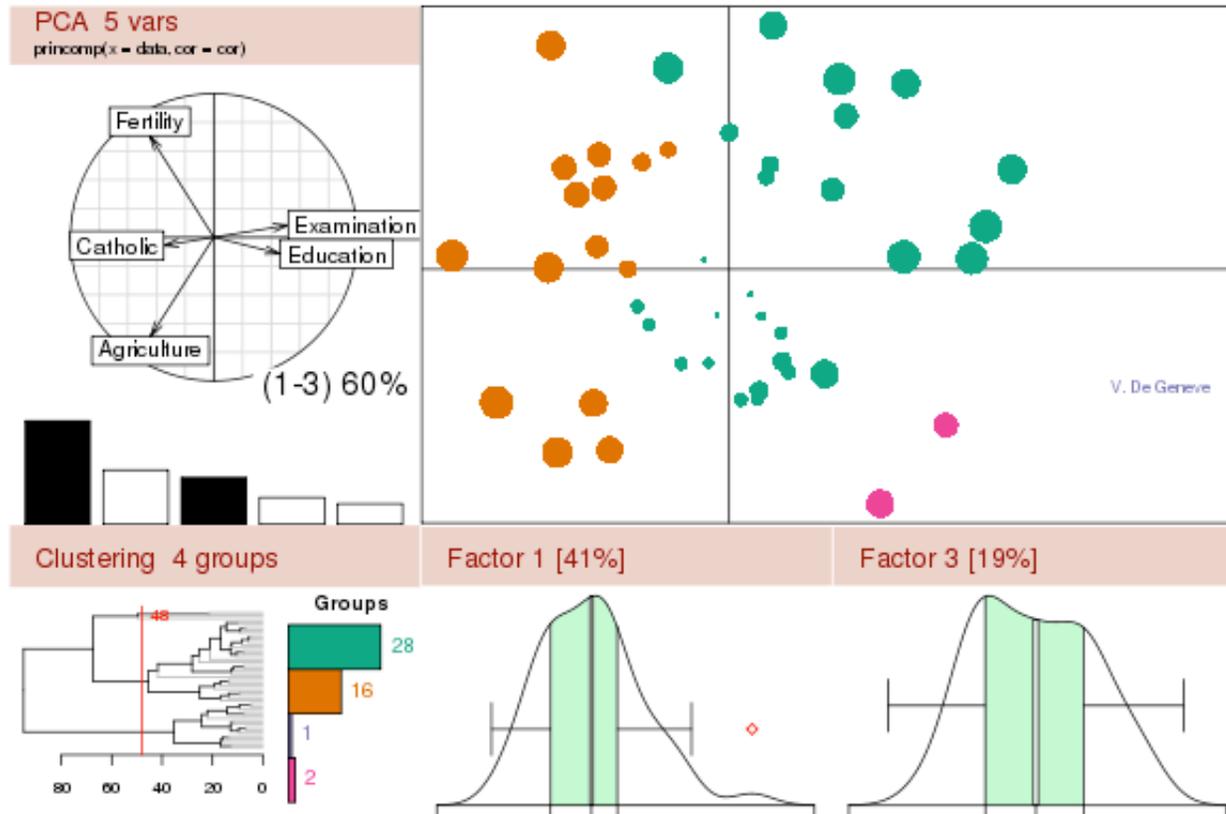


# R and Statistics (I)

Eric Lecoutre, 2004 competition



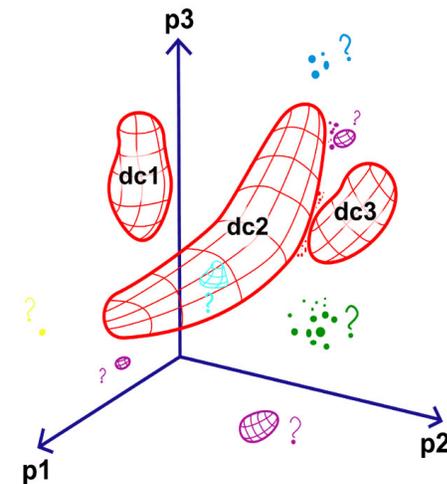
Ashish Mahabal

AyBi199, Caltech, 19 May 2011

# Statistics is extensively used

- 15000 astronomical studies per year
- 5% have “statistics” in their abstract
- 20% treat variable objects or multivariate datasets

A Generic Machine-Assisted Discovery Problem:  
Data Mapping and a Search for Outliers



However, it is not well understood

5 out of 4 people  
have trouble with  
Statistics.

(People also assume) it is misused

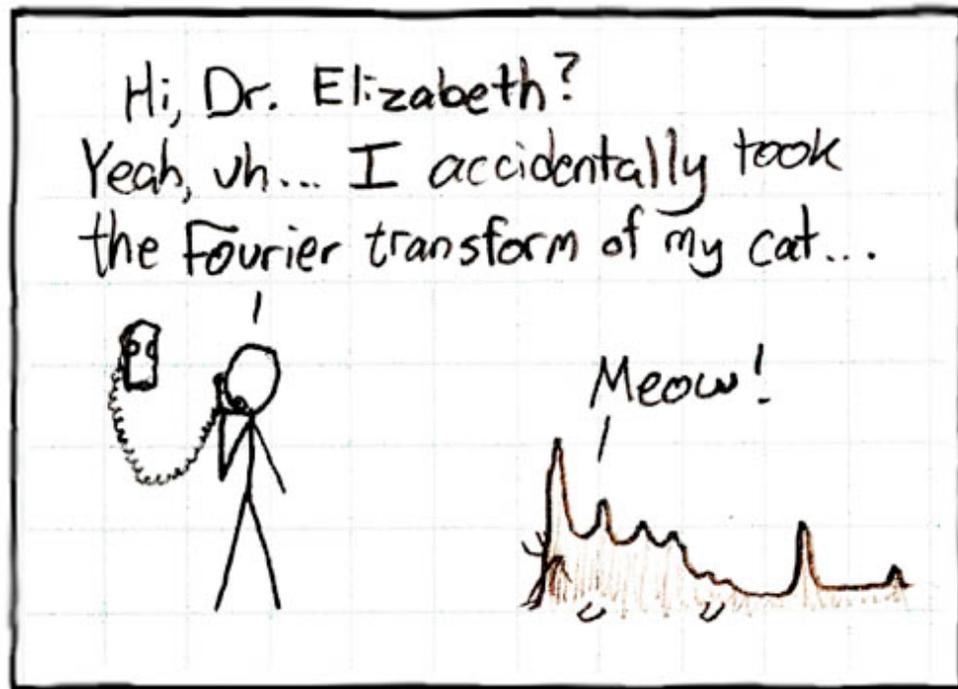
**There are lies, damned lies  
and statistics**

**-Benjamin Disraeli**

# Limited number of methods still dominate

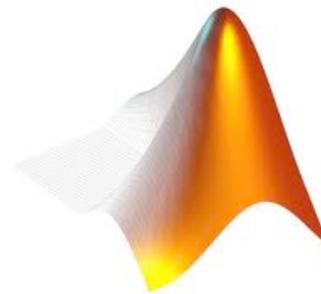
## Traditional methods: preWWII

- Fourier transform (Fourier 1807)
- Least sq. and chisq (Legendre 1805, Pearson 1901)
- Kolmogorov-Smirnov test (Kolmogorov 1933)
- Principal Component Analysis (Hotelling 1936)



# Advanced methods available in most systems

- Matlab
- Mathematica
- IDL
- Octave
- NumPy
- PDL

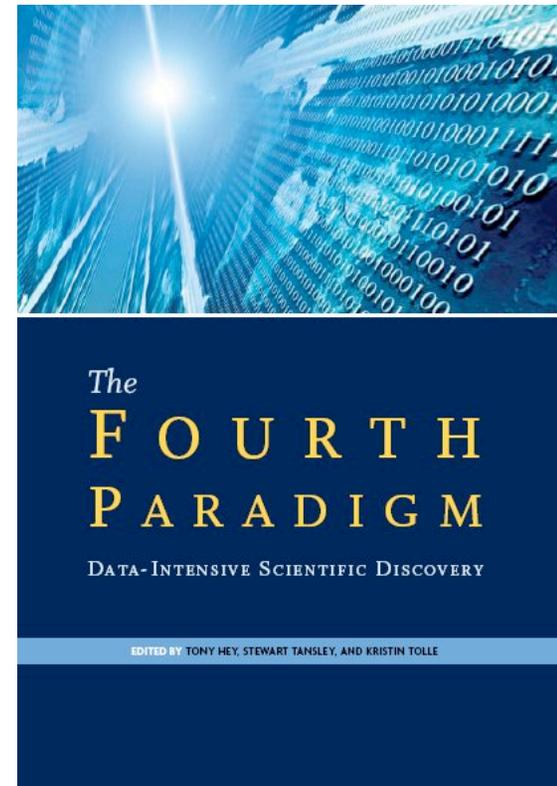


# Examples of available functions

- Descriptive statistics (e.g. boxplot)
- Two- and k-sample tests (e.g. Wilcoxon rank-sum test)
- Density estimation (e.g. Kernel smoothing)
- Correlation and regression (e.g. PCA)
- Censored data (e.g. Survival)
- Multivariate classification (e.g. H clustering)
- External functions (e.g. K-density)

# 4<sup>th</sup> paradigm, D2K, ...

- <http://research.microsoft.com/en-us/collaboration/fourthparadigm/>



# S and R

- S: John Chambers (Bell Labs)
- S-plus: 1988: Douglas Martin (UWash)
- R: 1993: Ross Ihaka, Robert Gentleman
  - Current version 2.13 (13 April 2011)
  - Lexical scoping (ala Scheme)
  - Procedural/functions
  - Object Oriented
  - Command line



# R follows S

- Linear and nonlinear modeling
- Statistical tests
- Time series analysis
- Classification
- Clustering
- ...

<http://www.r-project.org/>

(25 standard/recommended packages)

# Comprehensive R Archive Network

- <http://cran.r-project.org/>,
- <http://www.bioconductor.org/>
- Over 4300 (3/11) user contributed packages
- Strength: people contributed
- Weakness: organic growth – uniformity lost (e.g. plots)

[AMORE](#)

A MORE flexible neural network package

[ARES](#)

Allelic richness estimation, with extrapolation beyond the sample size

[AcceptanceSampling](#)

Creation and evaluation of Acceptance Sampling Plans

[AdMit](#)

Adaptive Mixture of Student-t distributions

[AdaptFit](#)

Adaptive Semiparametric Regression

[AlgDesign](#)

AlgDesign

[Amelia](#)

Amelia II: A Program for Missing Data

[AnalyzefMRI](#)

Functions for analysis of fMRI datasets stored in the ANALYZE or NIFTI format

[Animal](#)

Analyze time-coded animal behavior data

# More extensively used

- 43% data-miners use R (Rexer's Annual Data Miner Survey in 2010; Boston; 735 in 60 countries)
- <http://rgl.neoscientists.org/about.shtml>  
(3D visualization with interface to R)
- RapidMiner  
<http://rapid-i.com/content/view/181/190/>)
- Weka (<http://www.cs.waikato.ac.nz/ml/weka/>)  
R interface

# Not so a few years ago ...

# VOStat

- Columns are autoselected (and can be deselected)
- Parameter choices for functions are conveniently placed
- Can be used from your own webpages on tables residing elsewhere
- Java/perl
- ASCII/fits

Column1:	Column2:	Column3:	Column4:	Column5:
<input type="text" value="date1"/>	<input type="text" value="id1"/>	<input type="text" value="date2"/>	<input type="text" value="id2"/>	<input type="text" value="ra"/>
Column6:	Column7:	Column8:	Column9:	Column10:
<input type="text" value="dec"/>	<input type="text" value="B-R"/>	<input type="text" value="R-I"/>	<input type="text" value="r-i"/>	<input type="text" value="i-z1"/>
Column11:	Column12:	Column13:	Column14:	Column15:
<input type="text" value="i-z2"/>	<input type="text" value="R-i"/>	<input type="text" value="I-z1"/>	<input type="text" value="I-z2"/>	<input type="text" value="I-I"/>

## Multivariate classification

[Kmeans partitioning\(m\)](#)

[H clustering\(m\)](#)

Apply cuts?  YES  NO

Clusters:

Metric:

Height to cut at:

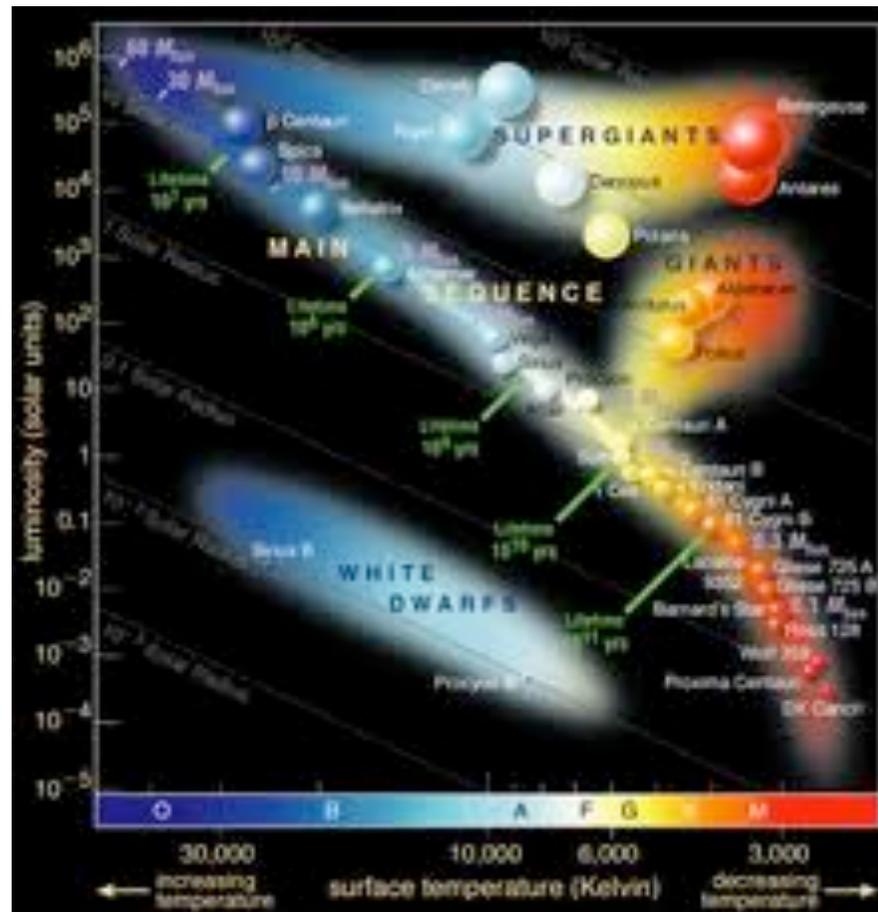
Max. iterations:

Method:

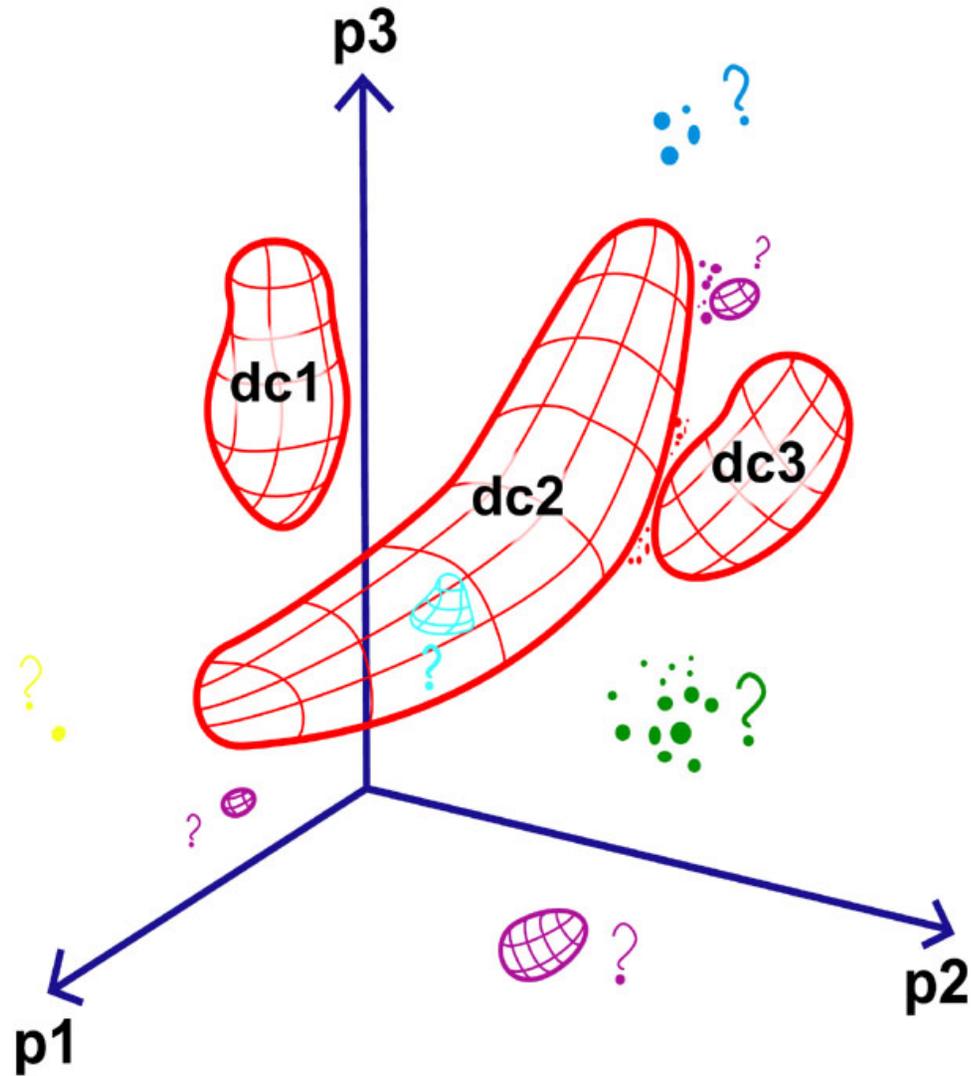
Clusters:

# Toy Demos

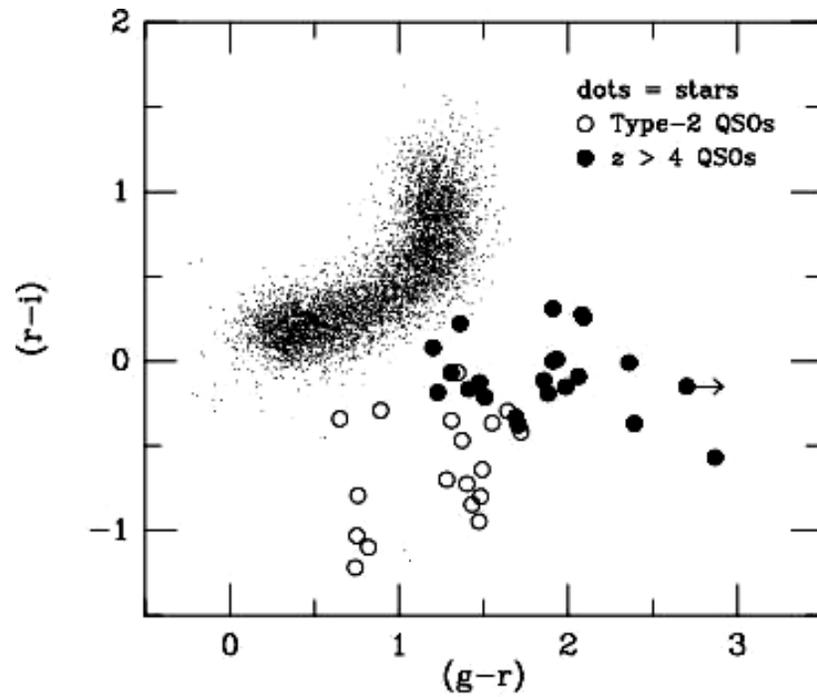
- Rediscovering HR diagram
- Rediscovering FP of Globular Clusters
- Looking for outliers in color-color space



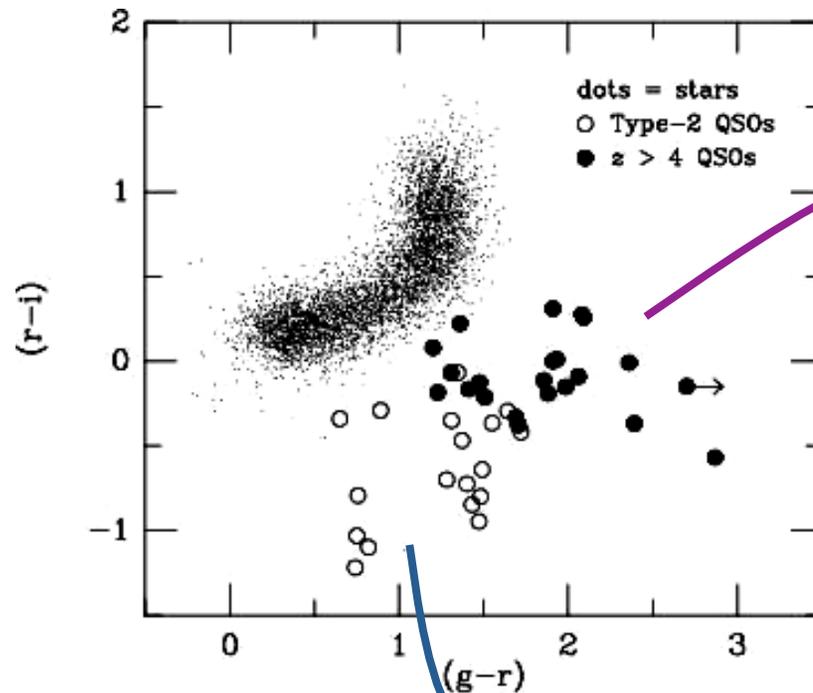
## A Generic Machine-Assisted Discovery Problem: Data Mapping and a Search for Outliers



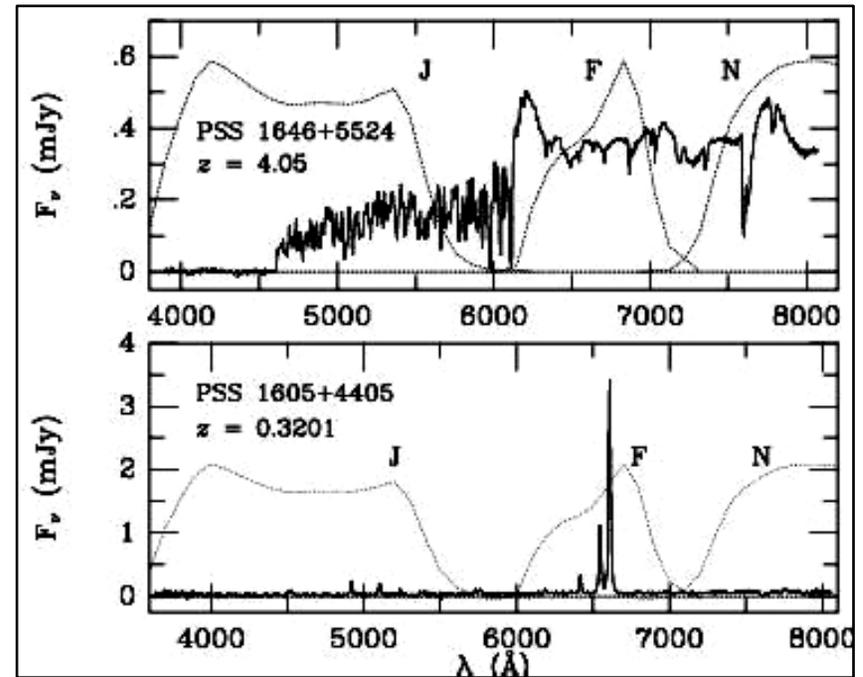
# An Example: Discoveries of High-Redshift Quasars and Type-2 Quasars



# An Example: Discoveries of High-Redshift Quasars and Type-2 Quasars



High- $z$  QSO



Type-2 QSO

# Simple Clustering Analysis: Gaussian Mixture Modeling

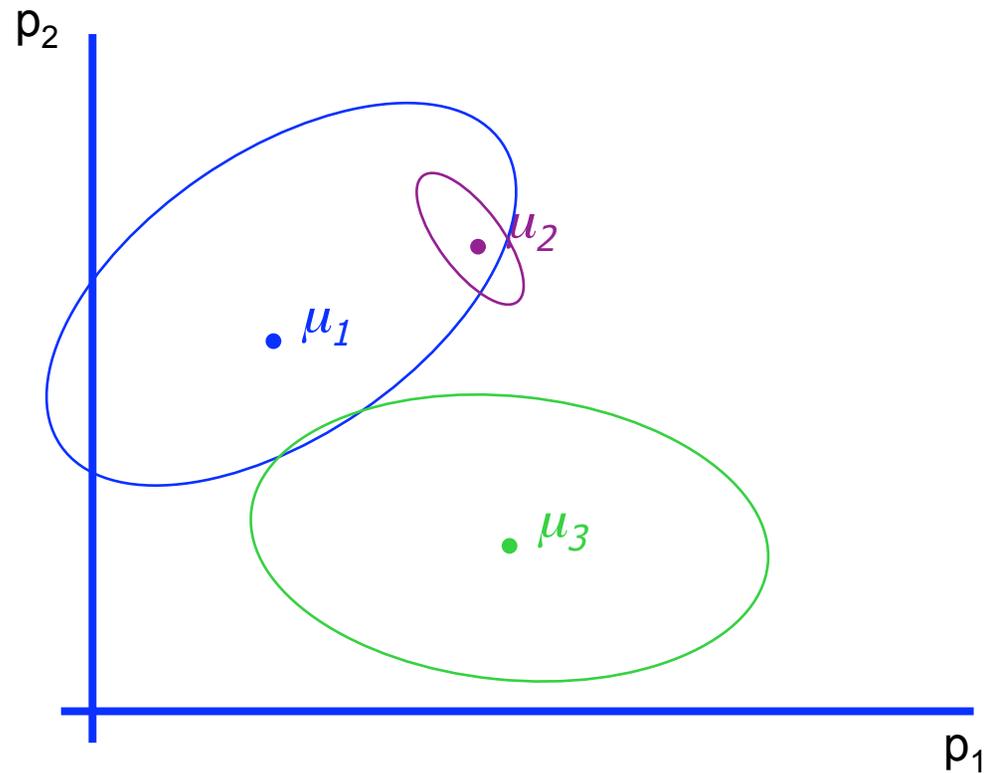
## Assumptions:

- There are  $k$  Gaussian components. The  $i$ 'th component is called  $w_i$
- Component  $w_i$  has an associated mean vector  $m_i$ , and a covariance matrix  $S_i$

## The challenge:

- Find  $k$  and all  $m_i$  and  $S_i$

**The ugly reality:** Things are seldom Gaussian



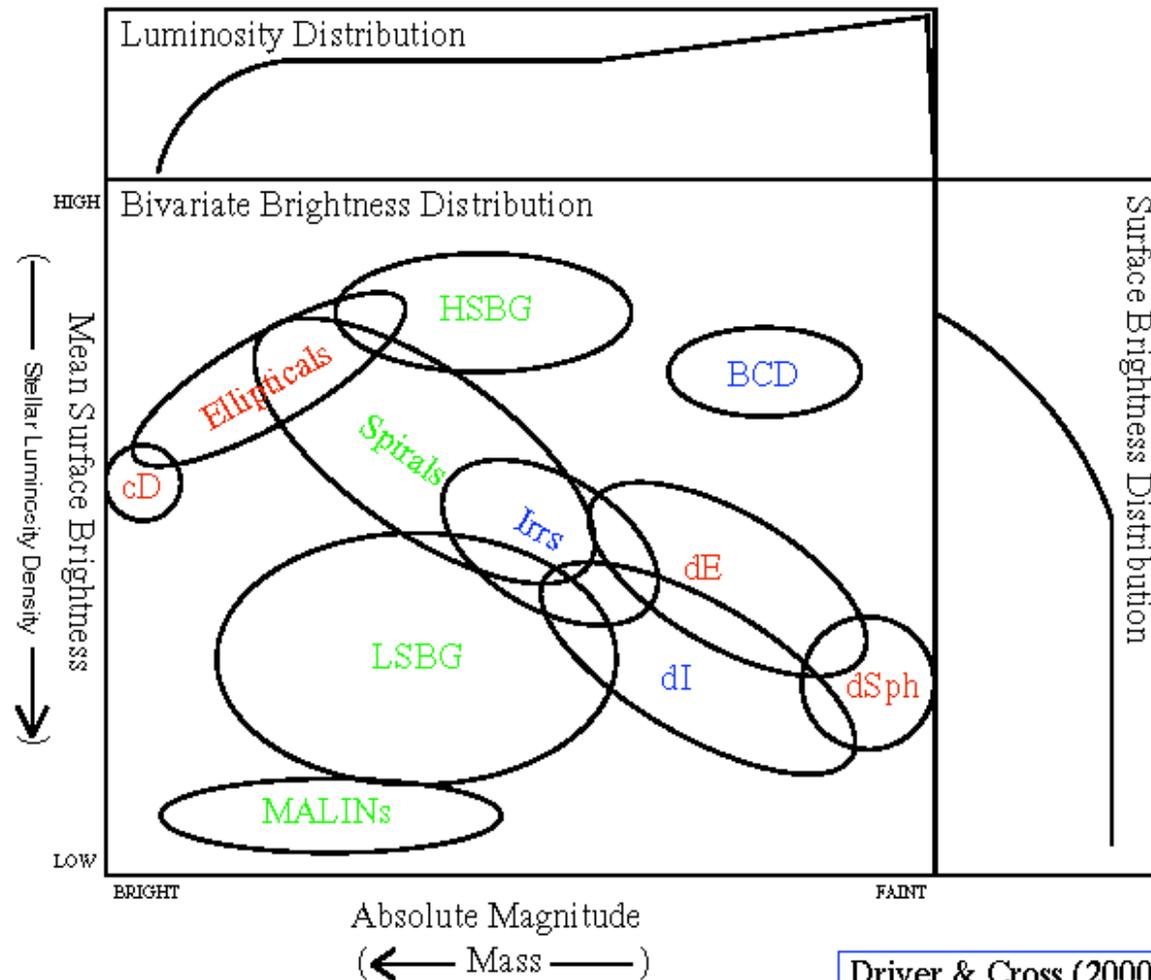
# Clustering Analysis:

How many different kinds of things do we have here, and who belongs to what group, with what probability?

## An example:

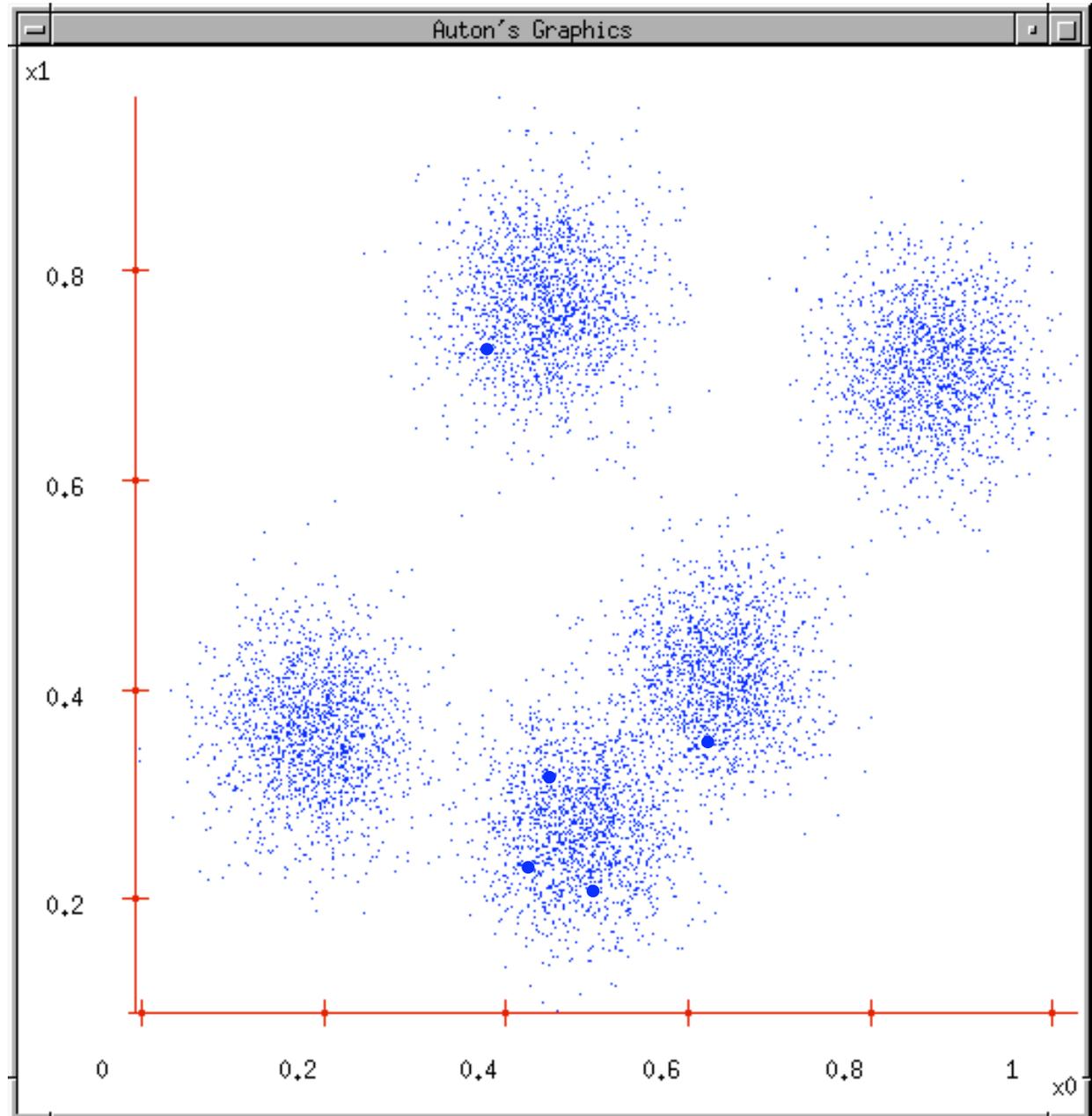
The bivariate luminosity and surface brightness distribution of galaxies.

(Also: subclustering, merged images, etc. etc.)

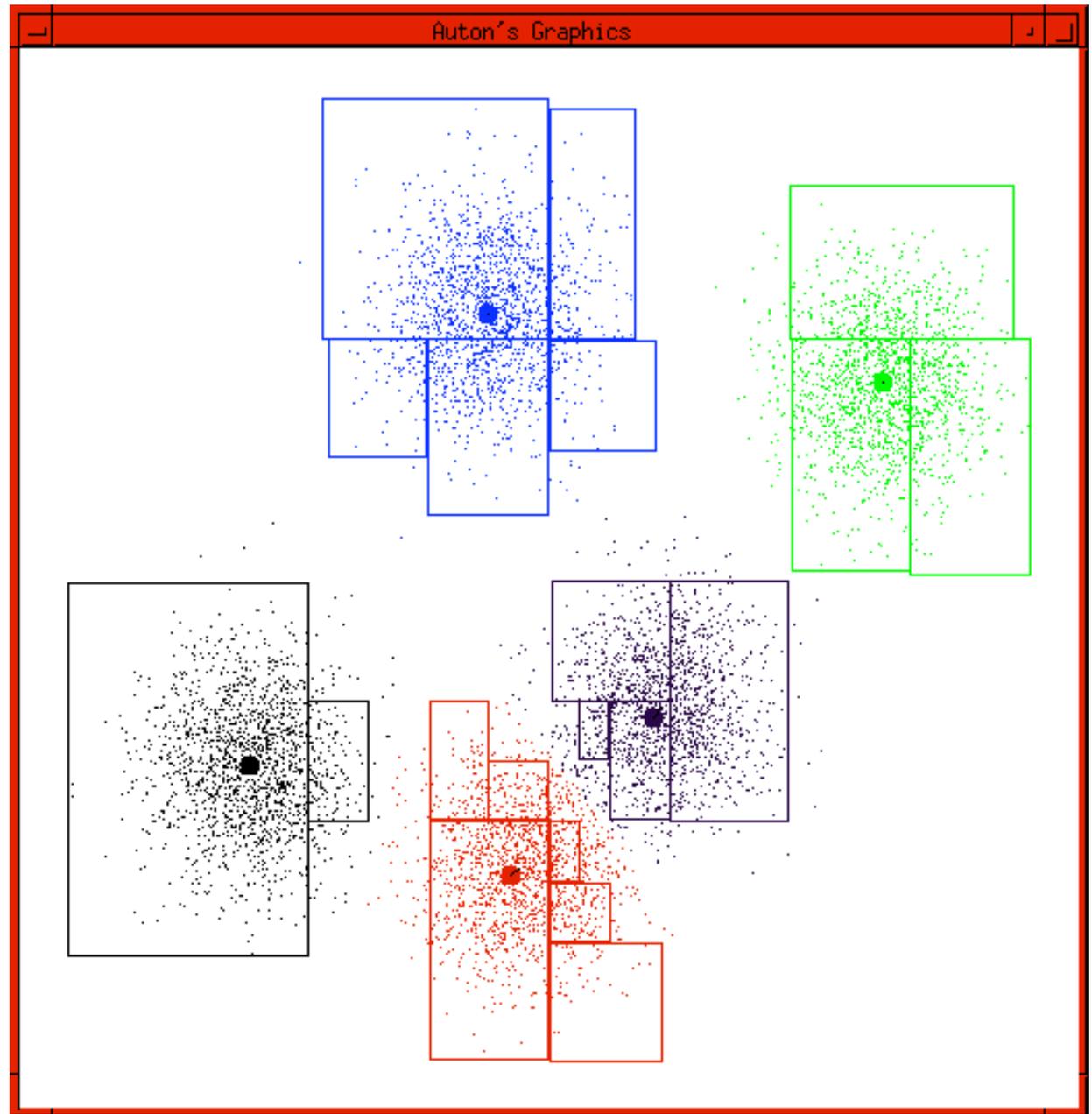


# K-means

1. Ask user how many clusters they'd like.  
(*e.g. k=5*)
2. Randomly (?) guess k cluster Center locations
3. Associate each data point with its nearest center
4. Compute the new mean centers
5. Iterate until some convergence criterion is reached

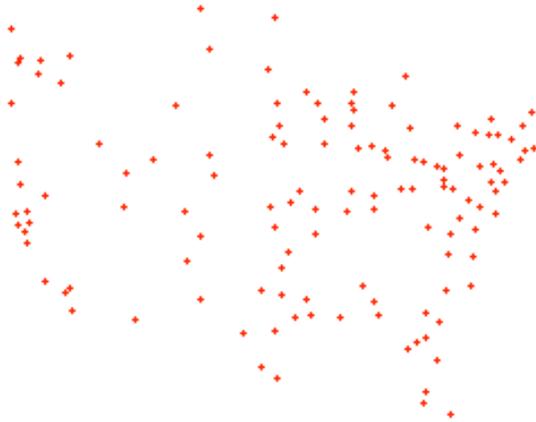


K-means  
terminates



# Minimal spanning trees

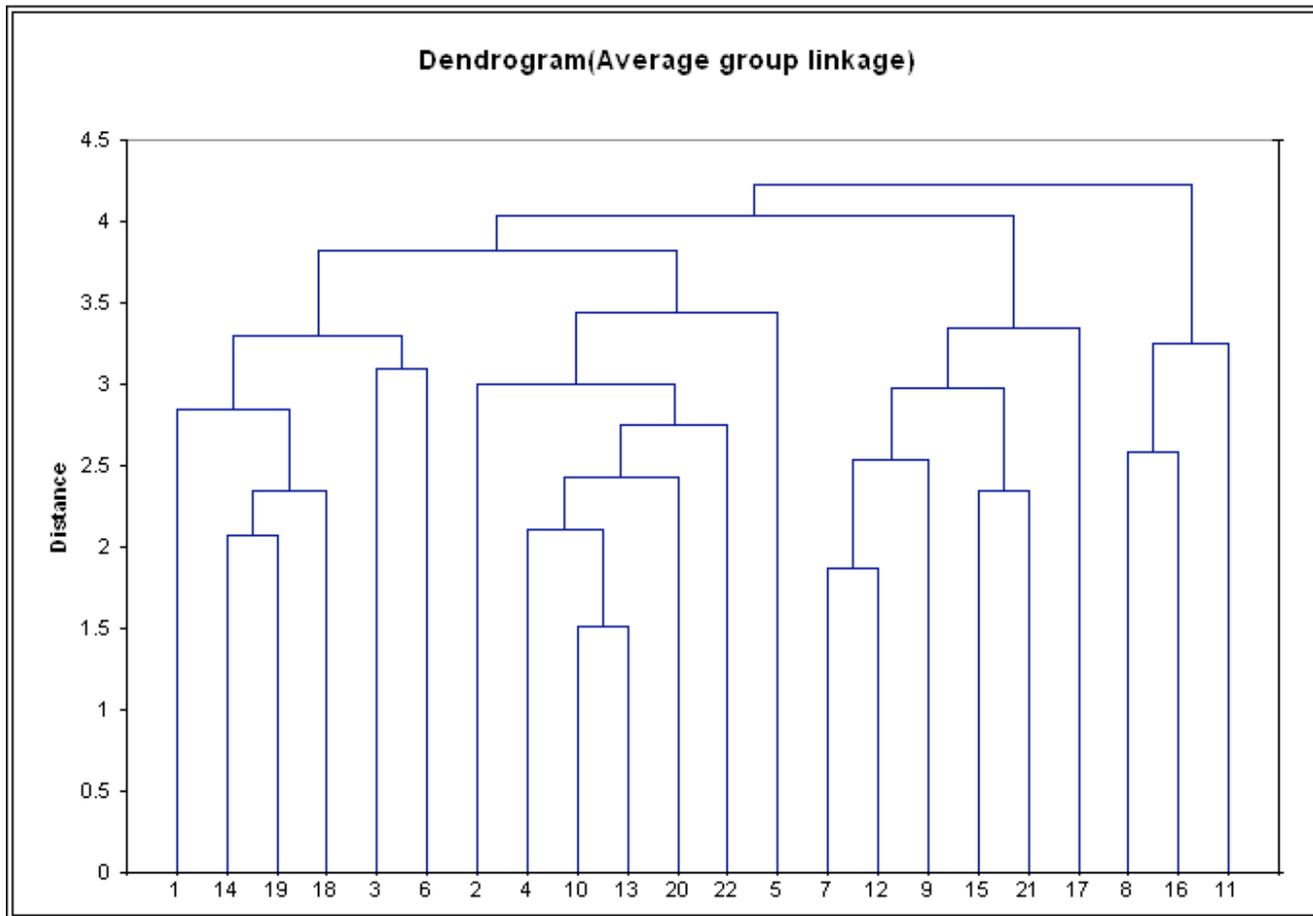
Minimum Spanning Tree



[www.combinatorica.com](http://www.combinatorica.com)

- Choose a point A and connect it to its nearest neighbor, B
- Now choose a point which is closest to either A, or to B
- Continue till all points are covered
- Cut-off at a required length

# Hierarchical clustering

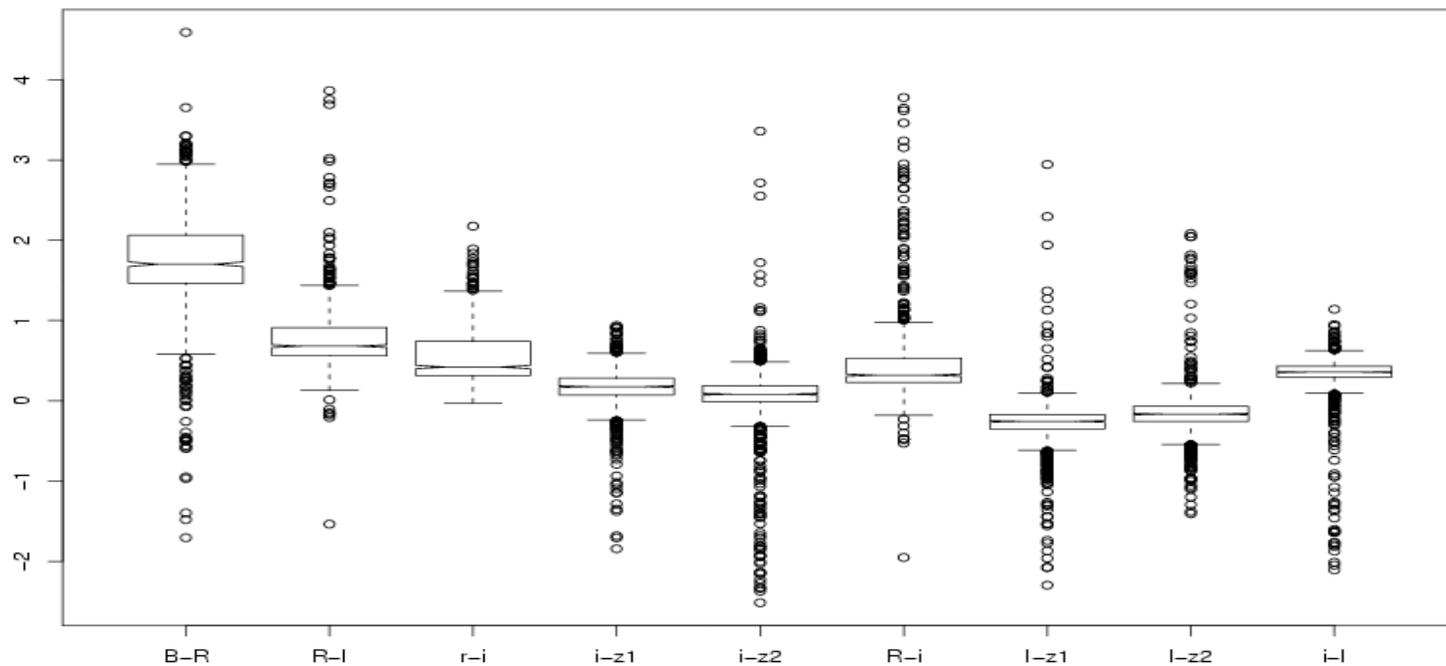


# Exploring outliers

- Palomar-QUEST synoptic sky survey
- 9 mix-and-match colors from 8 filters
- Aim: finding outliers in color-color space for spectroscopic follow-up
- 1000 random objects

# Boxplot

- Reveals relationships between colors (mean, median, overlap, outliers)



# Clustering

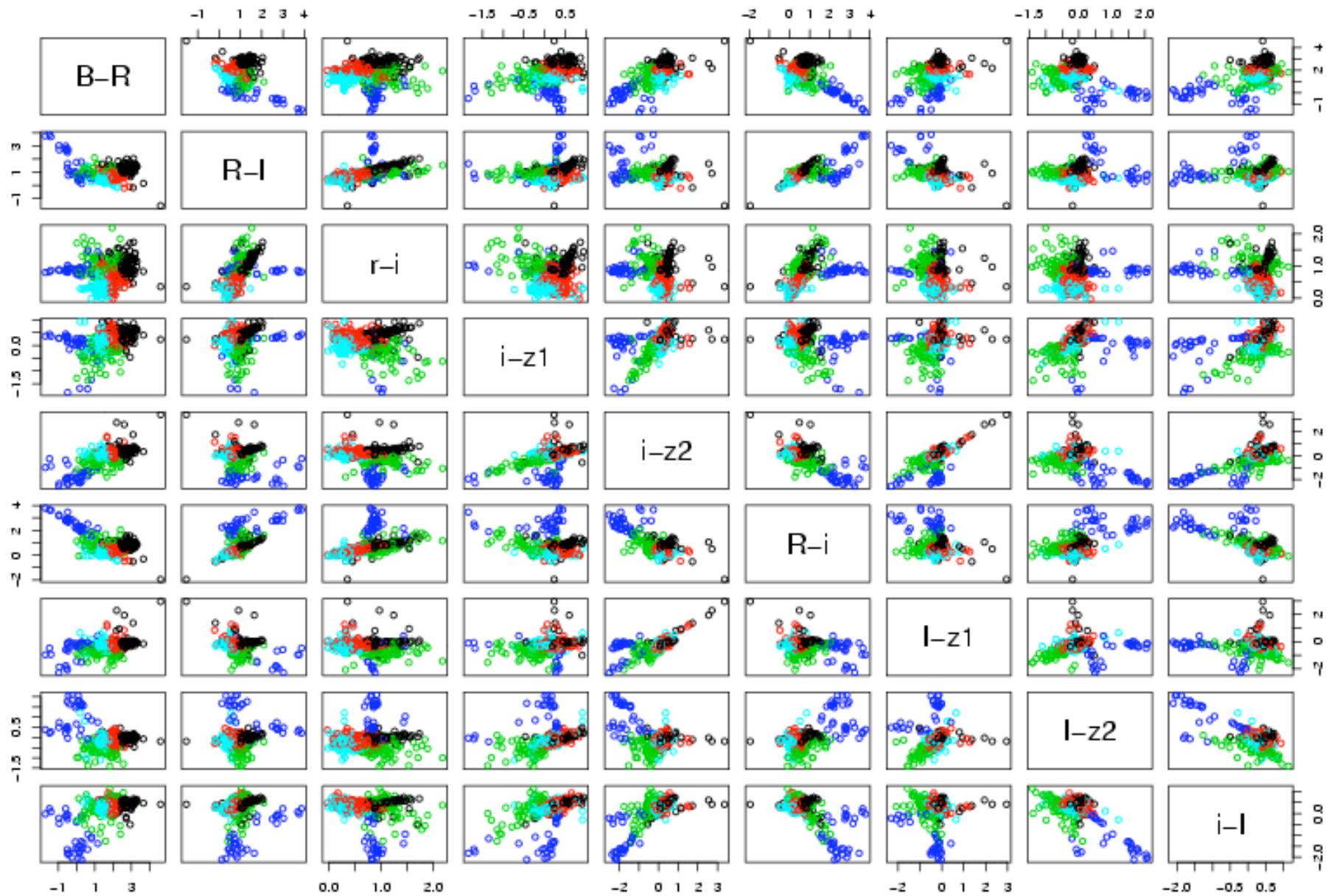
- K-means provides various cluster centers along with withinss and a list of possible outliers

```
> print(cl$size)
[1] 75 122 480 289 33

> print(cl$centers)
      x2.1553  x0.8833  x0.563  x0.2347  x0.1909  x0.5069  x0.1855
1  1.4074840 0.9671000 1.0442640 -0.29106000 -0.51805867 0.7100160 -0.77514267
2  2.6638713 1.1741434 0.9580811 0.40006393 0.39761967 0.7380221 -0.03850164
3  1.5062098 0.5789365 0.3302465 0.12387542 0.05890729 0.2437696 -0.27625958
4  2.0228934 0.7910471 0.5455412 0.24857820 0.15998754 0.4003003 -0.23075917
5 -0.1626848 1.5104515 0.8905485 -0.08033333 -1.67197273 2.5554939 -0.62693030
      x0.1417  x0.3764
1 -0.54814400 0.2570840
2 -0.03605738 0.4361213
3 -0.21129146 0.3351669
4 -0.14216851 0.3907467
5 0.96470909 -1.0450424

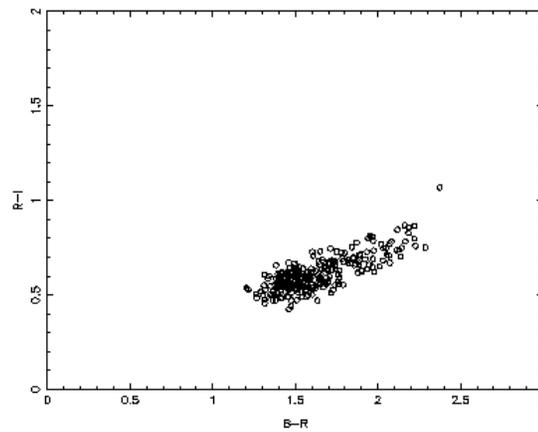
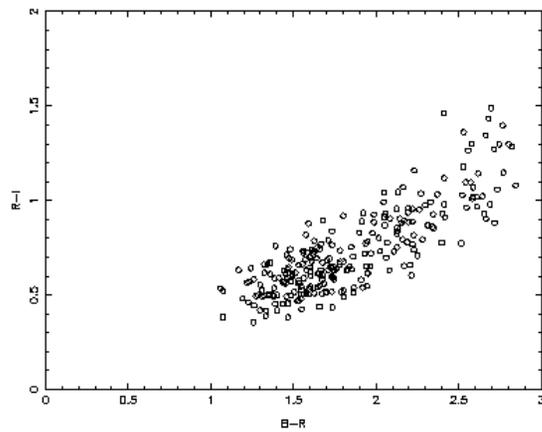
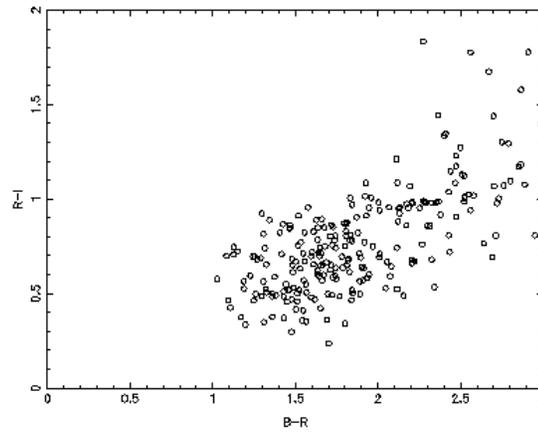
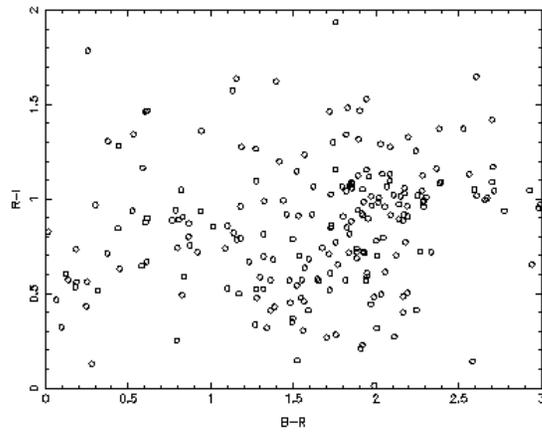
> print(cl$withinss)
[1] 118.08204 126.88979 95.40461 87.19068 142.91592

> print(cl$cluster)
[1] 1 4 3 2 3 3 3 4 3 3 3 3 3 3 3 4 4 3 3 4 3 3 3 3 3 4 5 3 3 3 3 3 3 3 3 5
```



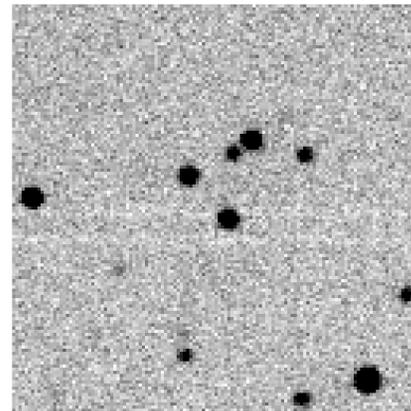
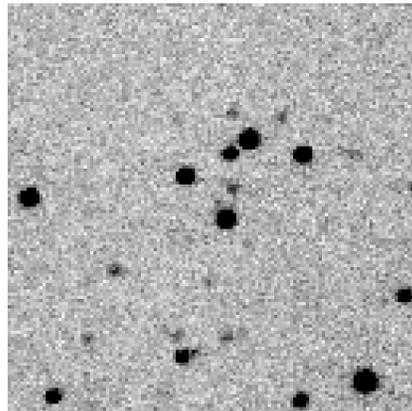
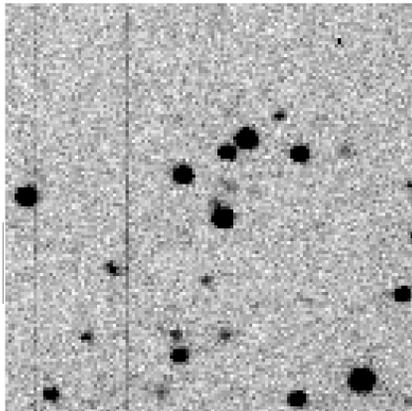
# K-density

- Probability - density association for outliers



# Visual confirmation

(found from 1000 random objects)



# Running R

1. Create a separate sub-directory, say `work`, to handle a particular problem.

```
$ mkdir work  
$ cd work
```

2. Start the R program with the command

```
$ R
```

3. At this point R commands may be issued (see
4. To quit the R program the command is

```
> q()
```

You can optionally save data.

# Getting help

- `help(solve)`
- `?search`
- `help("[[")`
- `help.start()`     # this is for html help
- `??matrix`
- `example(pairs)`

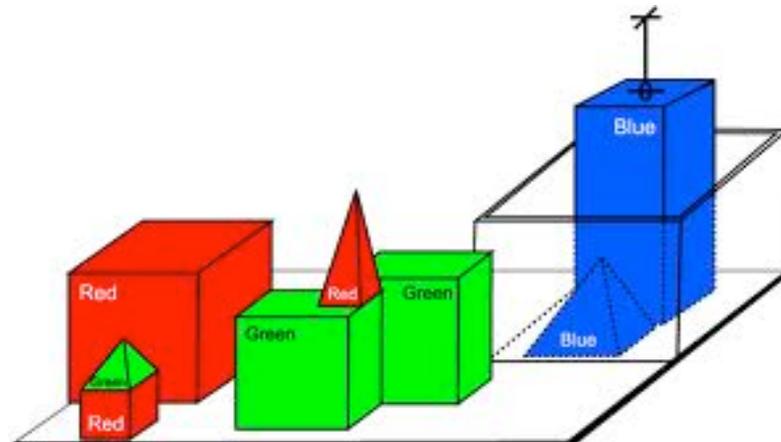


- source is like <
- sink is like >
- .Rhistory, .Rdata
- ls()/objects(), rm() deal with objects
- ls()
- rm(list = ls())

# Dealing with tables/objects (R frame)

- `X = read.table("foo",header=TRUE)`
- `objects()`
- `objets(X)`
- `names(X)`
- `X`
- `Name1`
- `X$Name1`
- `attach(X)`
- `Name1`

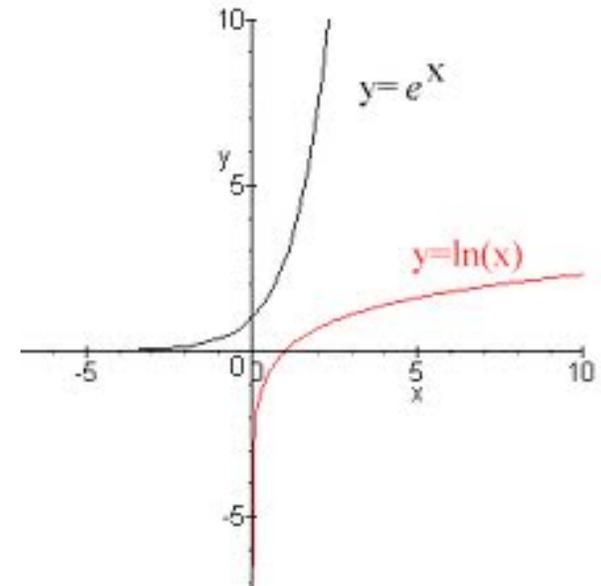
Num	Name1	Name2
1	1.1	3.3
2	4.4	5.4



# Assignments

- `x <- c(10.4, 5.6, 3.1, 6.4, 21.7)`
- `assign("x", c(10.4, 5.6, 3.1, 6.4, 21.7))`
- `c(10.4, 5.6, 3.1, 6.4, 21.7) -> x` (!)
- `1/x` # 0.09,0.17,0.32,0.15,0.04
- `y <- c(x,0,x)` # 10.4,.. ,21.7,0,10.4,..,21.7
- `v <- rep(x) + y + 1` # x repeated 2.2 times, 1 11
- `var = sum((x-mean(x))^2)/(length(x)-1)`

# Simple/standard functions



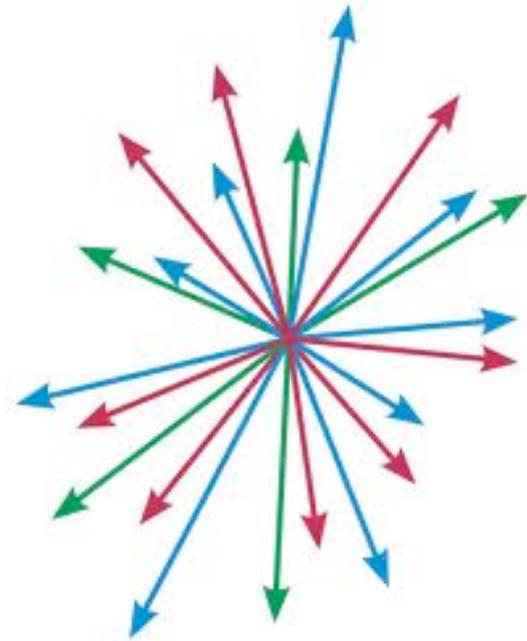
- $+ - * / ^$
- log, exp, sin, cos, tan, sqrt
- range, min, max, length, sum, var, prod, sort
- sort.list, order, pmax, pmin
- `sqrt(-17+0i)` # overloaded operators

# Sequences

- `1:30` # 1,2,3,
- `n <- 10; 1:n-1; 1:(n-1)` # : has precedence
- `2*1:15` #2,4,...,30
- `seq()` with named params: to, from, by, length
  - `s4 <- seq(length=51, from=-5, by=.2)`
  - Along can be used only by itself to create same sized vector as another `1:length(vector)`
- `s5 <- rep(x, times=5)` # `x1 x2 .. Xn x1 x2 ...`
- `s6 <- rep(x, each=5)` # `x1 x1 x1 x1 x1 x2 x2 ..`

# Logical vectors

- `n <- x >13`      # conditional
  - TRUE, FALSE, NA
  - `length(n) == length(x)`
  - `c1 & c2`      # intersection
  - `c1 | c2`      # union
  - `!c1`      # negation
  - FALSE = 0 and TRUE = 1 when coerced
  - Missing values, NA, NaNs `is.nan(x)`



# Indexing

- `x[1:10]` # get first 10
- `x[-(1:5)]` # leave out first 5
- `x[is.na(x)] <- 0` # replace missing values by 0
- `y[y < 0] <- -y[y < 0]` OR `y <- abs(y)`

- 
- `labs <- paste(c("X","Y"), 1:10, sep="")`  
`== c("X1", "Y2", "X3", "Y4", "X5", "Y6", "X7",  
"Y8", "X9", "Y10")`

# Classes of objects and unclass()

- Matrices
- Factors (categorical data)
- Data matrices
- Functions
- (also numeric, character, logical, raw)
- Vectors are atomic (all elements of one mode)
  - Coercion easy
- Lists are non-atomic (are recursive too)

# Arrays and matrices

- `dim(z) <- c(3,5,100)` # 3-d array with size
- `c(a[2,1,1], a[2,2,1], a[2,3,1], a[2,4,1],  
a[2,1,2], a[2,2,2], a[2,3,2], a[2,4,2])`
- `a[,,]` # the entire array
- `x <- array(1:20, dim=c(4,5))` # 4 by 5 array
- `i <- array(c(1:3,3:1), dim=c(3,2))` # 3x2 array
- `x[i] <- 0` # set elements 9, 6, 3 of x to 0

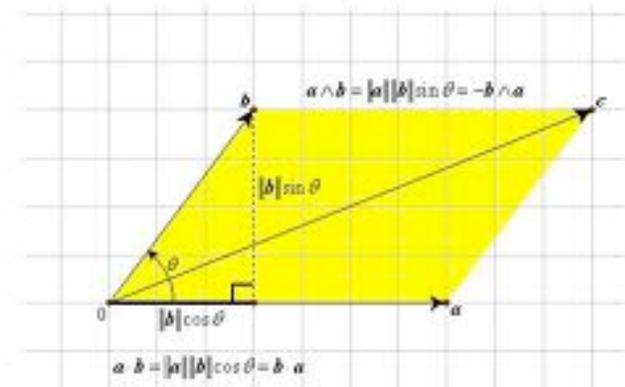
# Outer products, functions

- `ab <- a %o% b`
- `ab <- outer(a, b, "*")`

Generalized

- `f <- function(x, y) cos(y)/(1 + x^2)`
- `z <- outer(x, y, f)`

- `A * B` # element by element matrix product
- `A %*% B` # matrix multiplication
- `"%!%" <- function(X, y) { ... }`



# Lists (and data.frames=restricted)

- `Lst <- list(name="Fred", wife="Mary", no.children=3, child.ages=c(4,7,9))`
- Always numbered
- `Lst[[4]]` # returns `[1] 4 7 9`
- `Lst[[4]][2]` # returns `7`
- `Lst[4][2]` # returns `Null`
- `Lst[3]` # returns `$no.children [1] 3`

# Reading from files

- `HousePrice <- read.table("houses.data", header=TRUE)`
- `read.table(file, header = FALSE, sep = "", quote = "\"", dec = ".", row.names, col.names, as.is = !stringsAsFactors, na.strings = "NA", colClasses = NA, nrows = -1, skip = 0, check.names = TRUE, fill = !blank.lines.skip, strip.white = FALSE, blank.lines.skip = TRUE, comment.char = "#", allowEscapes = FALSE, flush = FALSE, stringsAsFactors = default.stringsAsFactors(), fileEncoding = "", encoding = "unknown")`

`read.csv, read.csv2, read.delim, read.delim2`

# Accessing built-in datasets

©2002 Shannon Burns

www.shannonburns.com



"I hope that wasn't our pilot."

- `data()`
- `data(AirPassengers)`
- `?AirPassengers`
- `new <- edit(AirPassengers)`
- `x<-array(c(AirPassengers[1:144]),dim=c(12,12))`
- `pairs(x)`

# Conditionals

- `if (expr_1) expr_2 else expr_3`
- `for (name in expr_1) expr_2`
- `while (condition) expr`

- Scope
- Arguments
- Customizing
- Factors
- Contrasts

# Plotting

- `plot(x, y)` # scatterplot
- `plot(xy)` # scatterplot from 2-col matrix
- `plot(x)` # timeseries or real/img
- `plot(f)` # barplots for factors
- `plot(f, y)` # boxplots for factors
- `pairs(X)`
- `hist()`, `dotchart()`, `image()`, `contour()`, ...
- `points()`, `text()`, `math`, `multiple`, `interactive`

Demo

# colors and classification

- `d2 = read.table("dataset2.Rframe",header=TRUE)`
- `objects()`
- `names(d2)`
- `umg`
- `d2$umg`
- `attach(d2)`
- `umg`
- `plot(umg,gmr)`
- `pairs(d2)`

- `demo(graphics)` to see some graphics capabilities
- `library(ggplot2)`
- `help(diamonds)`
- `dsmall <- diamonds[sample(nrow(diamonds), 100), ]`
- `qplot(carat, price, data=dsmall, shape=cut)`
- `dsmall`
- `qplot(carat, price, data=diamonds, alpha=1/(500))`
- `qplot(carat, price, data=diamonds, geom=c("smooth", "point"))`
- `qplot(carat, data=diamonds, geom="density", colour = color)`