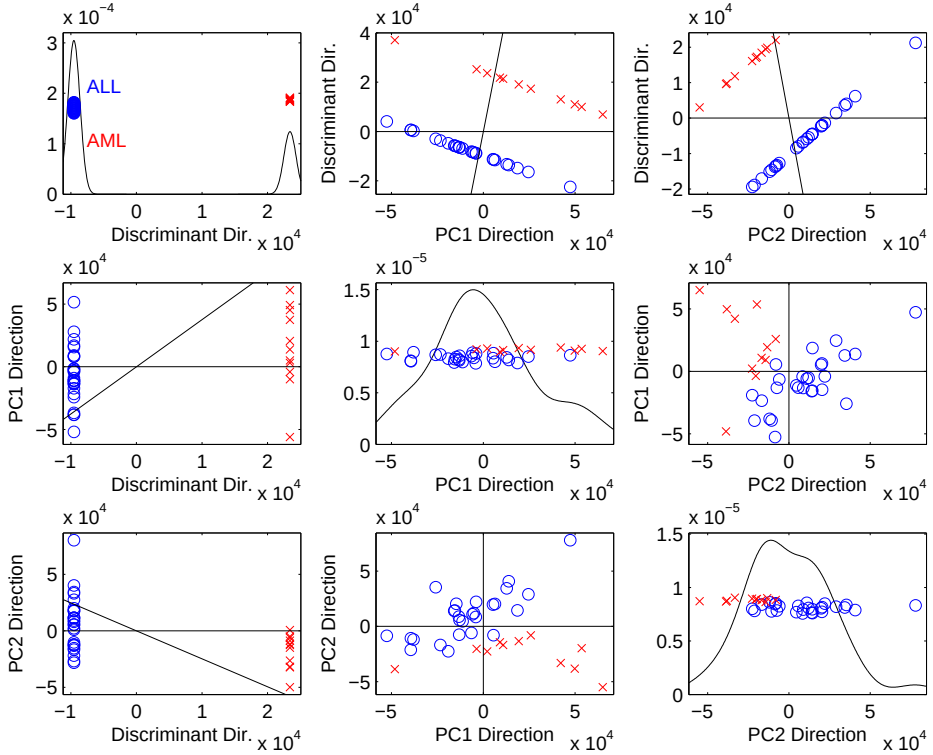
Golub data

Scatterplot matrix using the first three Principal Component Scores. A pattern there?



Golub data

Scatterplot matrix using the a liniear combination of all variables (that leads a good separation of two groups) and two Principal Component Scores. Better pattern?



Next: review on matrix algebra.