

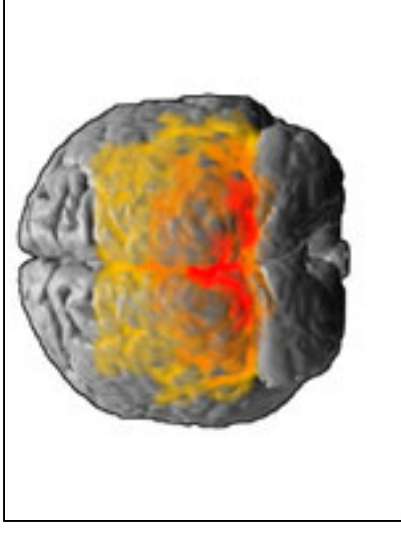
Application of data visualisation in particle physics

Steve Watts

BITlab

School of Engineering and Design
Brunel University, West London, UK

University of Manchester – from Jan ‘07

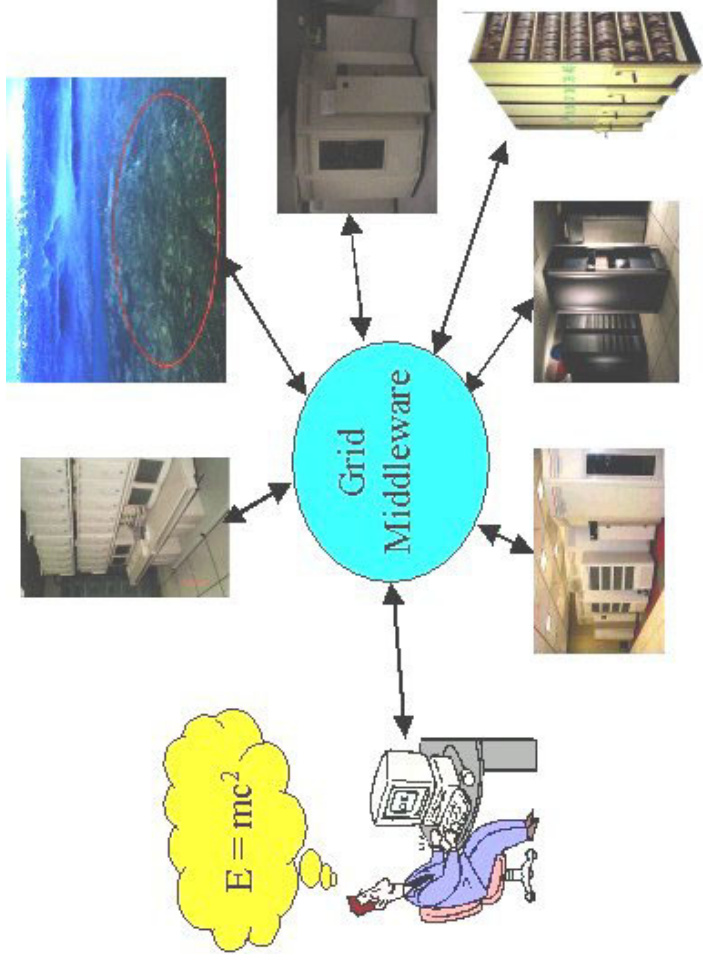


NOTE: “The visual cortex is the most massive system in the human brain and is responsible for higher-level processing of the visual image. It lies at the rear of the brain (highlighted in the image), above the cerebellum”

There is more to data visualisation than histograms, scatterplots and x/y plots.

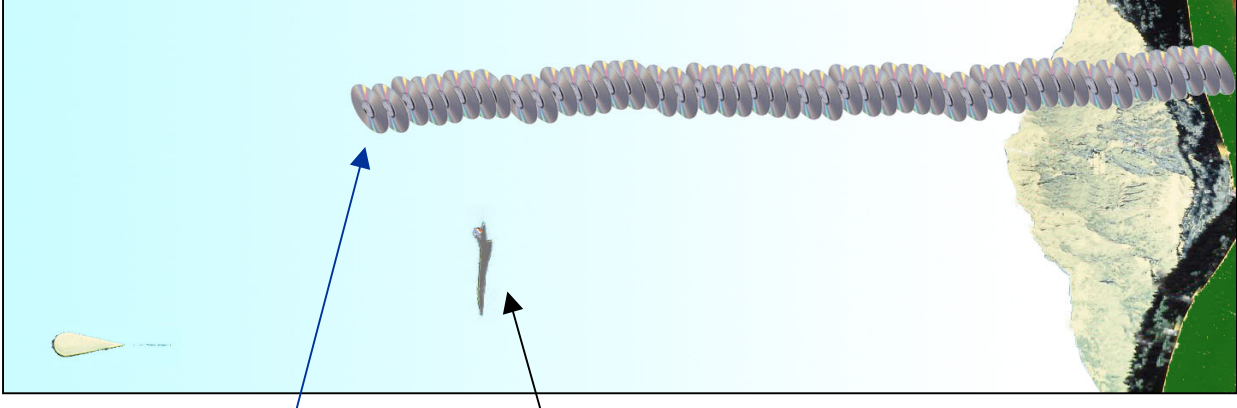
Edinburgh 8 November 2006

- WHAT SPARKED THE INTEREST ???
- INTRODUCTION TO DATA MINING
- DATA VISUALISATION
(history, look at a PP dataset, **parallel coordinates**, **brushing**, **pruning**...)
- CLASSIFICATION ALGORITHMS
Analysis of **wine dataset** (**Decision Trees**, **SVM**, **kNN**)
Links to visualisation – e.g. **GRAND Tour**, **Radviz**, **polyviz**
- ANALYSIS of PP dataset with different techniques
- OTHER USEFUL VISUALISATION TECHNIQUES
(**survey plots**, **heat maps**, **mosaic display**)
- DIY (Do it yourself) – some advice.
- CONCLUSIONS



CD stack with
1 year LHC data
(~ 20 km)

(Ex-)Concorde
(15 km)



GRID computing gives massive computing power.
No excuse for not being smarter with data analysis techniques

Thanks to Steve Lloyd for the nice pictures.....

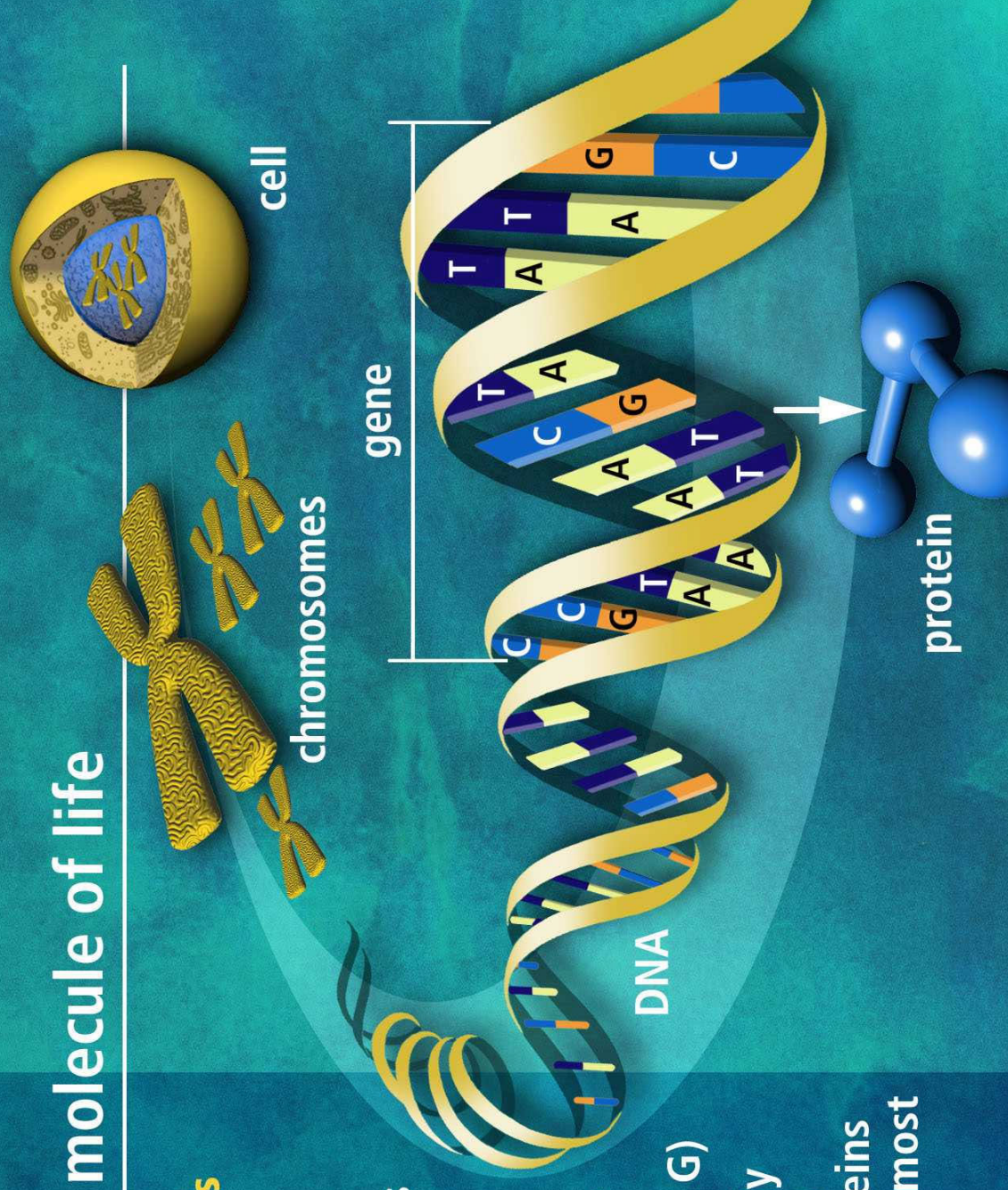
MANY AREAS OF MODERN SCIENCE, ENGINEERING,
HUMANITIES AND ARTS HAVE A DATA OCEAN TO SWIM IN !!!

DNA the molecule of life

Trillions of cells

Each cell:

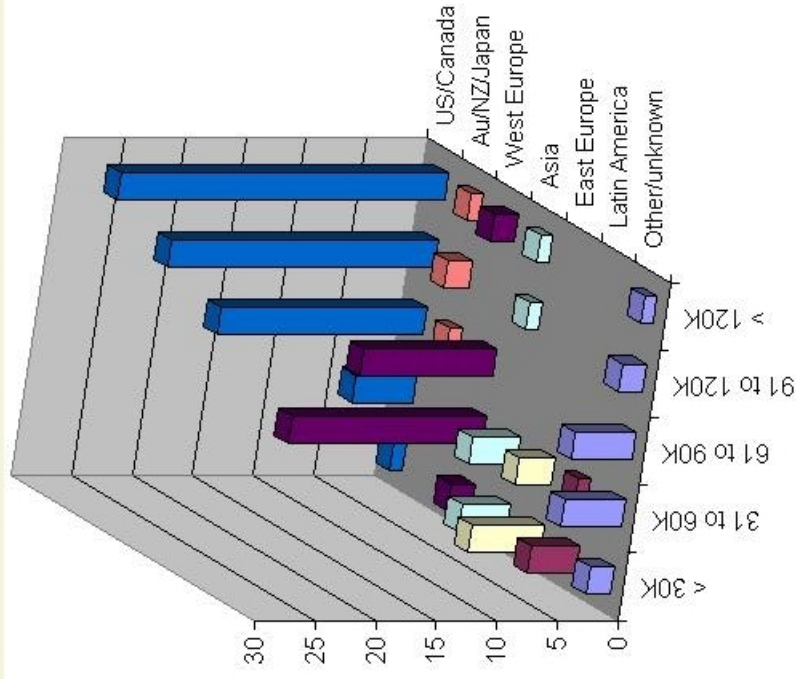
- 46 human chromosomes
- 2 meters of DNA
- 3 billion DNA subunits (the bases: A, T, C, G)
- Approximately 30,000 genes code for proteins that perform most life functions



Data mining, also known as knowledge-discovery in databases (KDD), is the practice of automatically searching large stores of data for patterns. To do this, data mining uses computational techniques from statistics and pattern recognition.
en.wikipedia.org/wiki/Datamining

http://www.kdnuggets.com/polls/2006/data_miner_income_by_region.htm

The following graph shows the breakdown of income (salary) by region, with number of respondents on the vertical axis (excluding students). (Note: the poll asks for income to include data miners who work for a company as well as self-employed).



The message is clear!

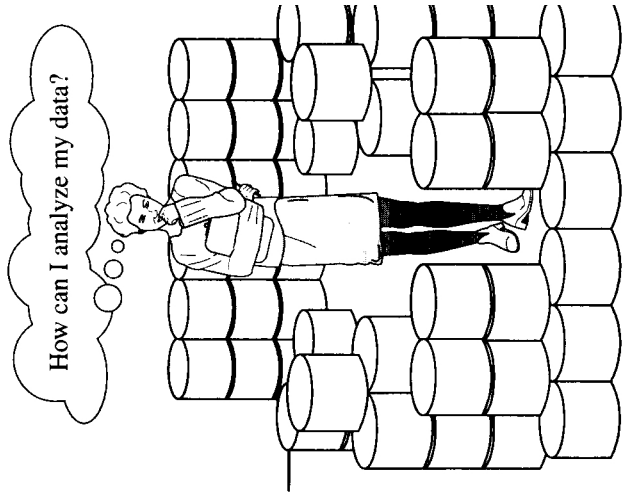


Figure 1.2 We are data rich, but information poor.

**Data Mining:
Concepts and Techniques
2nd ed. Jiawei Han
Micheline Kamber**

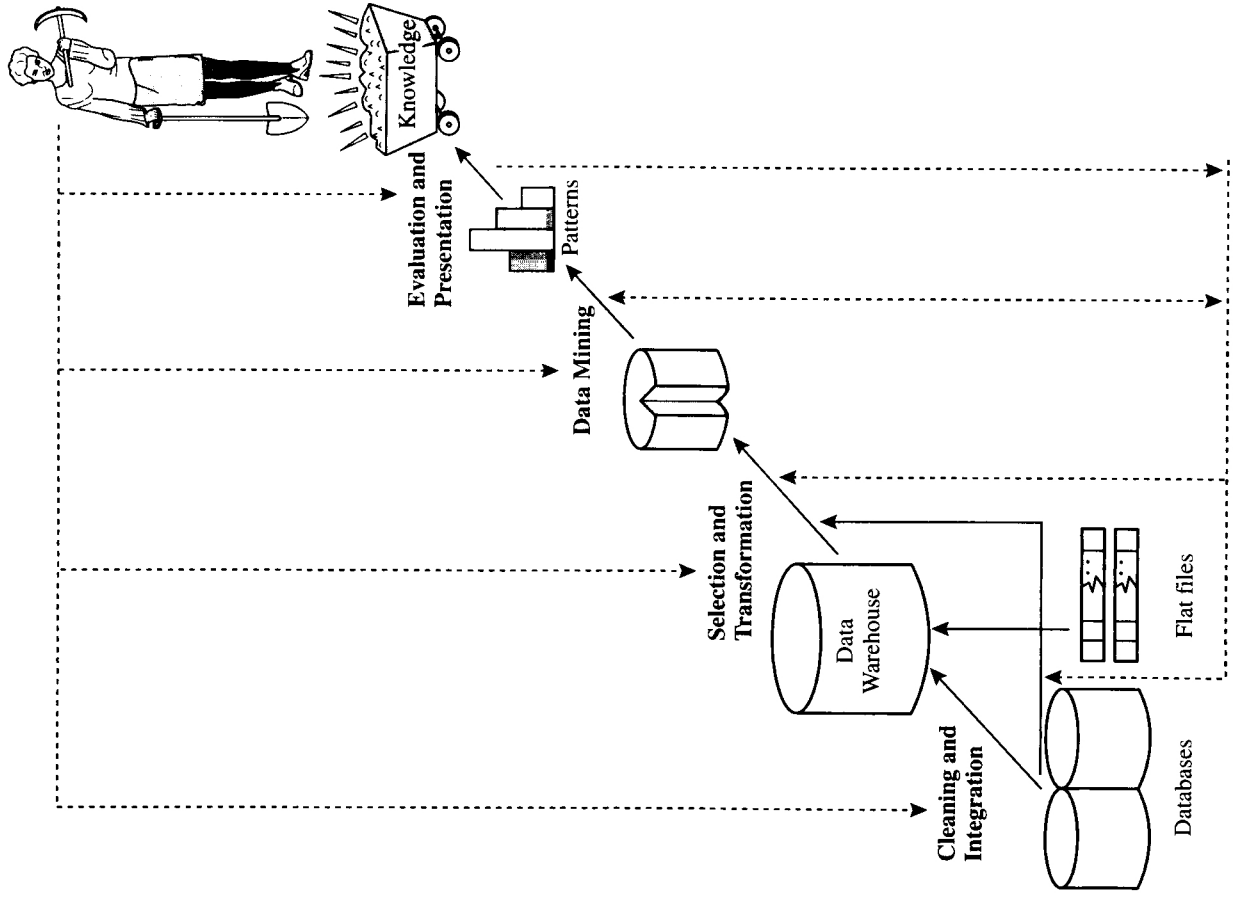


Figure 1.4 Data mining as a step in the process of knowledge discovery.



[project](#) - [software](#) - [book](#) - [publications](#) - [people](#) - [related](#)

“We are drowning in information
and starving for knowledge”

Rutherford D Roger

“Information is not knowledge”
Albert Einstein

Data Mining: Practical Machine Learning Tools
and Techniques (Second Edition)

Ian H. Witten, Eibe Frank

Morgan
Kaufmann
June 2005
525 pages
Paper
ISBN
0-12-088407-0



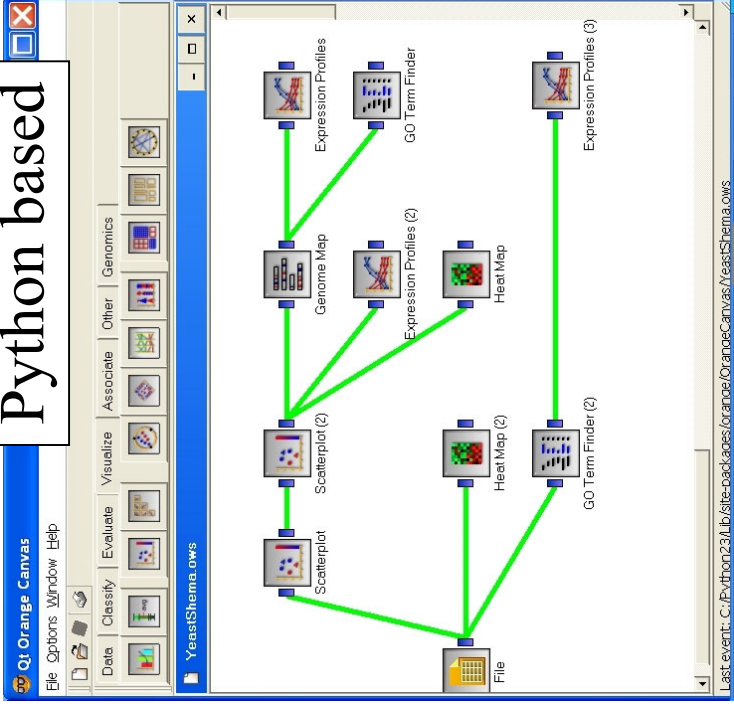
Eibe Frank and Ian
Witten



Statistical
Learning
KEY TEXT

WEKA Machine Working Workbench
Waikato Environment for Knowledge Analysis

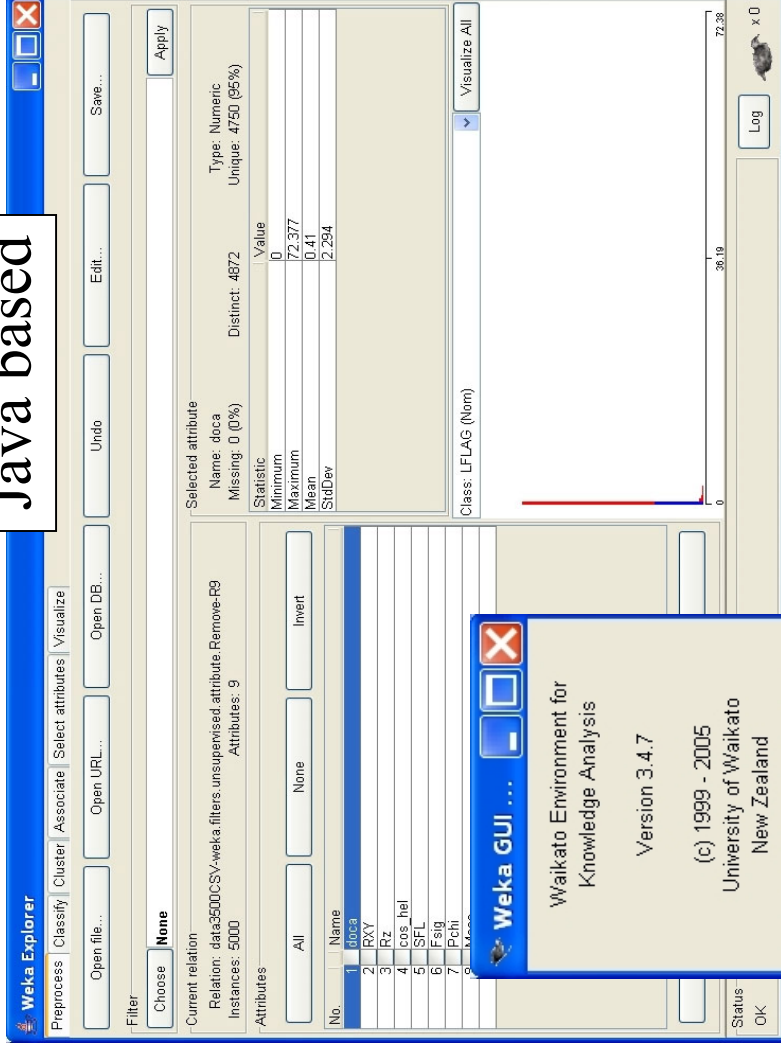
Python based



<http://www.ailab.si/orange>

KEY TERMS
Preprocess Data
Classify
Cluster
Associate
Visualisation

Java based

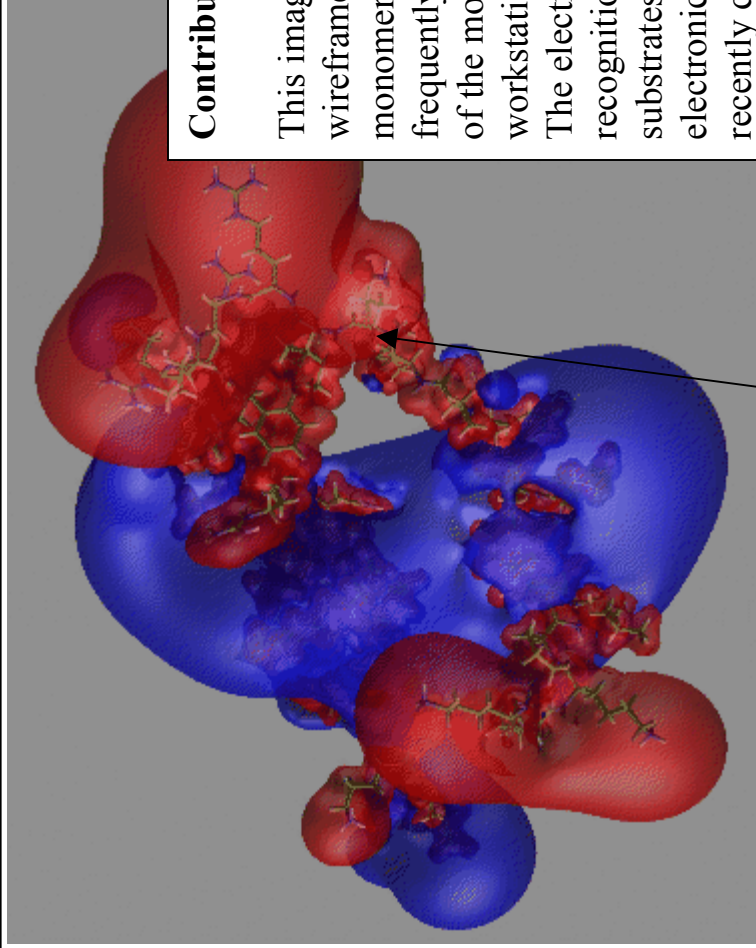


Knowledge Flow
Similar to ORANGE
intrinsic

<http://www.cs.waikato.ac.nz/~ml/weka/>

<http://www.msi.umn.edu/software/dx/tutorial/dx-images.html>

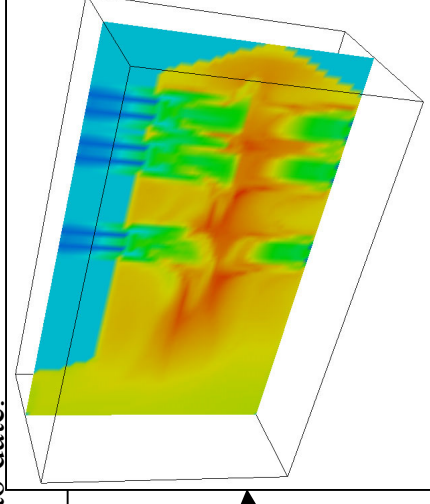
Examples of scientific visualisation



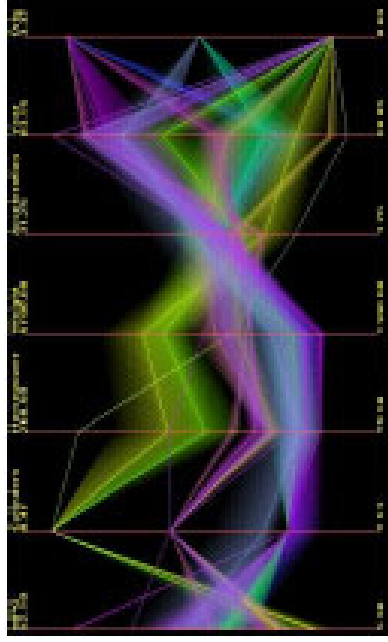
Contributors: Matt Challacombe and Eric Schwegler

This image shows a view of electrostatic potential iso-surfaces and a wireframe representation of the p53 tumor suppressor tetramerization monomer. Mutations in the p53 tumor suppressor are the most frequently observed genetic alterations in human cancer. The structure of the monomer's electrostatic potential has been rendered on an SGI workstation using iso-surfaces corresponding to -0.06 and $+0.06$ au. The electrostatic potential is widely implicated in molecular recognition, binding, and the enhanced diffusion of charged substrates. These results have been obtained from first principles electronic structure calculations using linear scaling Hatree-Fock theory recently developed at the University of Minnesota. Involving 3836 basis functions, this calculation was performed in 3 cpu days on an IBM RS6000 model 590 workstation, and is the largest Gaussian-based *ab initio* calculation performed to date.

AVS Express
Paraview - free !
Tecplot
IBM Data Explorer
VisIt - free



The **pseudocolor plot** (right) is used to map temperature to color on the same planar slice.



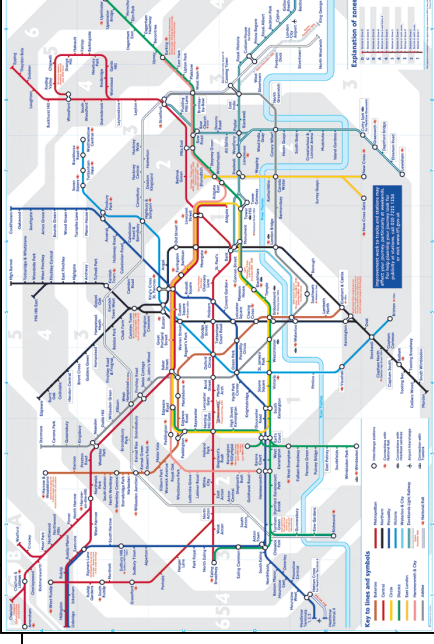
Information Visualization image shown courtesy of Matt Ward of Worcester Polytechnic Institute (WPI).

Information Visualisation

Displaying information to help the user understand it better. Abstraction of data.

Example above I would categorise as **Data Visualisation**

The London Tube map I would categorise as **Information Visualisation** – recommend you read Edward Tufte

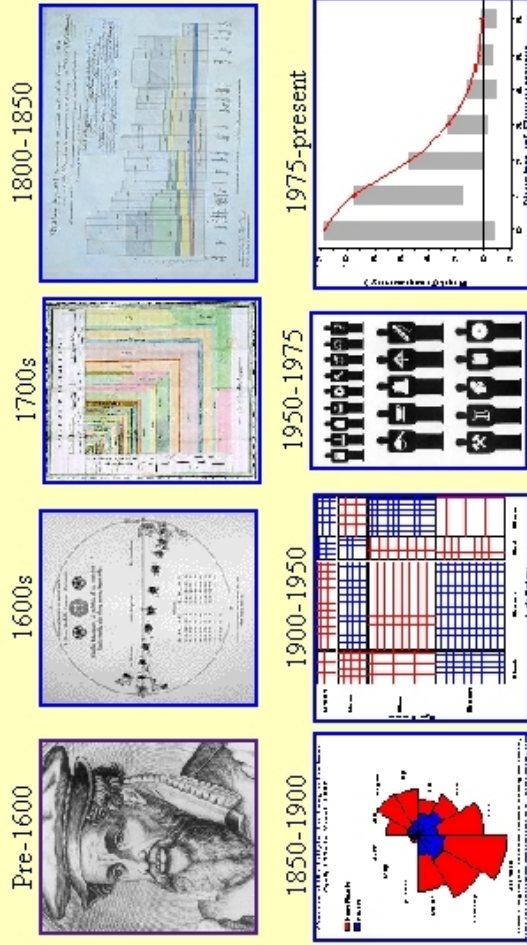


SciVis - late '80s
InfVis - late '90's

This is a vast new field - especially important for **data mining**

Milestones in the History of Thematic Cartography, Statistical Graphics, and Data Visualization

An illustrated chronology of innovations
by Michael Friendly and Daniel J. Denis



- [Up: Gallery](#)
- [Introduction](#)
- [1600s](#)
- [1700s](#)
- [1800+](#)
- [1850+](#)
- [1900+](#)
- [1950+](#)
- [1975+](#)
- [Search](#)

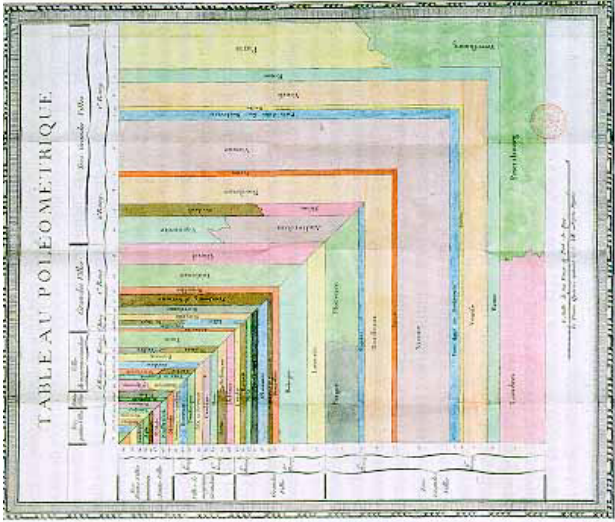
See also:

- [This document in PDF form, with active links. \(You need Adobe Acrobat Reader\)](#)
- [Chapter on the Milestone Project in C. Wehs and W. Gaul \(eds.\), Classification-- The Ubiquitous Challenge, Springer, 2005.](#)
- [Images from the JSM 2002 Technical Poster Session \[Thanks to Andy Mauromoustakos!\]:](#)
 - [Image1](#) (864 x 648; 123K);
 - [Image2](#) (864 x 648; 124K).

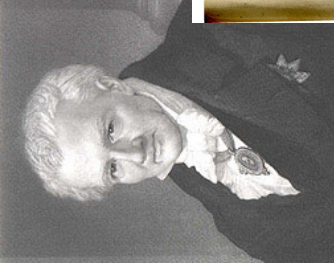
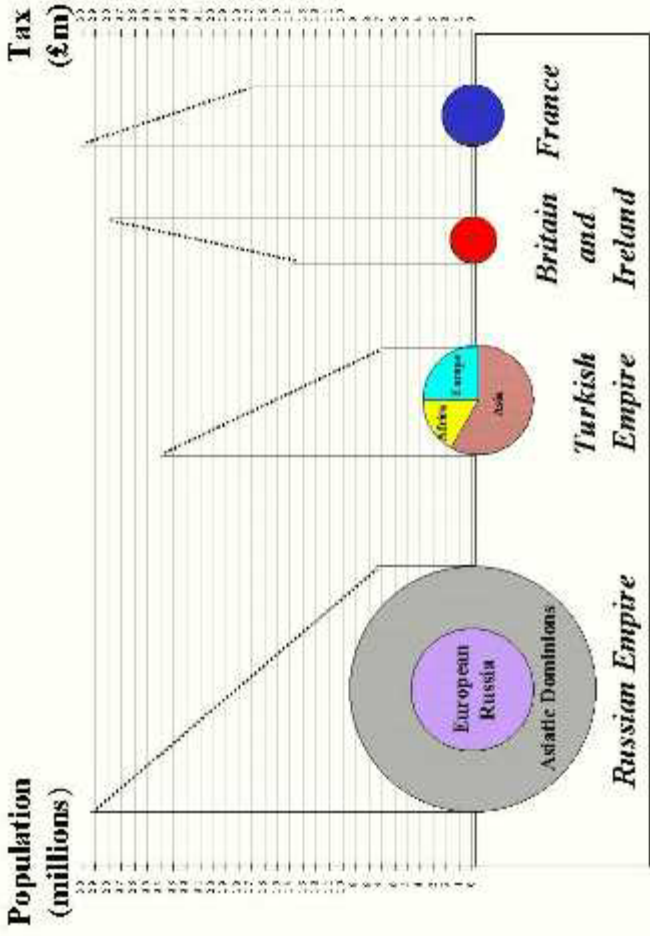
This web version is dedicated to Arthur H. Robinson (1915-2004), who inspired and encouraged our interest; to Antoine de Falguerolles, who initiated it, and to les Chevaliers des



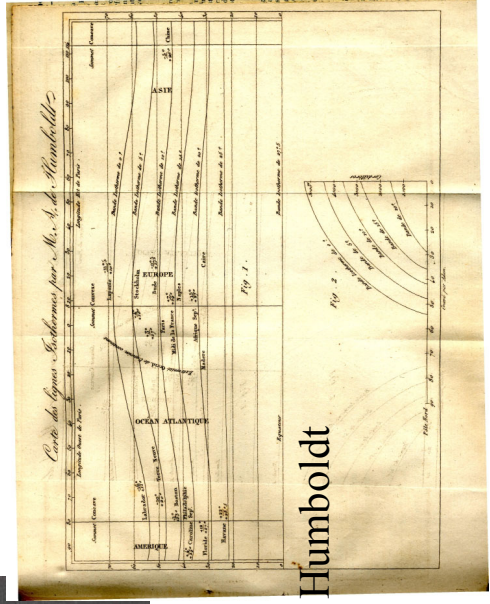
Luke Howard 1800
1st use of coordinate paper
in a research paper



Charles de Fourcroy
1782
“proportional squares”



William Playfair's chart
Invented pie-chart. 1801

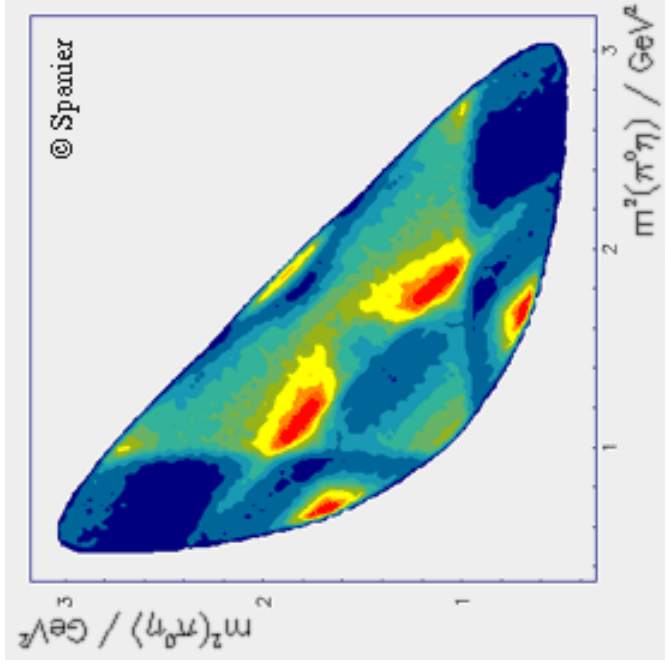


Humboldt's
isotherms
1817

Alexander Von Humboldt

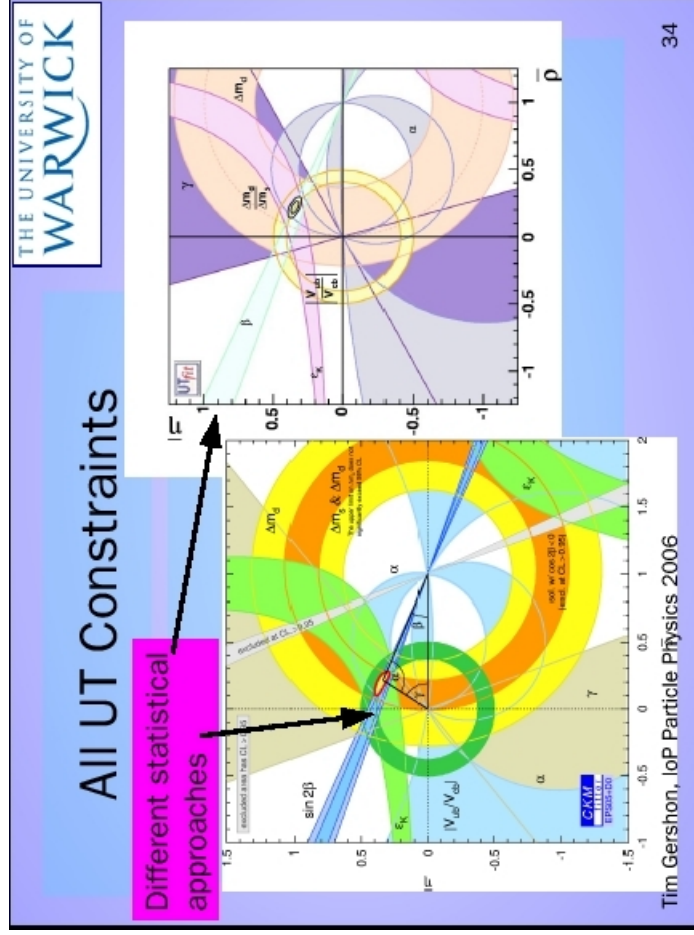


Prof. Dalitz FRS – 1925-2006



Dalitz Plot 1954

Some data visualisations from particle physics
Excluding event displays!



Status of the CKM matrix

Milestones: Section 9. 1975-present - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

http://www.math.yorku.ca/SCS/Gallery/milestone/sec9.html

Getting Started Latest Headlines

1975-present

Up: Milestones Introduction Related References Term Index

Pre-1600 1600s 1700s 1800+ 1850+ 1900+ 1950+ 1975+

Fourfold display Mosaic displays Table lens

9. 1975-present: High-D data visualization

It is harder to provide a succinct overview of the most recent developments in data visualization, because they are so varied, have occurred at an accelerated pace, and across a wider range of disciplines. It is also more difficult to highlight the most significant developments (and because we have focused on the earlier history), so there are presently areas and events unrepresented here.

With this disclaimer, a few major themes stand out:

- the development of a variety of highly interactive computer systems and more importantly,
- new paradigms of direct manipulation for visual data analysis (linking, brushing, selection, focusing, etc.)
- new methods for visualizing high-dimensional data (grand tour, scatterplot matrix, parallel coordinates plot, etc.);
- the invention of new graphical techniques for discrete and categorical data (fourfold display, sieve diagram, mosaic plot, etc.), and analogous extensions of older ones (diagnostic plots for generalized linear models, mosaic matrices, etc.) and,
- the application of visualization methods to an ever-expanding array of substantive problems and data structures.

These developments in visualization methods and techniques arguably depended on advances in theoretical and technological infrastructure. Some of these are: (a) large-scale software engineering; (b) extensions of classical linear statistical modeling to wider domains; (c) vastly increased computer processing speed and capacity, allowing computationally intensive methods and access to massive data problems.

In turn, the combination of these themes and advances now provides some solutions for earlier problems.

Done

Milestones in the history of thematic cartography, statistical graphics and data visualisation – M. Friendly and D. Denis Jan 2006

Big thankyou to Michael Friendly website
<http://www.math.yorku.ca/SCS/StatResource.html>

1975 to now High D data visualisation

Some key dates...selective list ..

- 1985 Alfred Inselberg **Parallel Coordinates**
- 1985 D. Asimov **Grand Tour**
- 1985 DataDescription Inc. Paul Velleman Cornell - **DataDesk**
- 1987 A. Becker and W. Cleveland **Linking and Brushing**
- 1998 A. Buja, D. Asimov, C. Hurley, J. McDonald **XGobi**
- 1990 **E. Wegman Statistical analysis and parallel coord. CrystalVision.**
- 1991 M. Friendly Mosaic Display and Categorical data
- 1999 L. Wilkinson “Grammar of Graphics”

Systemization of data and graphs and graph algebras in an OO framework.

Particle Physics Data - a problem in the analysis of a huge amount of multivariate data

What do we use ? Histograms and scatterplots. Sometimes use colour

Can one use the latest computer graphics technology or ideas that statisticians and computer scientists have dreamt up in the last decade...?

To illustrate, will use the “pollen dataset” to show use of parallel coordinates, brushing and pruning.
The Grand Tour.comes later.....

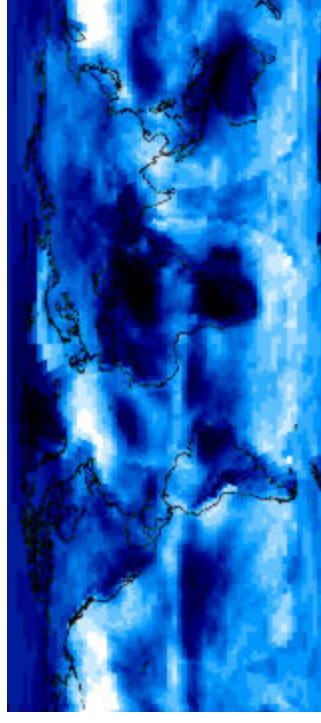
There are many other ideas

Data Exposition 2006

Sponsored by the Sections on Statistical Graphics, Statistical Computing, and Statistics and the Environment.

American Statistical Association

Have challenges each year
This is the 2006 one



Pollen Data Set

the **data set** from the 1986 JSM Exposition's **dataset** and was assembled by David Coleman of RCA Labs

JSM = Joint Statistical Meeting

Data Visualisation

Software

CrystalVision - E. Wegman

GGobi

XmdvTool

Orange

- **The data set:** The data are geographic and atmospheric measures on a very coarse 24 by 24 grid covering Central America. The variables are: elevation, temperature (surface and air), ozone, air pressure, and cloud cover (low, mid, and high). With the exception of elevation, all variables are monthly averages, with observations for Jan 1995 to Dec 2000. These data were obtained from the NASA Langley Research Center Atmospheric Sciences Data Center (with permission; see important [copyright terms](#) below).
- More details about the data, including descriptions of the variables, are available [here](#).
- Download the data as a [gzipped tar ball](#) or as a [zip file](#).
- There is also a [flyer](#) available.
- **The question:** The aim of the Data Expo is to provide a *graphical* summary of important features of the data set. This is intentionally vague in order to allow different entries to focus on different aspects of the data. For example, the focus can be on: the fact that the data are multivariate, or time-series, or spatial; or the fact that the data contain missing values; or the focus could even be on the *process* of exploring the data.
- Some obvious general questions that could be answered are: What are the important relationships between the variables? Are there any important trends in the data? Are there any important groupings or clusters in the data? Are there any unusual locations or time periods in the data set?

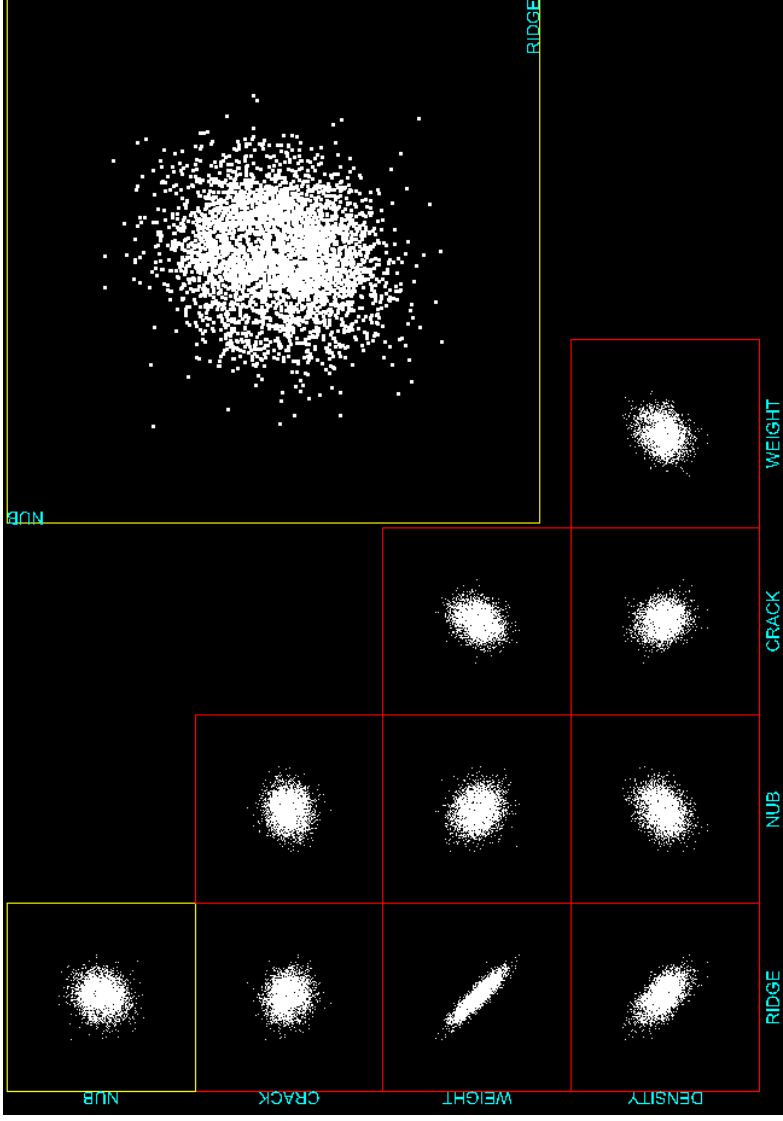
In graphics, a portion of each pixel's data that is reserved for transparency information. 32-bit graphics systems contain four channels -- three 8-bit channels for red, green, and blue (RGB) and one 8-bit alpha channel. The **alpha** channel is really a mask -- it specifies how the pixel's colors should be merged with another pixel when the two are overlaid, one on top of the other.

1) Try this on the pollen data set with CrystalVision

2) Now parallel coordinates.

Problem - how do you study an N-Dimensional space ($N > 2$) when you only have a flat screen ?

This is one solution - with **colour mixing** (blending) and the **alpha channel** (transparency) - is very powerful



Note:
Size of dots matters!

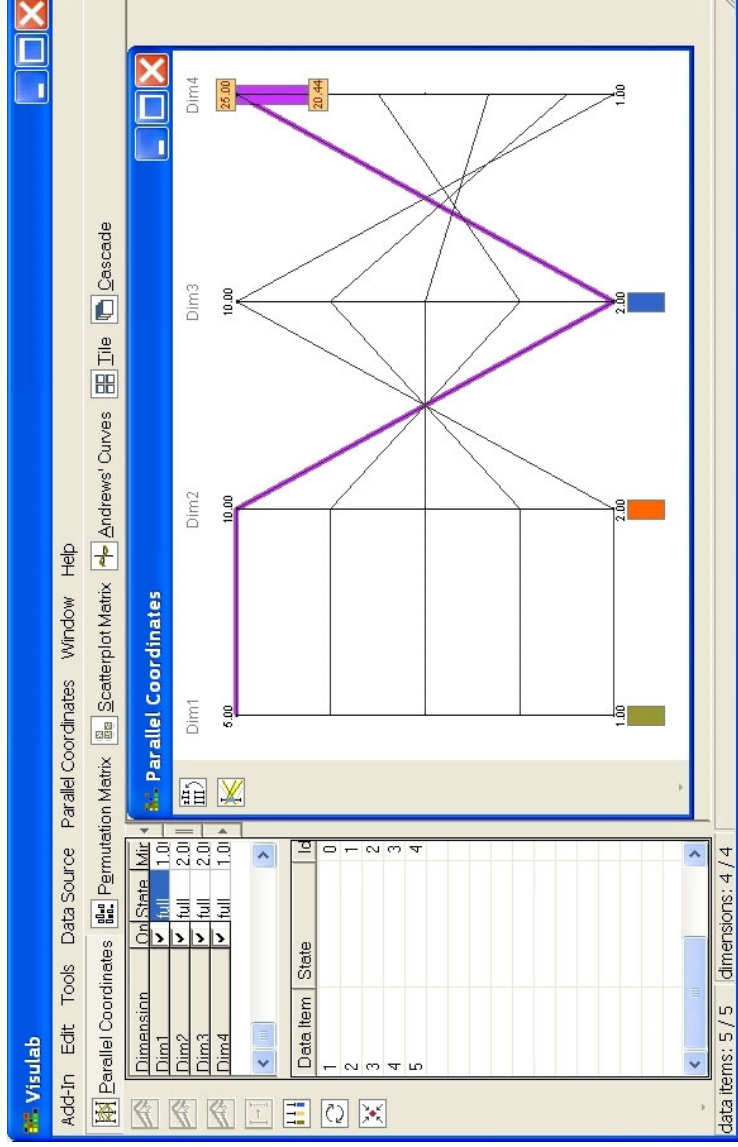
The pollen data - this is called a **scatter matrix**.
2D projections of this 5 variable space helps - but -

Greatly help matters using **colour** and the **alpha** channel

Introduction to Parallel Coordinates

| DataPoint | Dim1 | Dim2 | Dim3 | Dim4 |
|-----------|------|------|------|------|
| 1 | 1 | 2 | 10 | 1 |
| 2 | 2 | 4 | 8 | 4 |
| 3 | 3 | 6 | 6 | 9 |
| 4 | 4 | 8 | 4 | 16 |
| 5 | 5 | 10 | 2 | 25 |

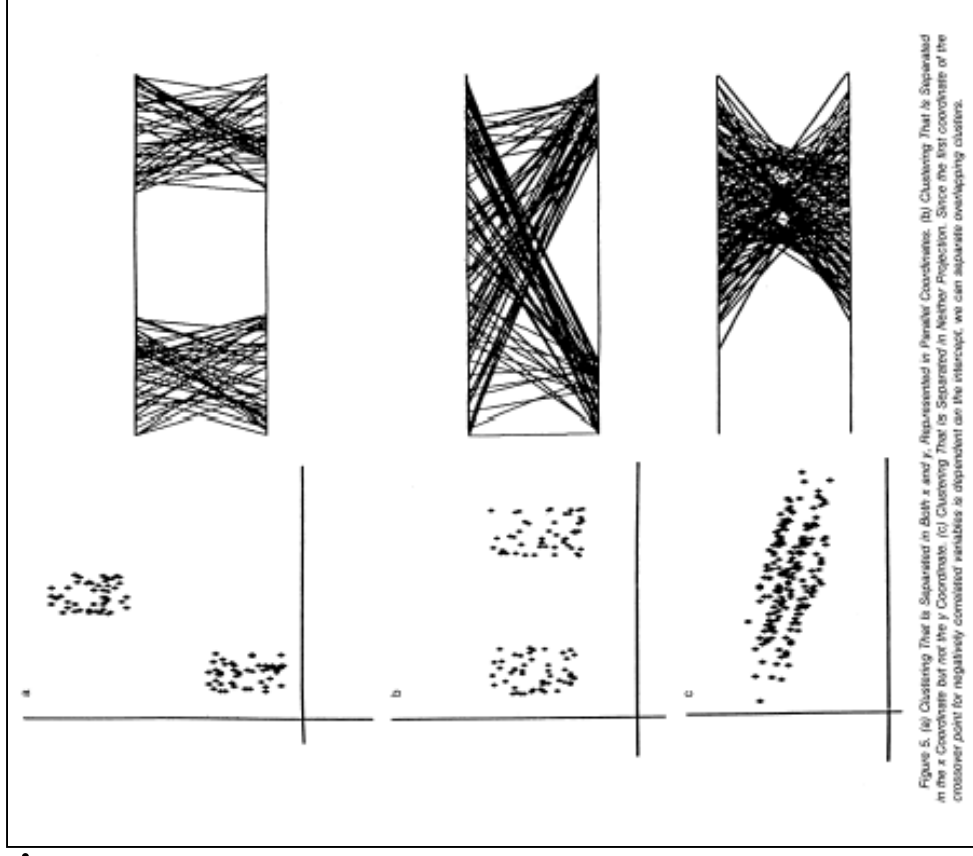
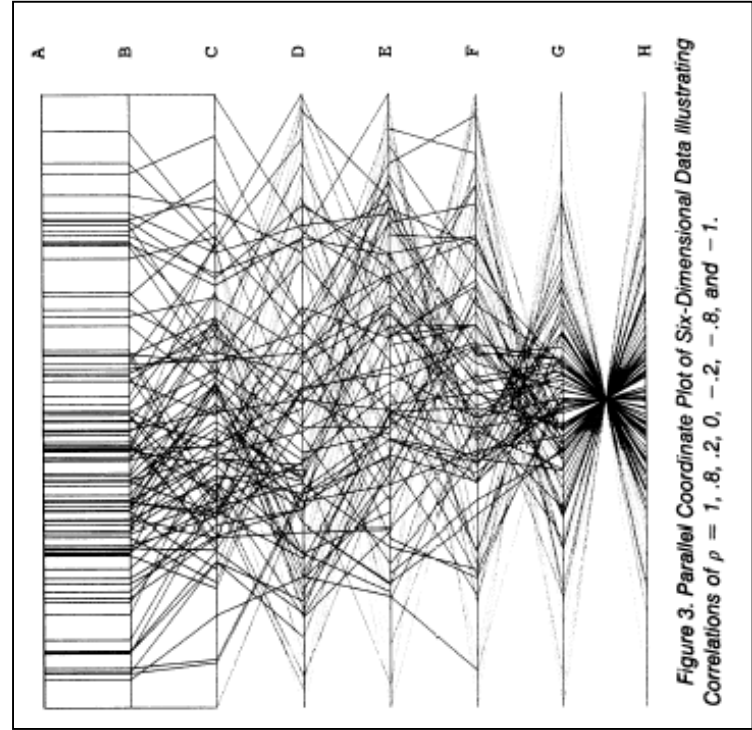
Simple Implementation with EXCEL plugin
<http://www.inf.ethz.ch/personal/hinterbe/Visulab/>

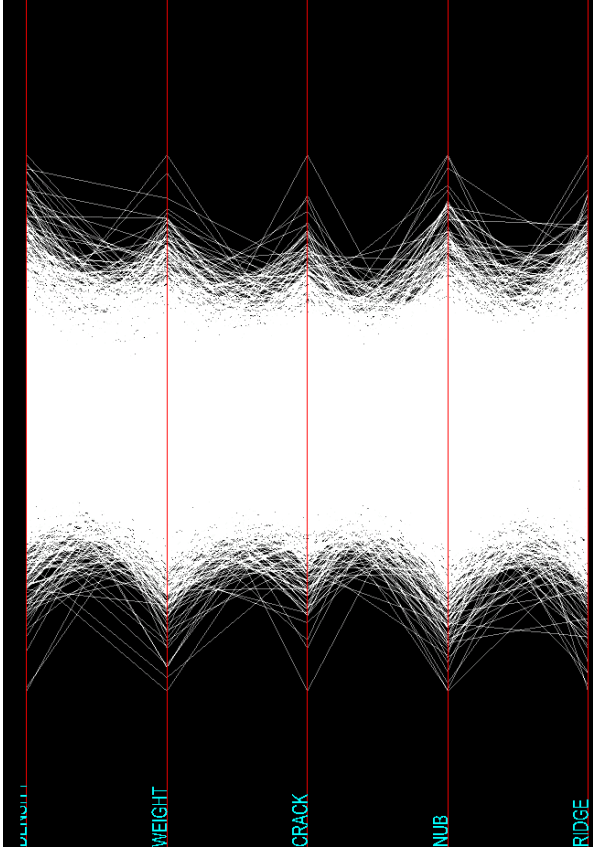


This also shows the idea of brushing

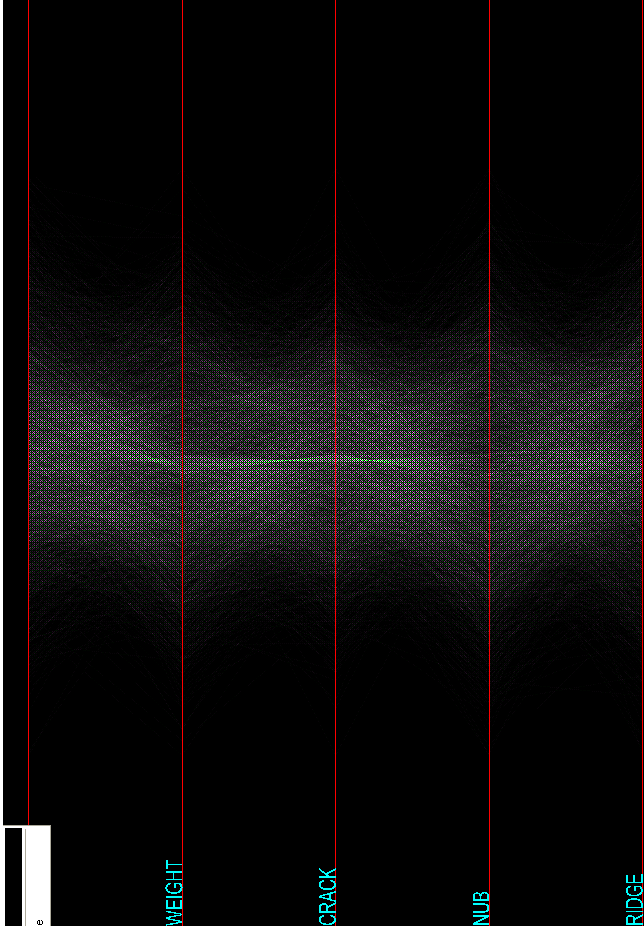


Wegman has done much on the use of parallel coords.
Some useful things to note.....





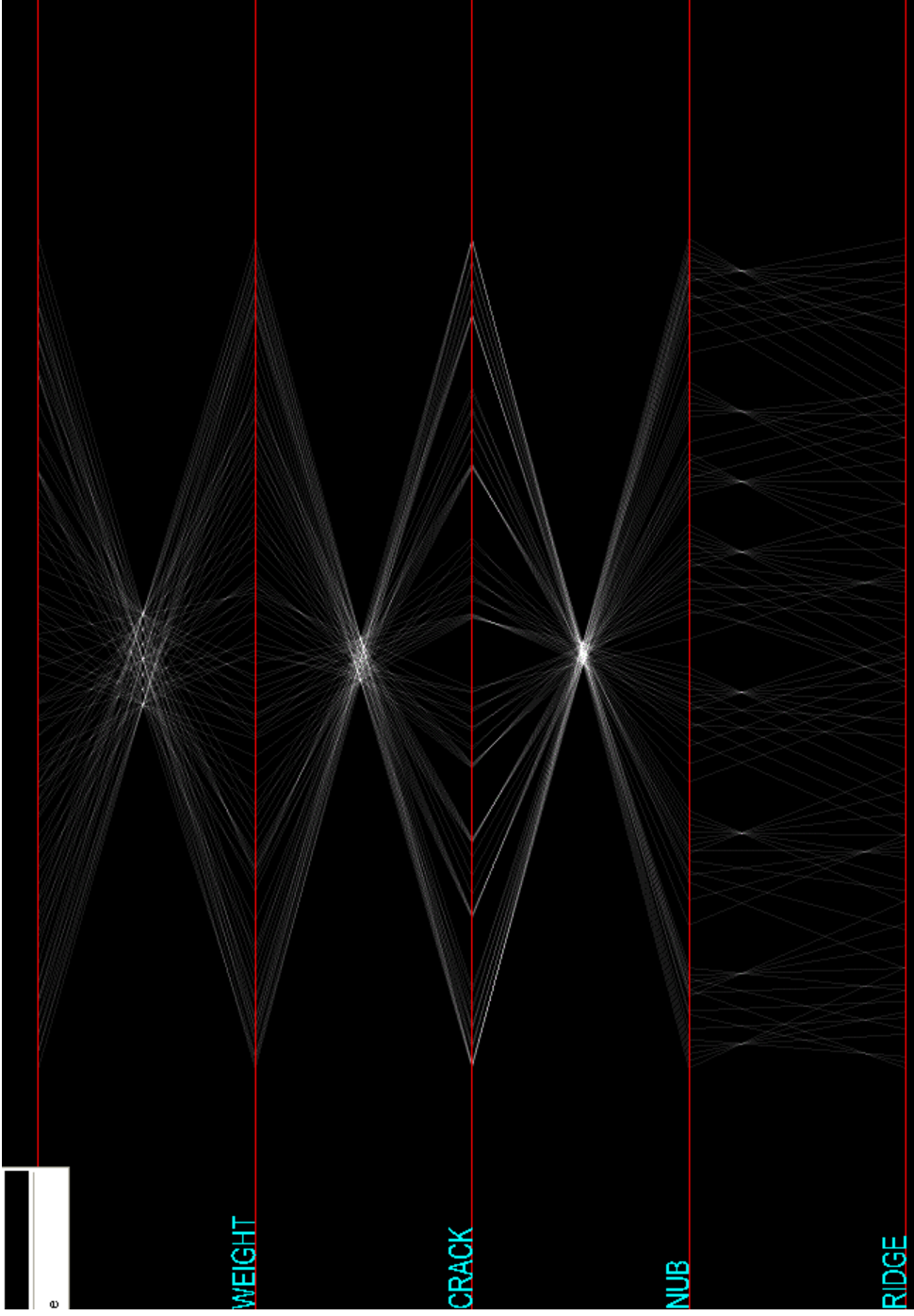
High alpha



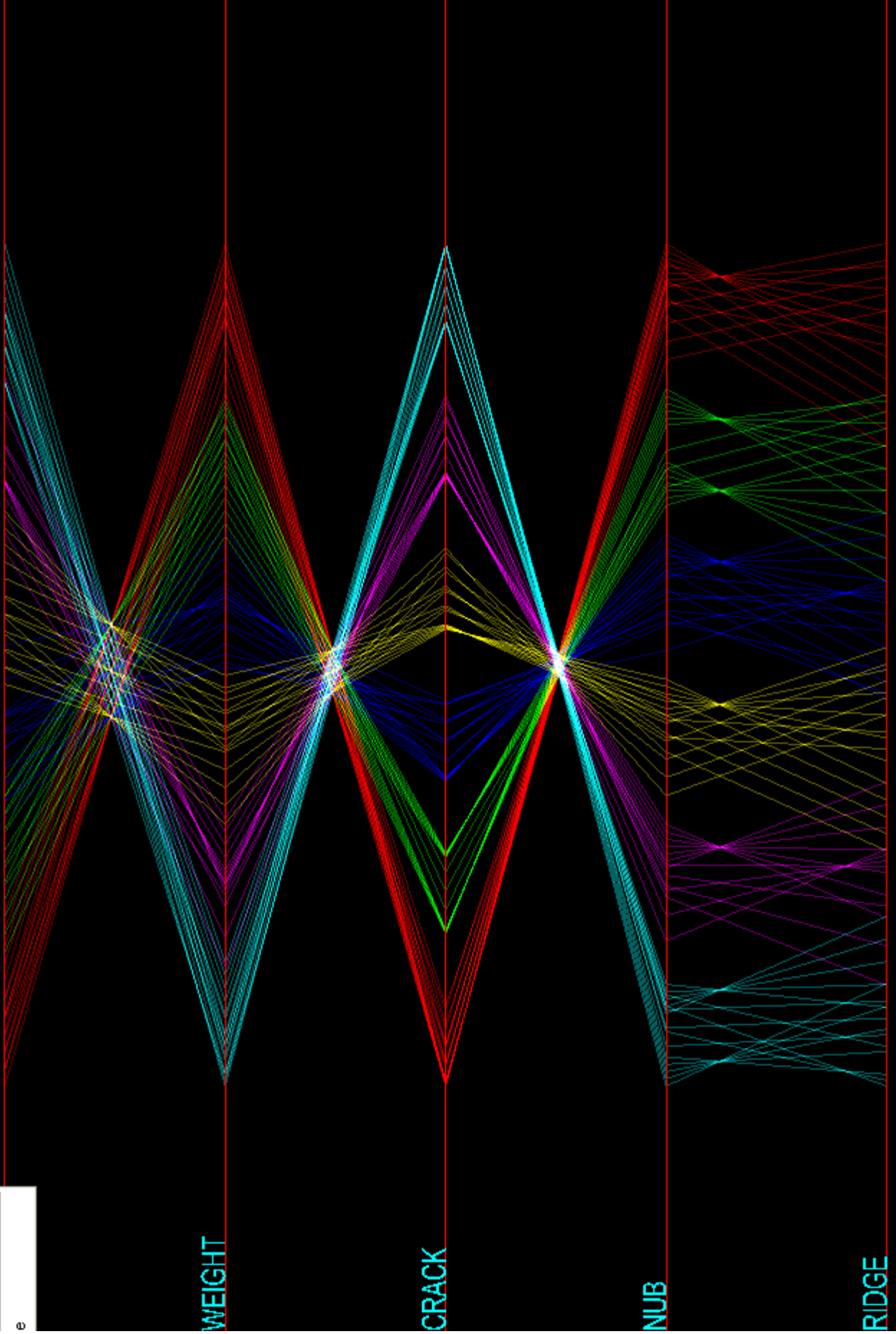
Low alpha

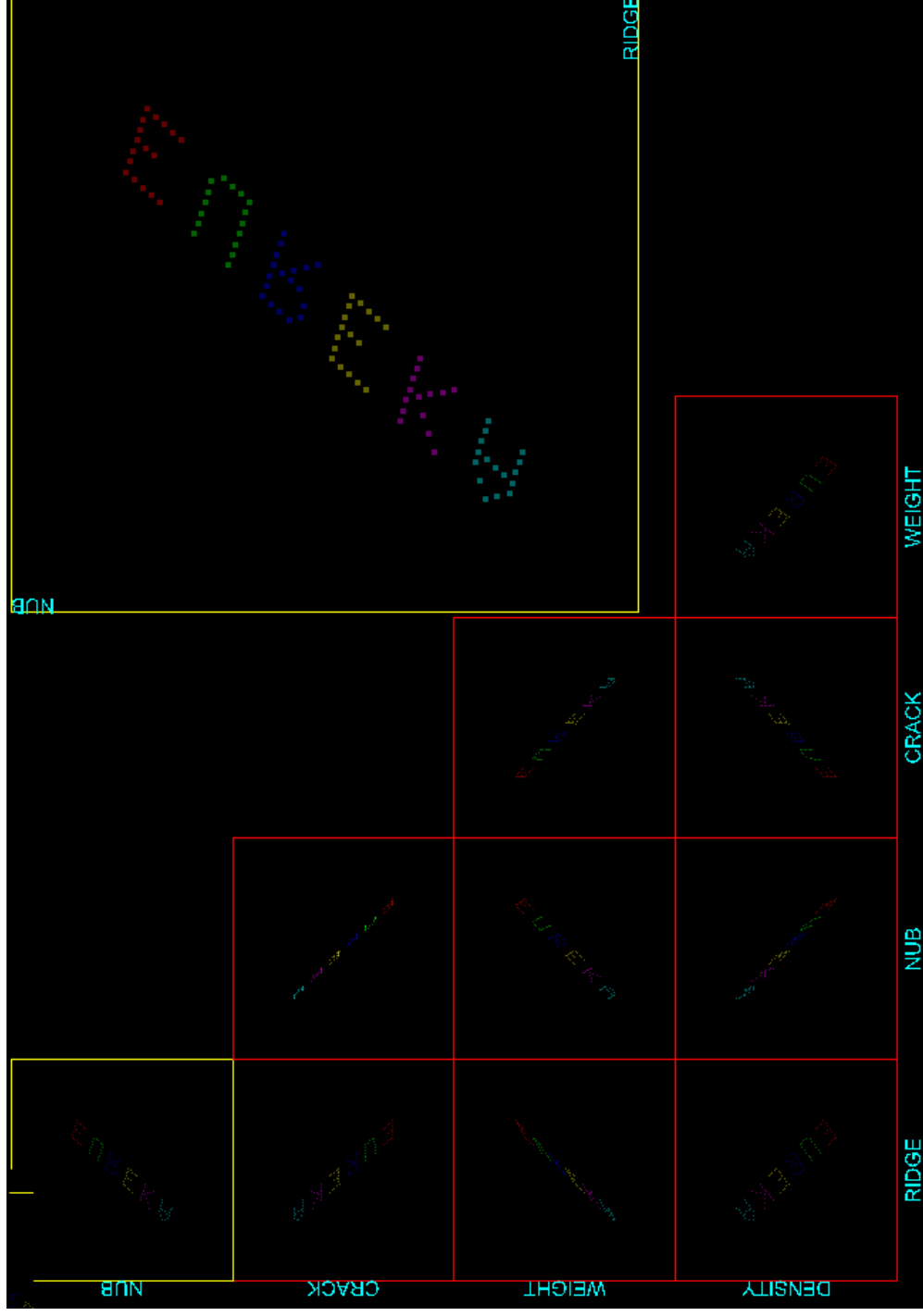
Now **brushing** - colour the data with chosen colours
and **pruning** - cut data you do not want

First lets PRUNE



e



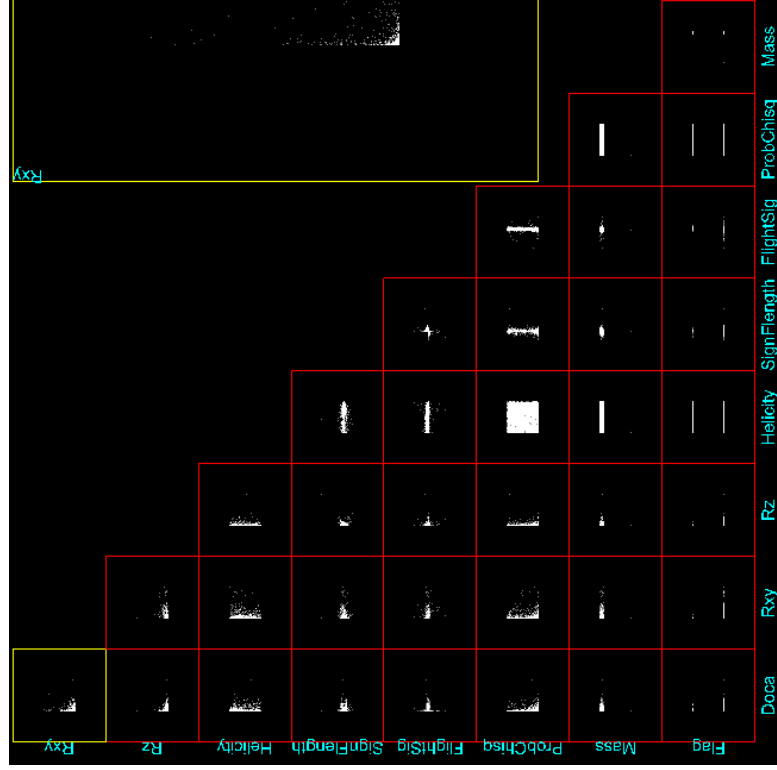


98/3848 points. $S/B = 2.6\%$

There are other features in the data. See E. Wegman
 Contrived example, but helps a newcomer to use this
 type of graph.

Now lets try some particle physics monte carlo data

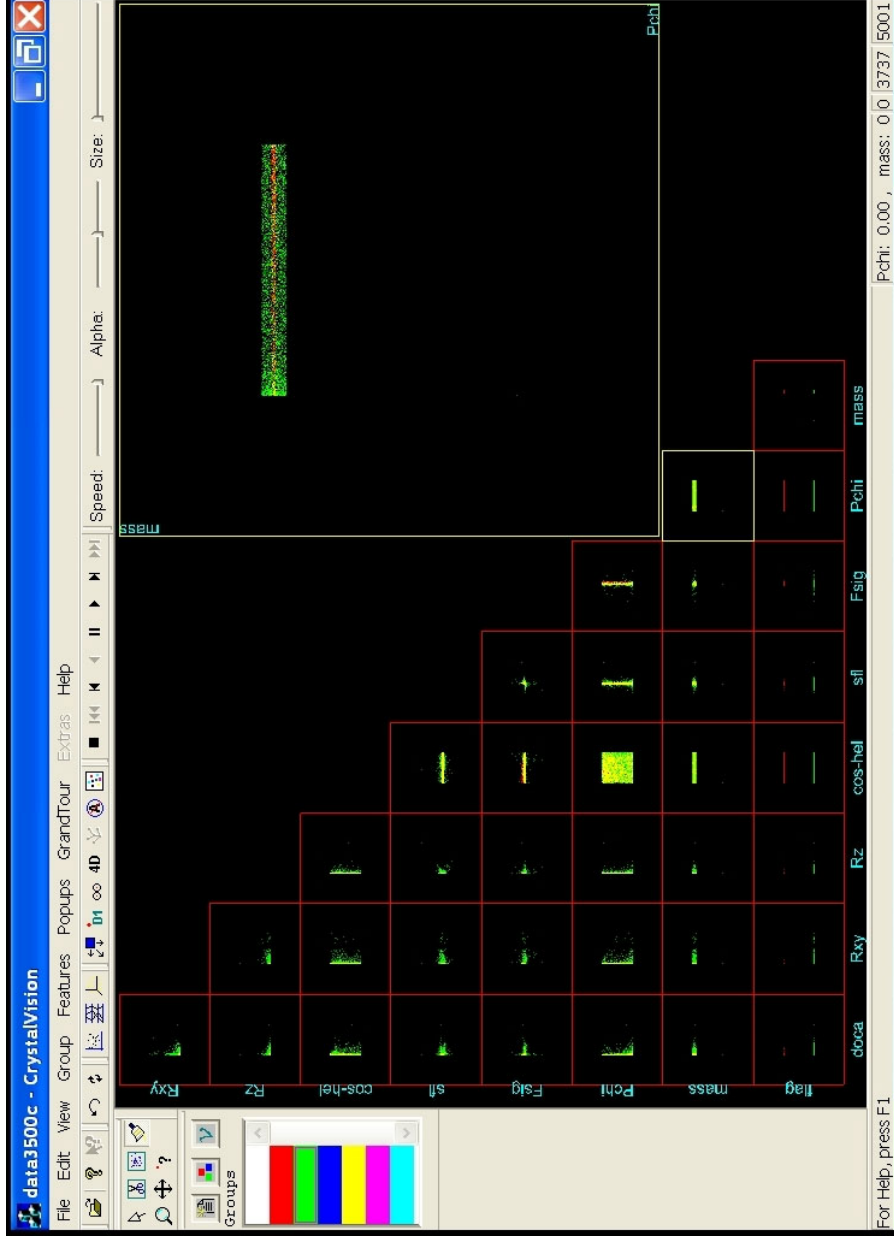
From Liliana Teodorescu - 1264 Kzero + 3734 background
(and a flag to tell us which is which ! Flag=1 S Flag=0 B
LT has shown how to use GEP on this dataset in another talk.



Doca = distance of closest approach
Rxy radius of cylinder for interaction region
Rz abs. half length of cylinder defining the IR
Cos_hel abs. Value of cosine of Ks helicity angle
SFL – signed flight length
Fsig stat. Sig. Of Ks flight length
Pchi chisq prob of Ks vertex
Mass – reconstructed mass of the Ks



CrystalVision – E. Wegman



CrystalVision
(E. Wegman)

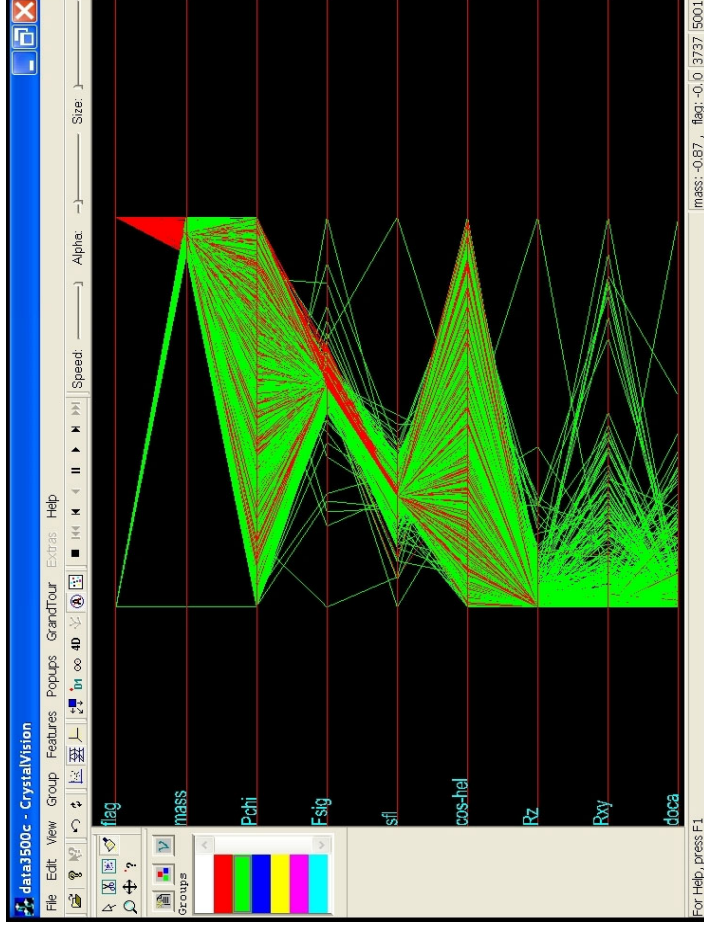
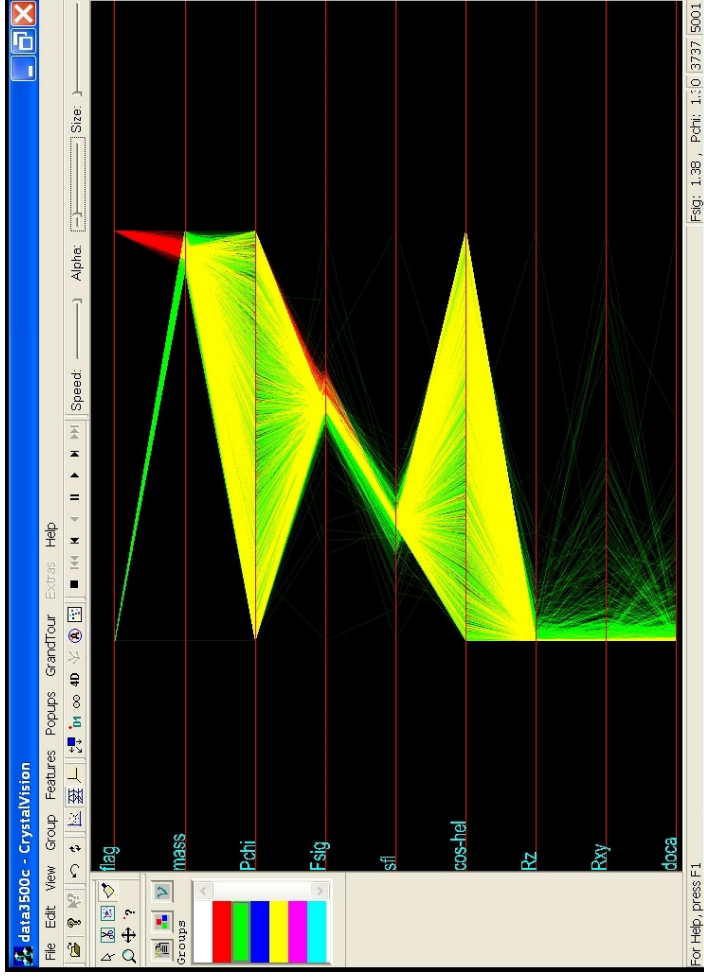
Has blending
and control of
intensity

VERY Powerful

Brush signal RED and background GREEN

If they overlap RED + GREEN = YELLOW (yellow)

Now go to parallel coordinates - adjust alpha



Note: See affect of turning alpha channel on and off

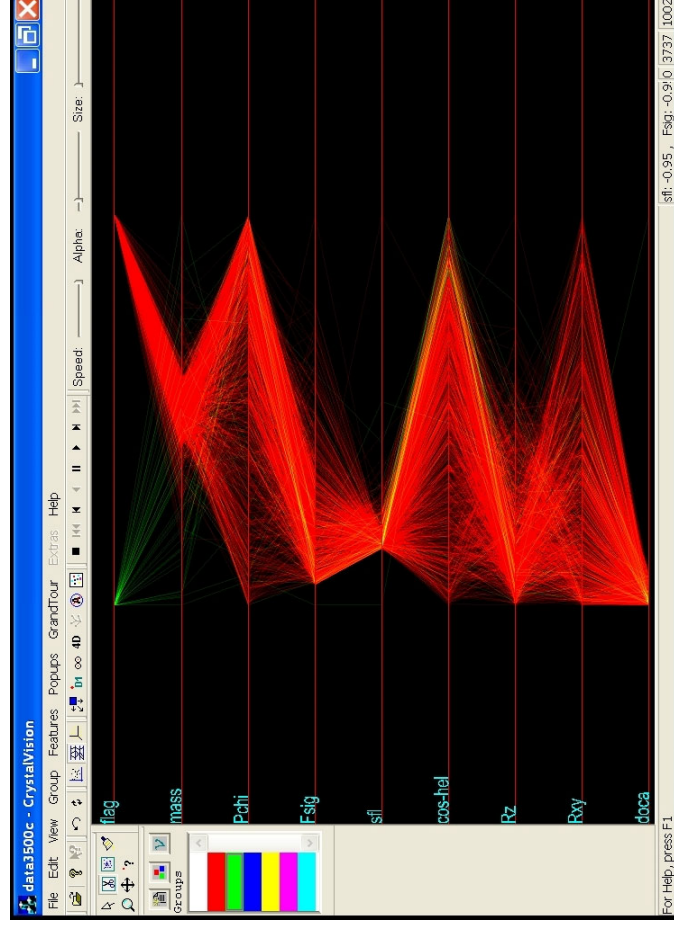
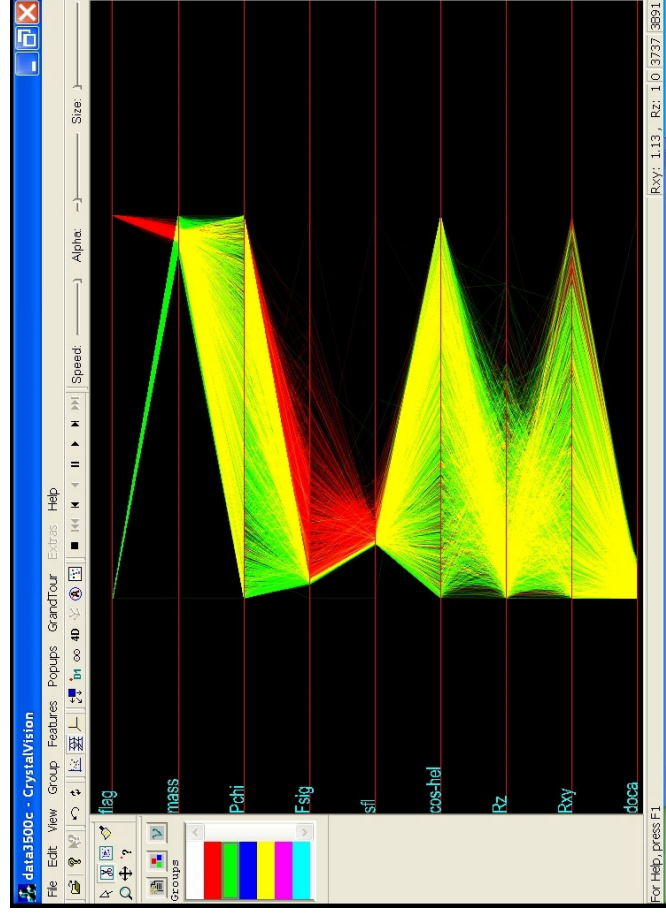
Note: Parallel Coords Vertical. Scales data between min. and max.

Immediately see that R_{xy} , Doca (and sfl less so) discriminate the background
Only variable where signal can be seen is Fsig.

How to clean up this data - “ what is the order of cuts ?”

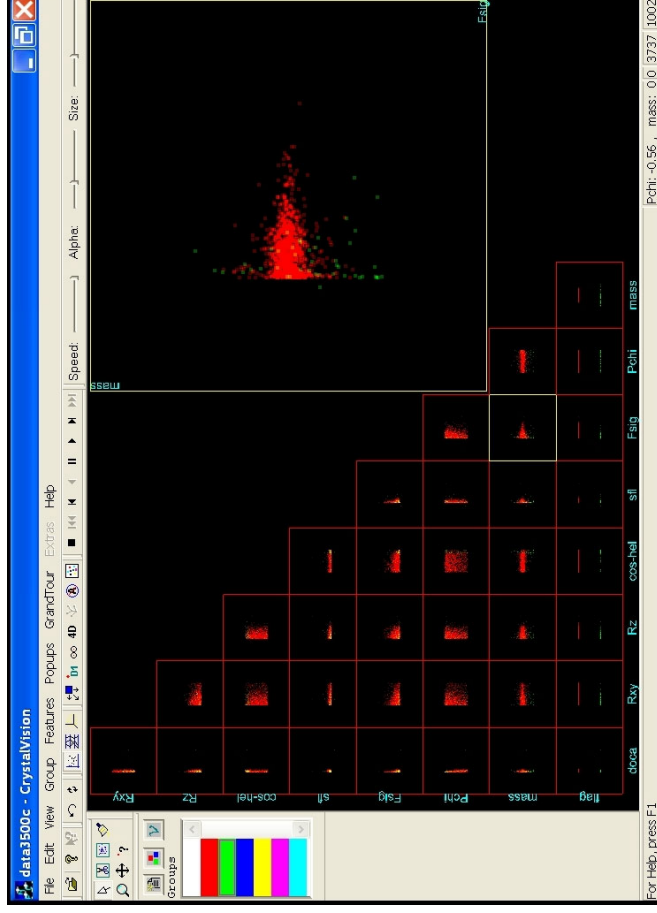
Remove obvious background (Prune **Doca** and **Rxy**)

Then select signal (**FSig**)



Takes just a couple of minutes to do this...

Back in scatterplot space



958 S 44 B 95% Purity 80% Efficiency
Did not spend long on this – Exploratory Visual Data Analysis

Powerful way to decide which variables matter and the order in which cuts should be applied.

Precursor to machine learning approachto be continued

Multivariate classifiers

An algorithm/tool that assigns a point in a multidimensional space to one of several possible categories e.g. signal or background.

- Cut (binary split or stump)
- Decision Trees
- Support Vector Machine (SVM)
(NOTE: radial basis function SVM equiv. to a type of Neural Net)
- Neural Net
- k nearest neighbours (kNN)
- VizRank
- Genetic Algorithm, Genetic Programming,
Gene Expression Programming (GEP) – can do other things also.
- etc.....

ViZRank – finding informative data projections in Functional genomics by machine learning

Bioinformatics applications note Vol 21 no. 3 2005 413-414
Gregor Leban et al.....Use **ORANGE**

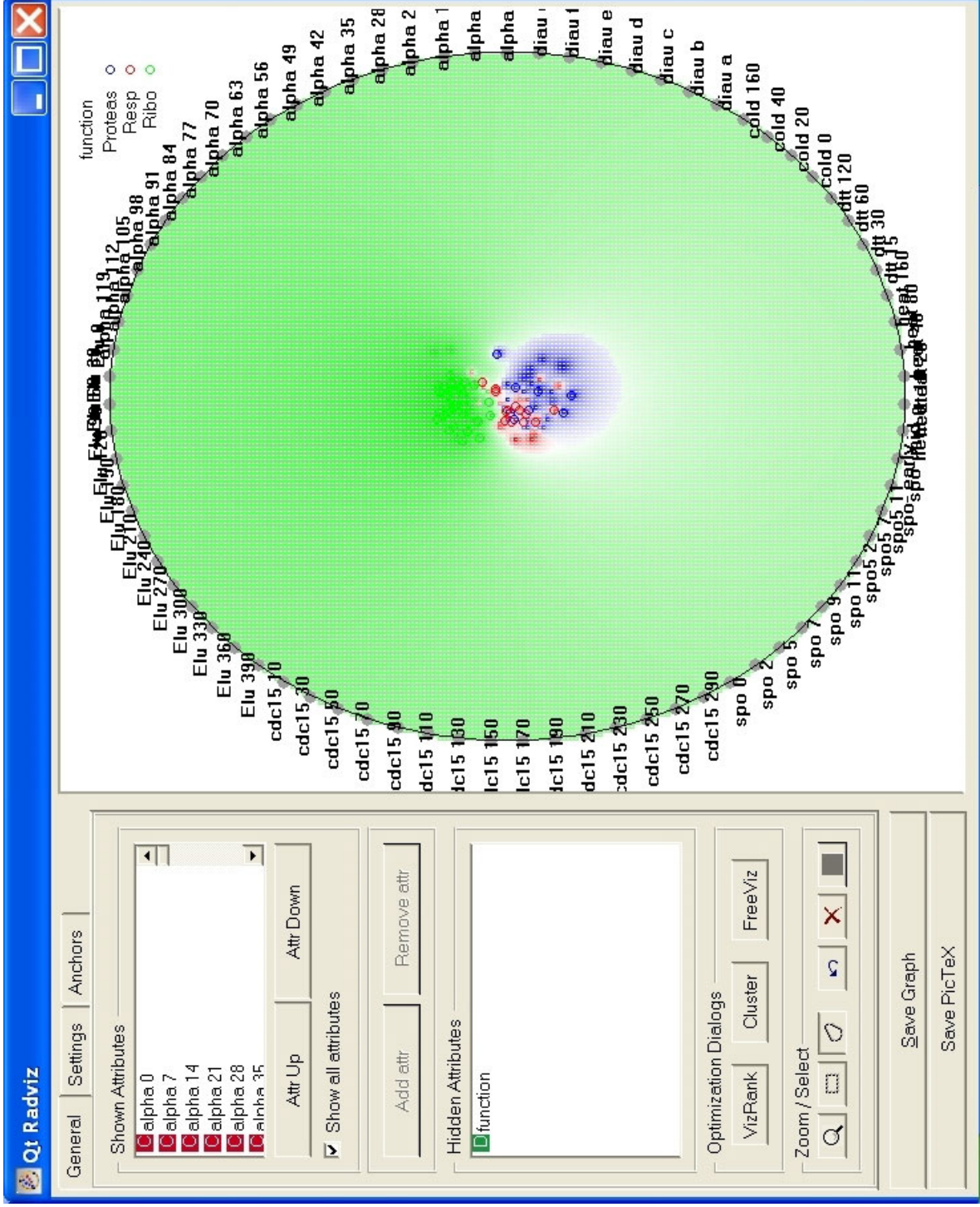
Project N-dimension space onto a reduced number of dimensions (use radviz or polyviz visualisation)

Rank projections using kNN classifier

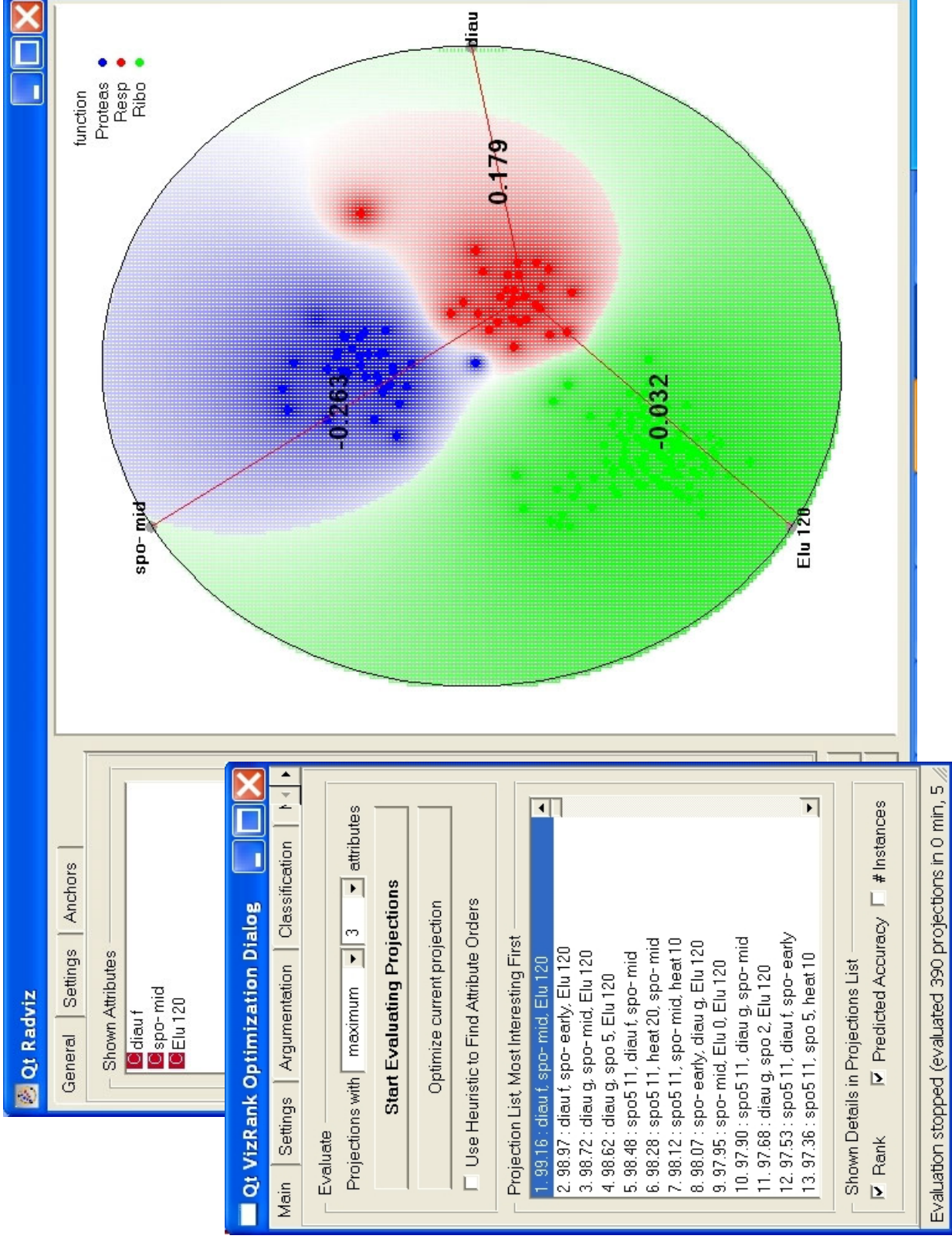
Yeast *Saccharomyces cerevisiae*

79 different DNA microassay hybridization measurements
Describe each gene.....which ones matter ?

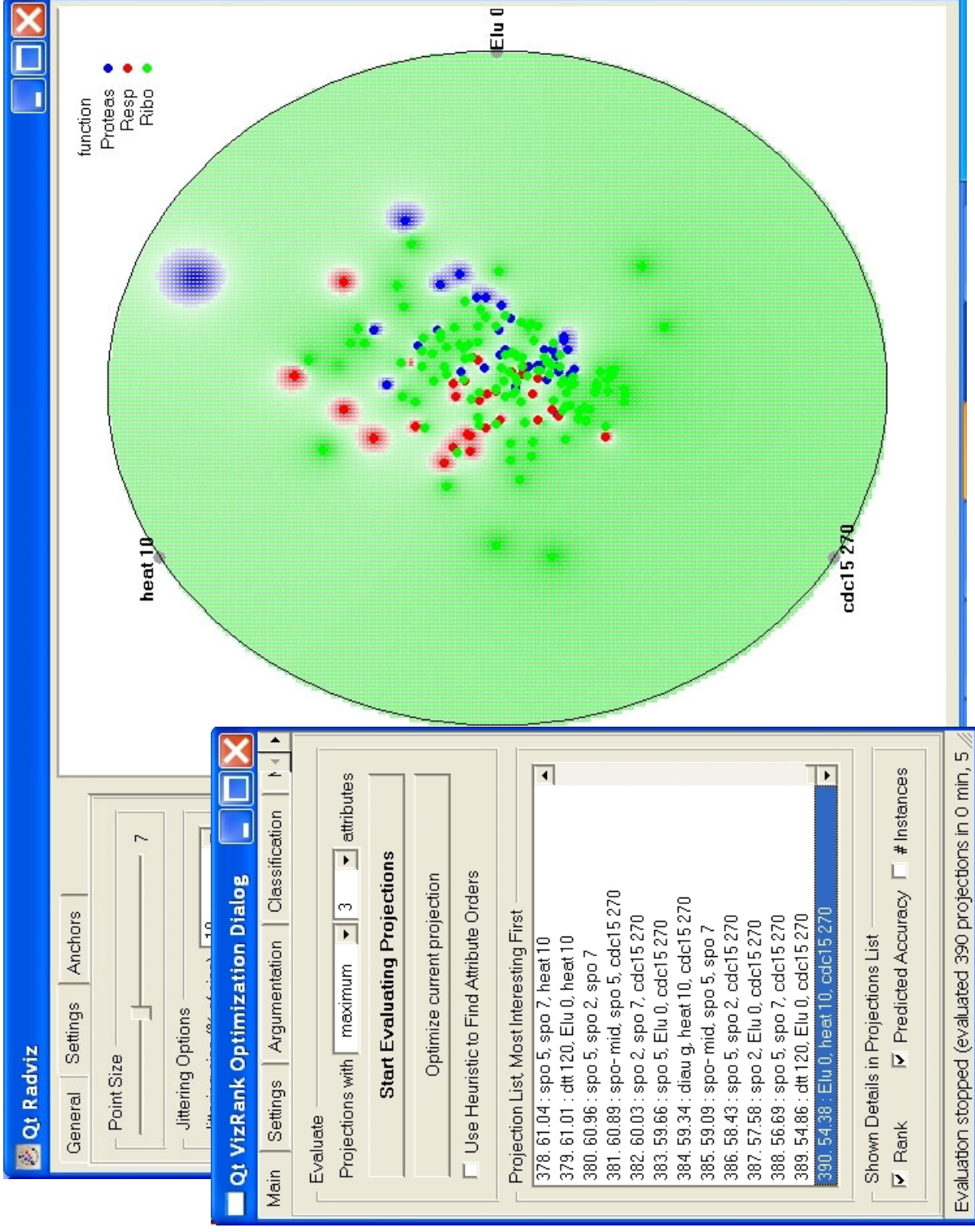
RadViz Visualisation – invented by P. Hoffman



Rank 3 attribute projections 99 %



Poorly ranked projection – 54%



Illustrate some other classifiers and visualisation using the wine dataset....

content

[Introduction 1.1 - Formal Text Mining Combined](#)

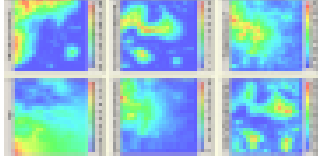
[KDDuggestions](#) : Datasets

See also [Datasets for Data Mining Comparison](#) and [KDD-CAT](#) results and data.

Datasets for Data Mining

- See first [UCI KDD Database Expository](#) – the most popular site for datasets used for research in machine learning and knowledge discovery.
- [Census](#), Data for Evaluating Learning in Video Experiments
- [KDD-CAT](#), a comprehensive source of US statistics and more.
- [IBM Repository for Research on Data Mining](#), Implementations and datasets.
- [Financial Data for Research on Data Mining](#), a large catalog of financial data sets
- [Genomic Data Resources](#), financial data including stocks, futures, etc.
- [Internet Links](#), includes financial data
- [Microsoft Image Server](#), aerial photographs and satellite images you can view and download.
- [MIT Center for Genomics and Computational Biology and Population Sciences](#), from MIT Whitehead Center for Genome Research.
- [MIT Center for Genomics and Computational Biology and Population Sciences](#), list of Datasets.
- [University of Toronto Machine Learning Repository \(MELOR\)](#), NASA data sets from planetary exploration, space and solar physics, life sciences, astrophysics, and more.
- [Public Data Catalog](#), a public catalog of financial data sets
- [SMD: Stanford Microarray Database](#), stores raw and normalized data from microarray experiments.
- [Sourceforge.net Research Data](#), includes historic and future activities on approximately 100 BSD projects and over 1 million registered users' activities at the project management web site.
- [STATSOCC: Statistics and Data](#)
- [UCR Time Series Data Mining Archive](#), offering datasets, papers, links, and code.
- [Unconquered Account Links](#)

[Data Mining Tools](#)
[Data Mining](#)
[Introduction](#)



[Baseline Algorithms and Experiments](#)
[Mining Activities on the KDD Repository](#)

UCI KDD Repository

It would be great if a particle physics database existed for algorithm evaluation

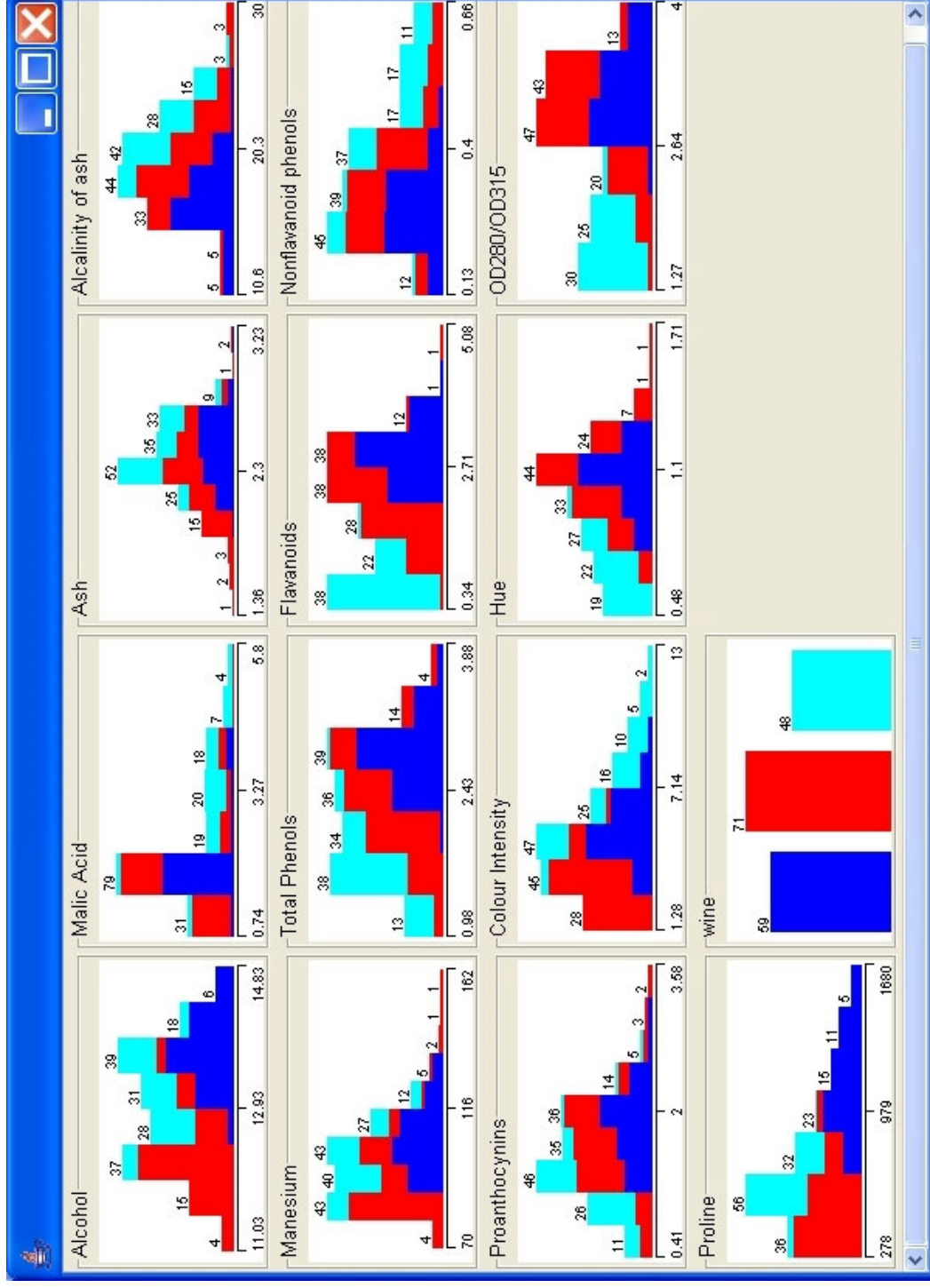
[KDDuggestions](#) : Datasets

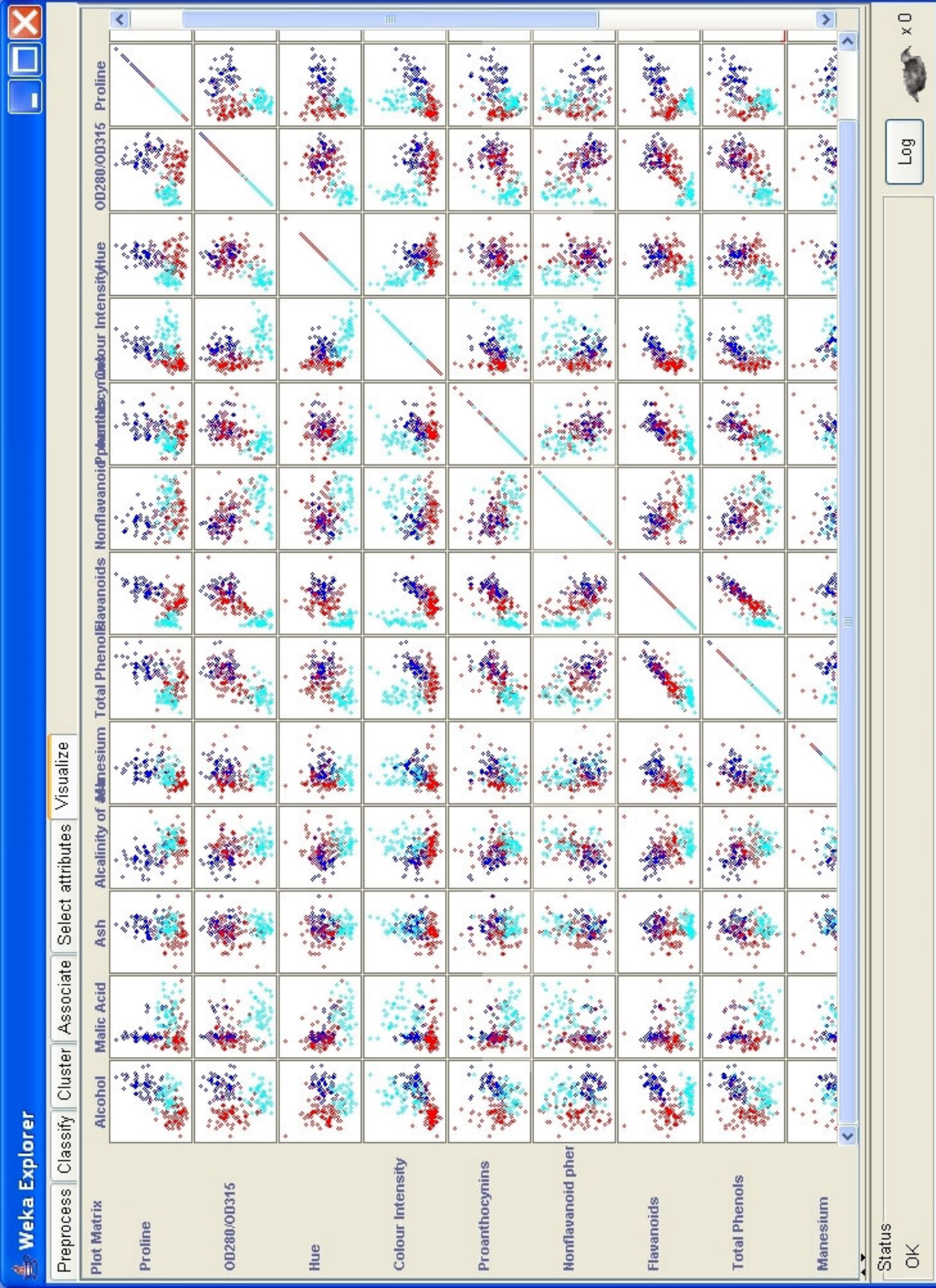
Copyright © 2008 KDDuggestions. [Subscribe](#) to KDDuggestions!

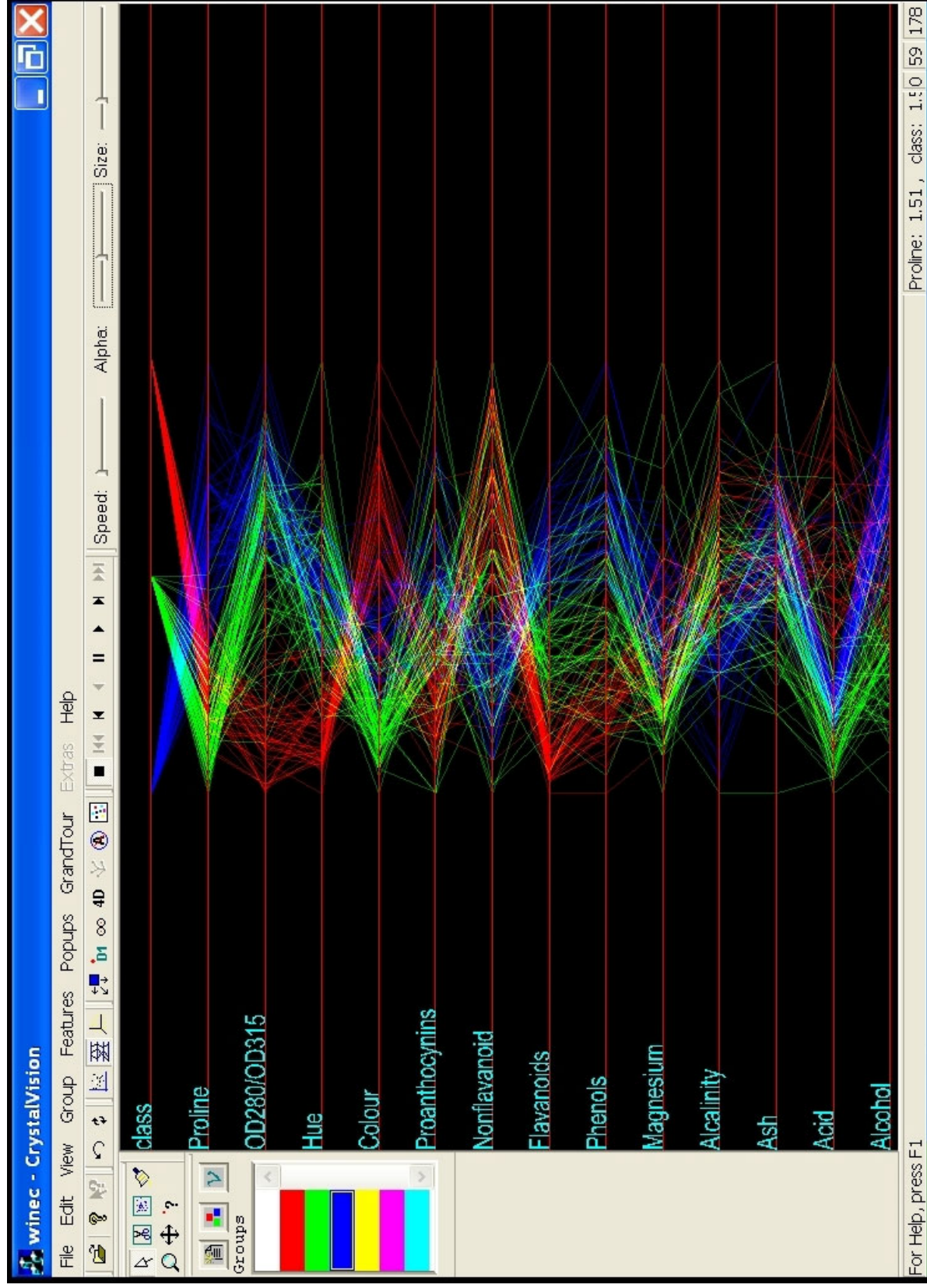
THE WINE DATA SET

4. Relevant Information: -- These data are the results of a chemical analysis of wines grown in the same region in Italy but derived from three different cultivars. The analysis determined the quantities of **13 constituents found in each of the three types of wines.**
- I think that the initial data set had around 30 variables, but for some reason I only have the 13 dimensional version. I had a list of what the 30 or so variables were, but a.) I lost it, and b.), I would not know which 13 variables are included in the set. **!!**
5. Number of Instances class 1 - 59 class 2 - 71 class 3 - 48
6. Number of Attributes 13

Use WEKA - histogram of all the wine dataset

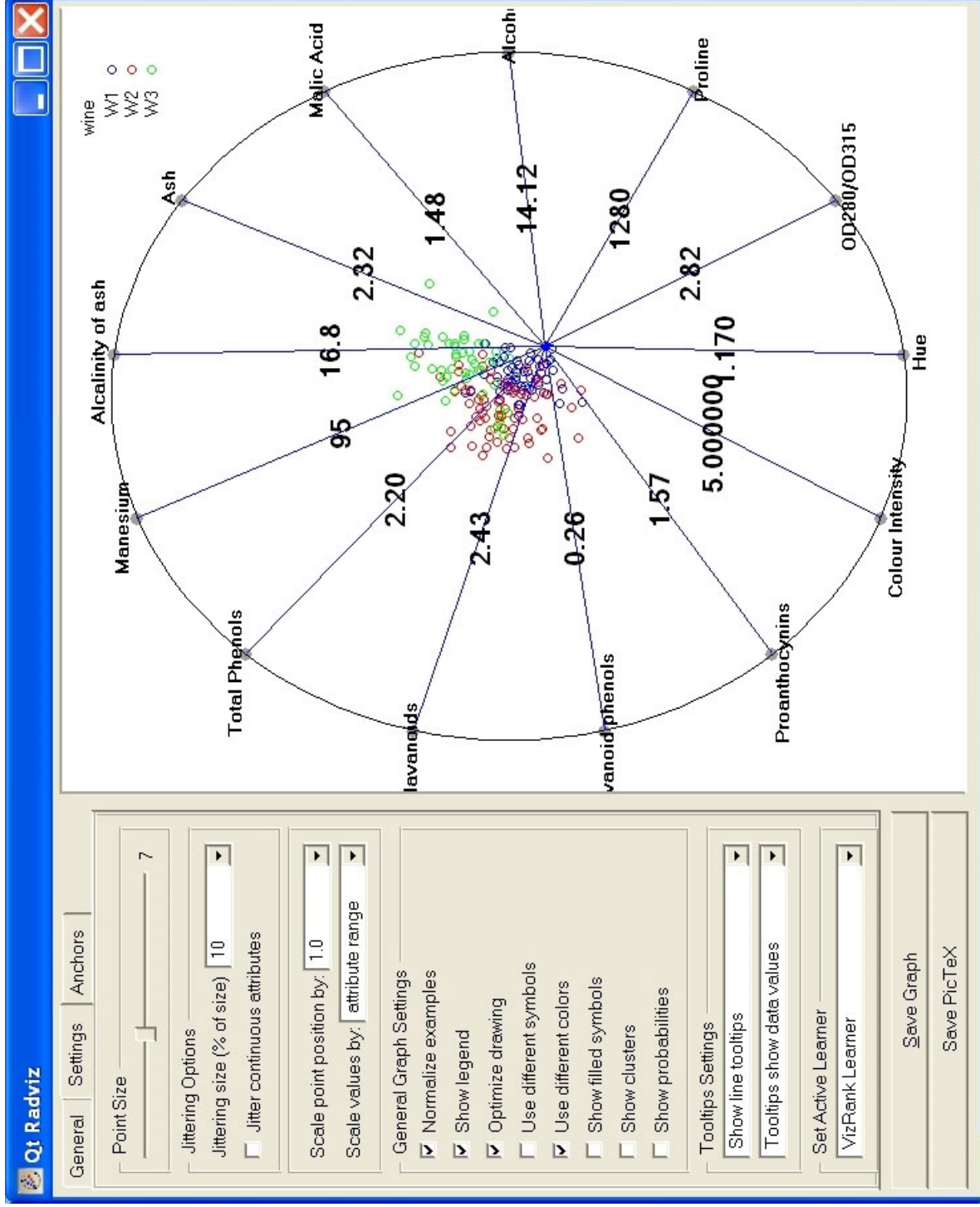


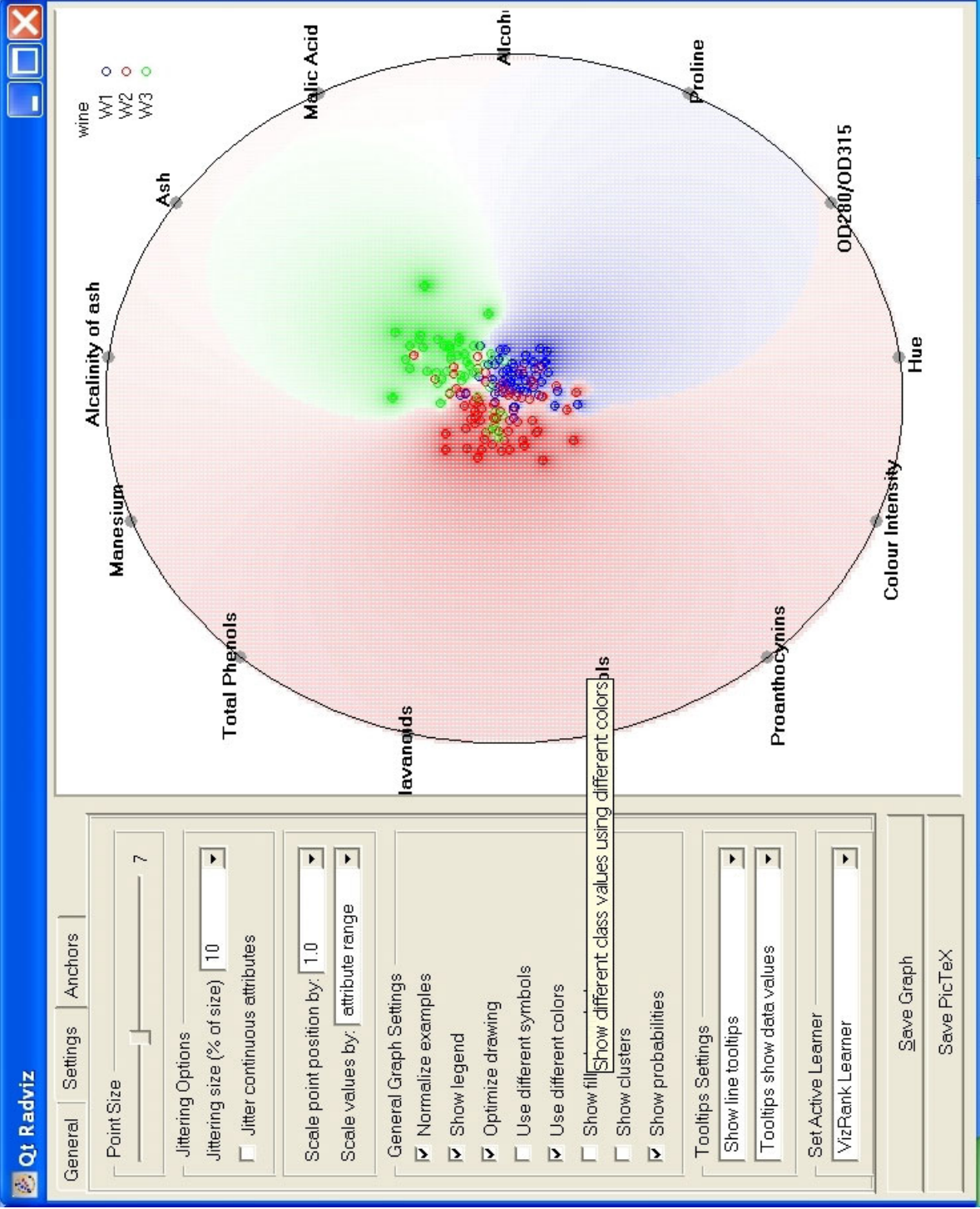




Once you get used to it, this plot contains a lot of information

Wine dataset....





Qt Radviz

General Settings Anchors

Point Size

Jittering Options

Jittering size (% of size)

Jitter continuous attributes

Scale point position by:

Scale values by:

General Graph Settings

Normalize examples

Show legend

Optimize drawing

Use different symbols

Use different colors

Show fill

Show clusters

Show probabilities

Tooltips Settings

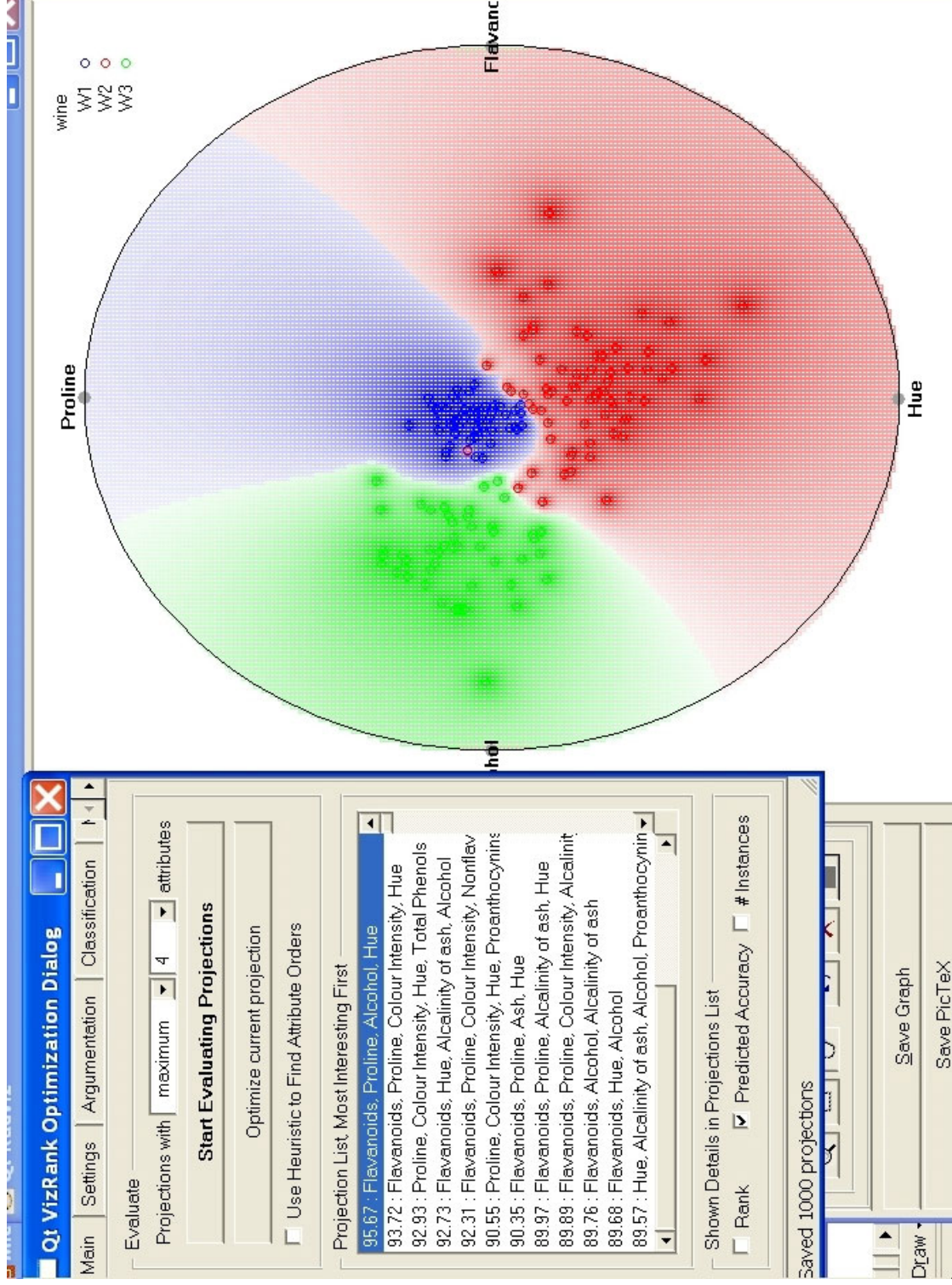
Set Active Learner

Save Graph

Save PicTeX

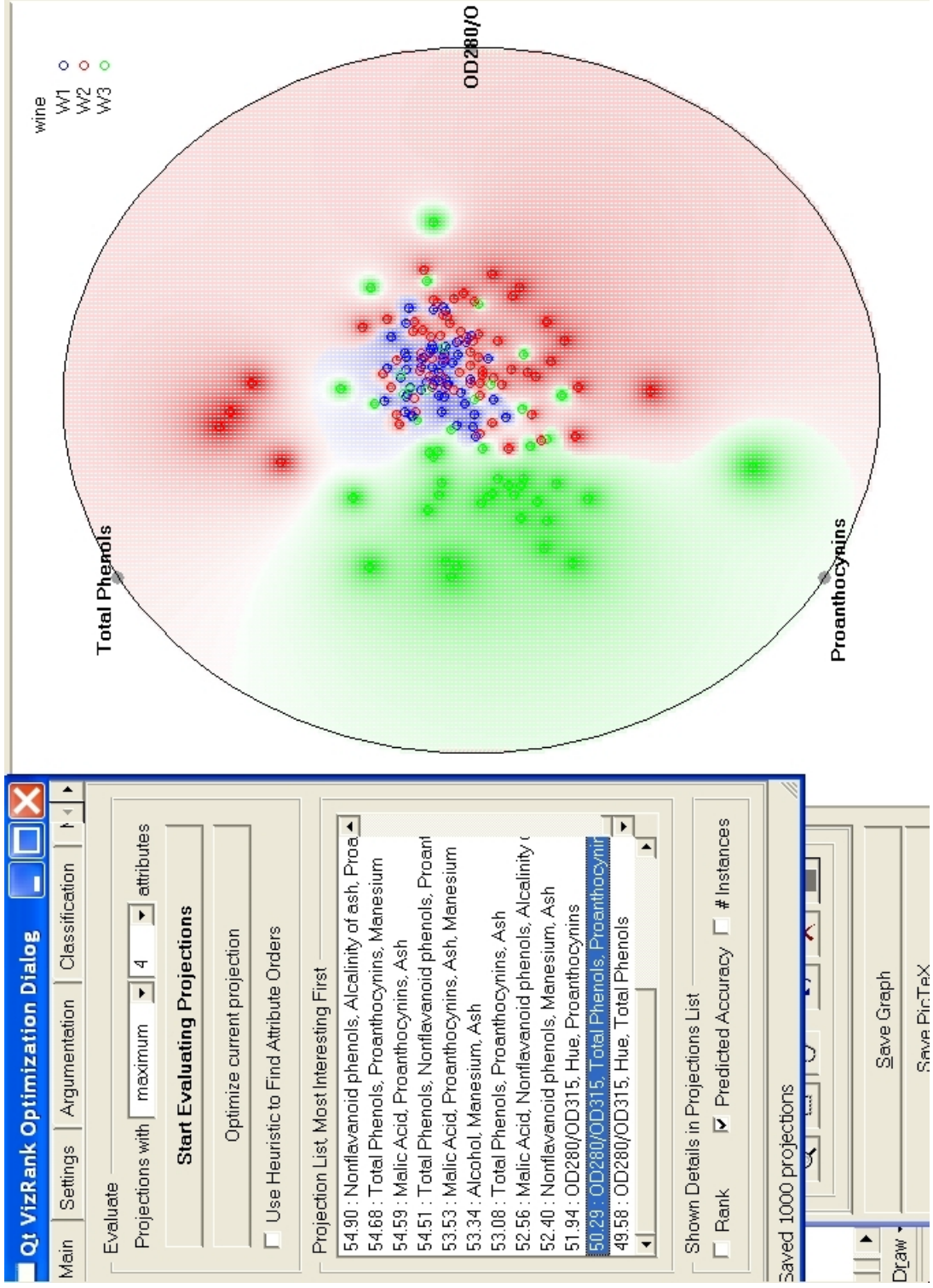
Show different class values using different colors

Flavanoids, colour, hue, alcohol, proline matter.....

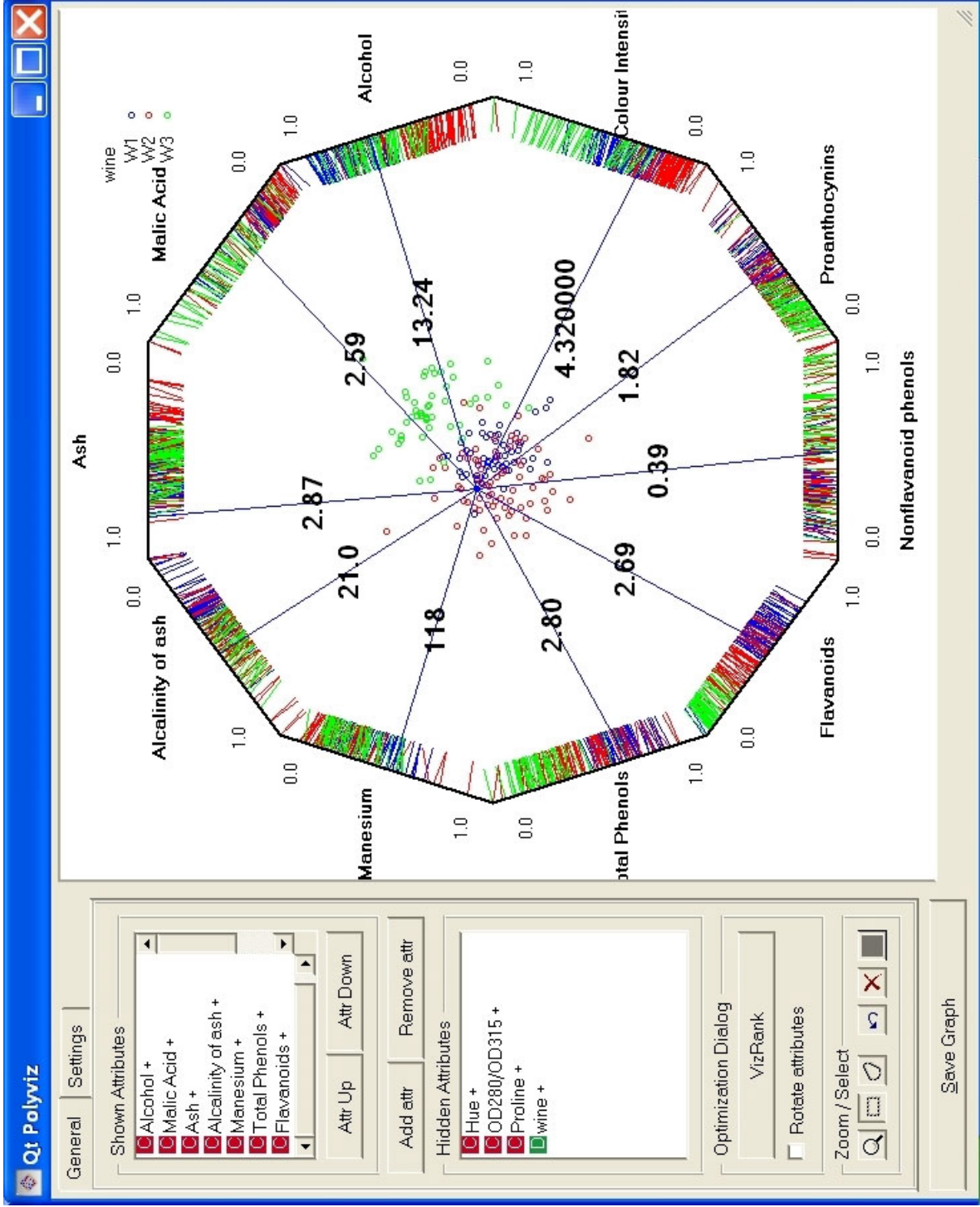


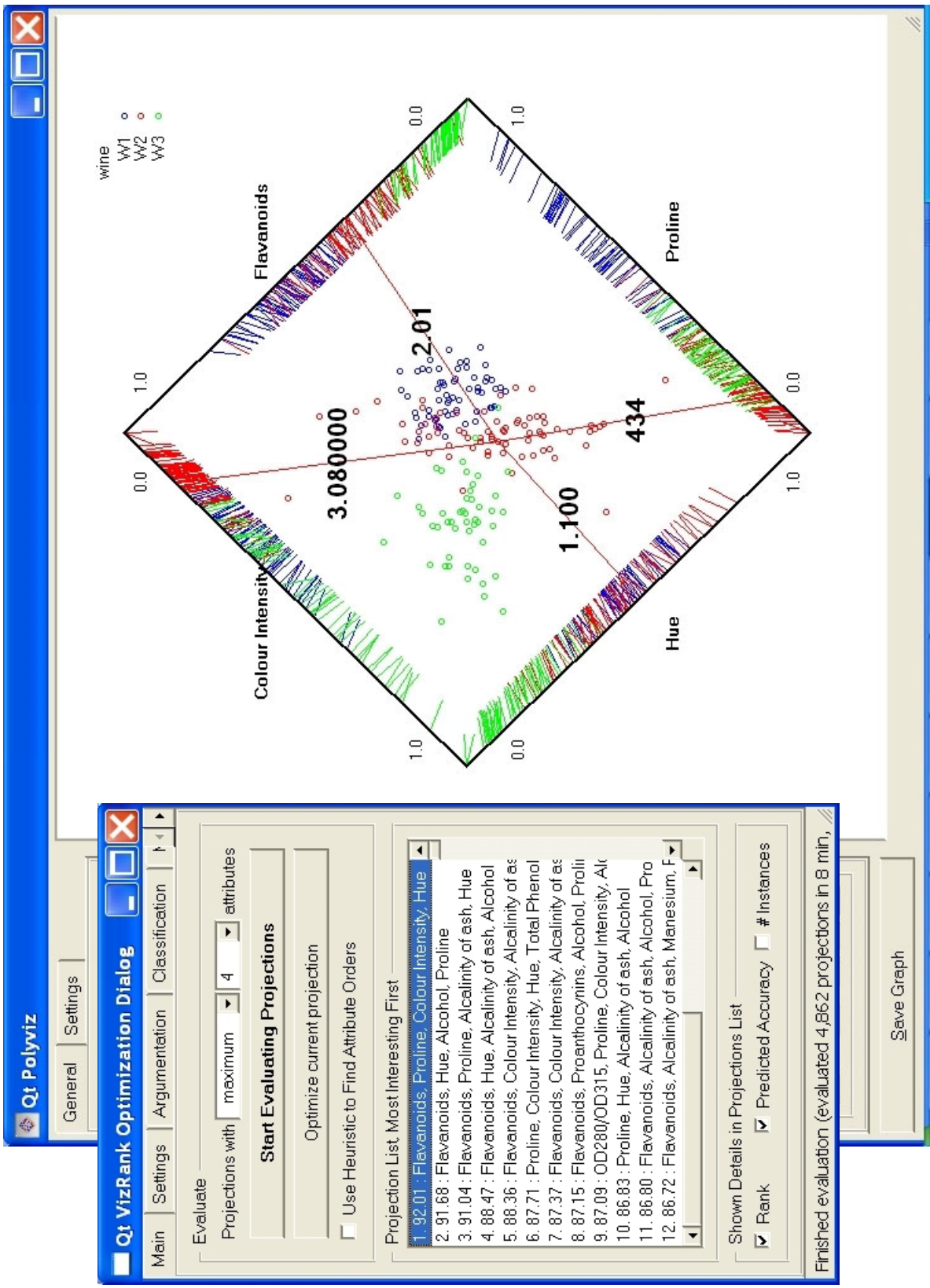
VIZRank algorithm applied....

50% selection.....wines overlap.....



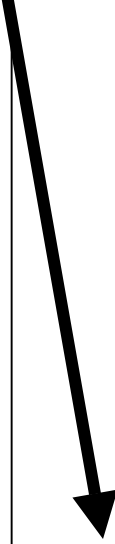
Polyviz – radviz + value of variable indicated





The **GRAND** tour

2D projections of an N-D space - choose suitable axes of rotation and an algorithm that ensures you explore all the space.
(The maths is complicated – See E. Wegman or Asimov



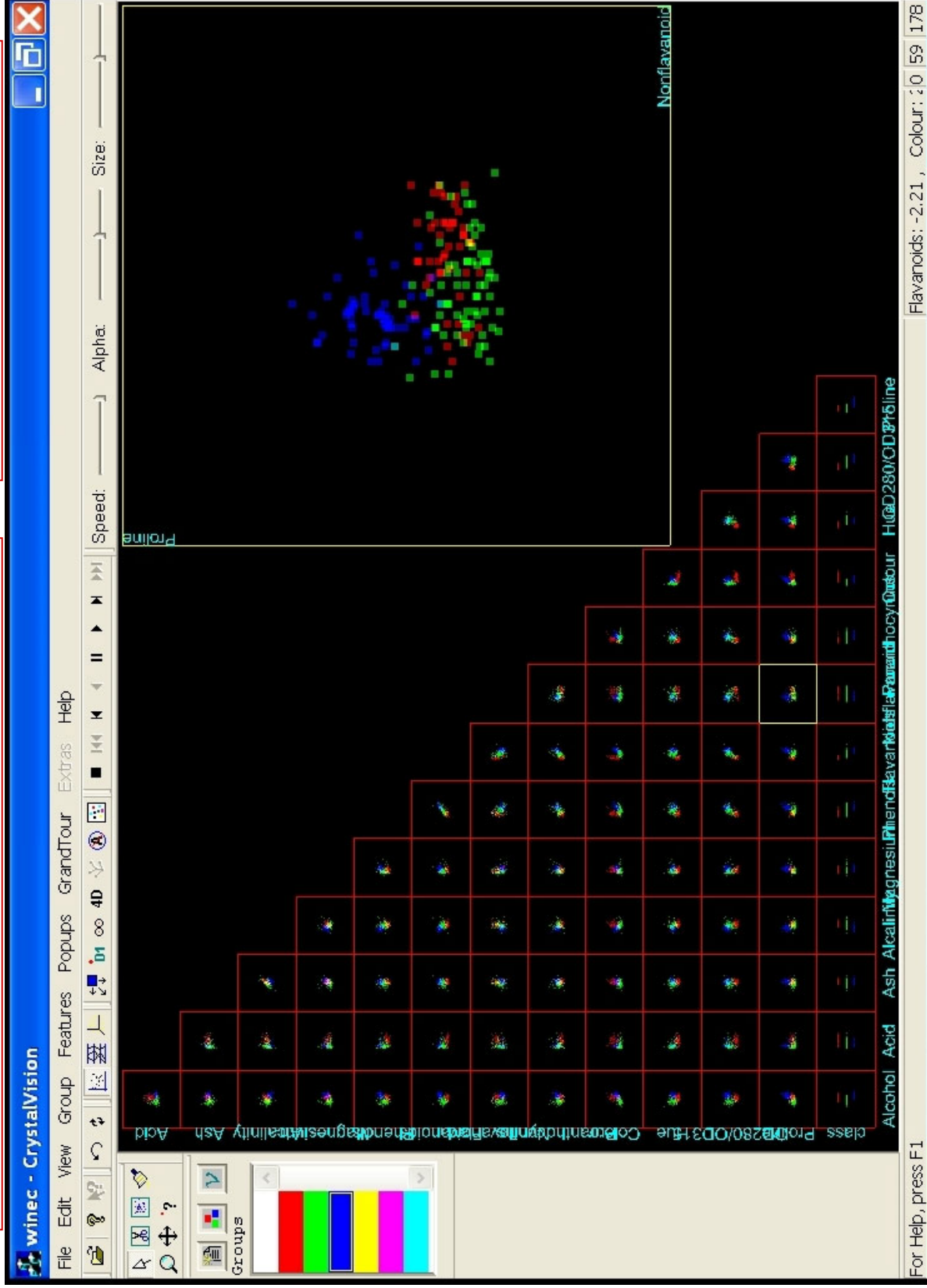
The Grand Tour via Geodesic Interpolation of 2-frames*

Daniel Asimov and Andreas Buja†
Report RNR-94-004, February 1994

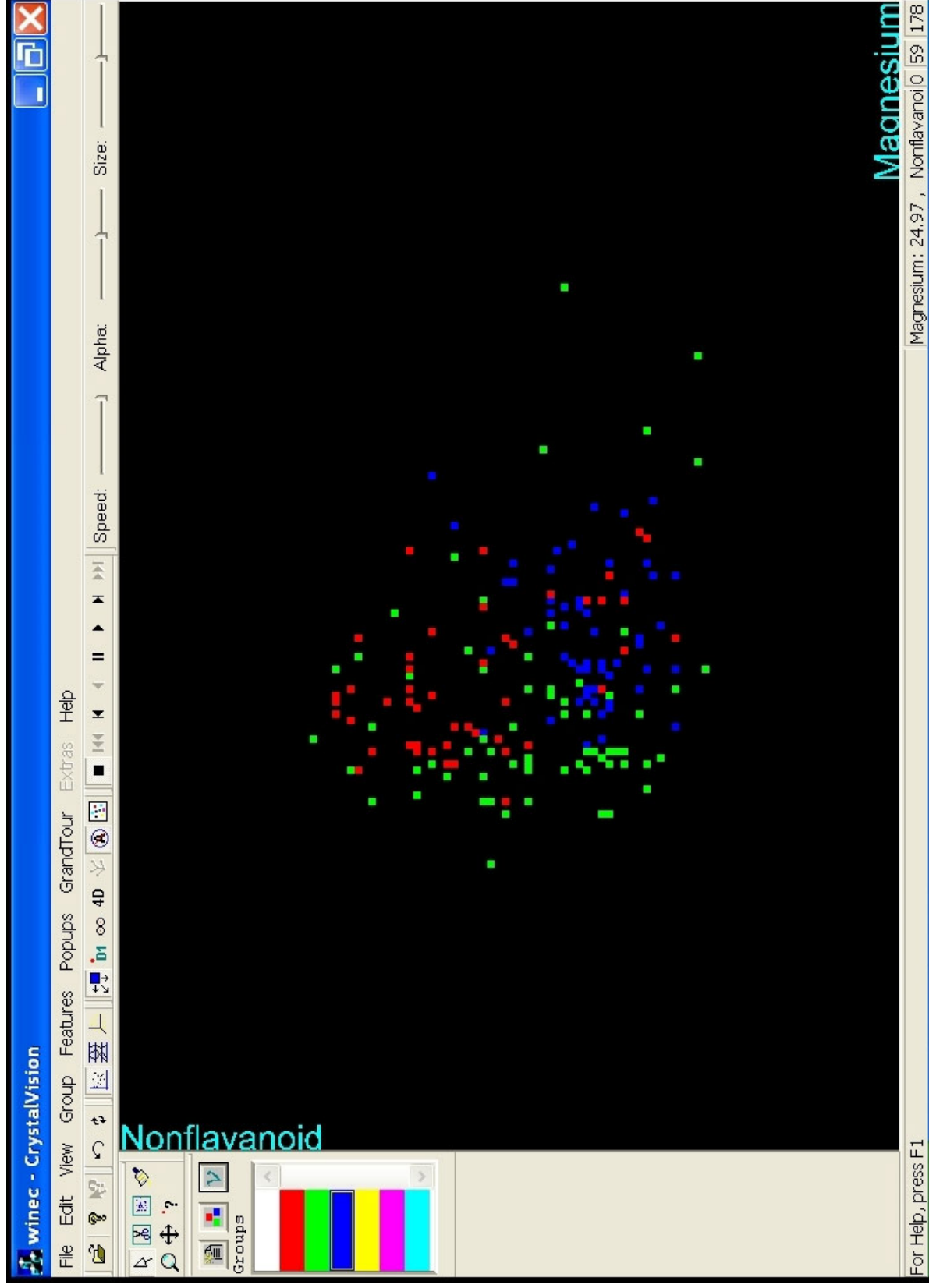
Facinating idea – useful for looking for clusters in data

Grand Tour of the wine dataset 1

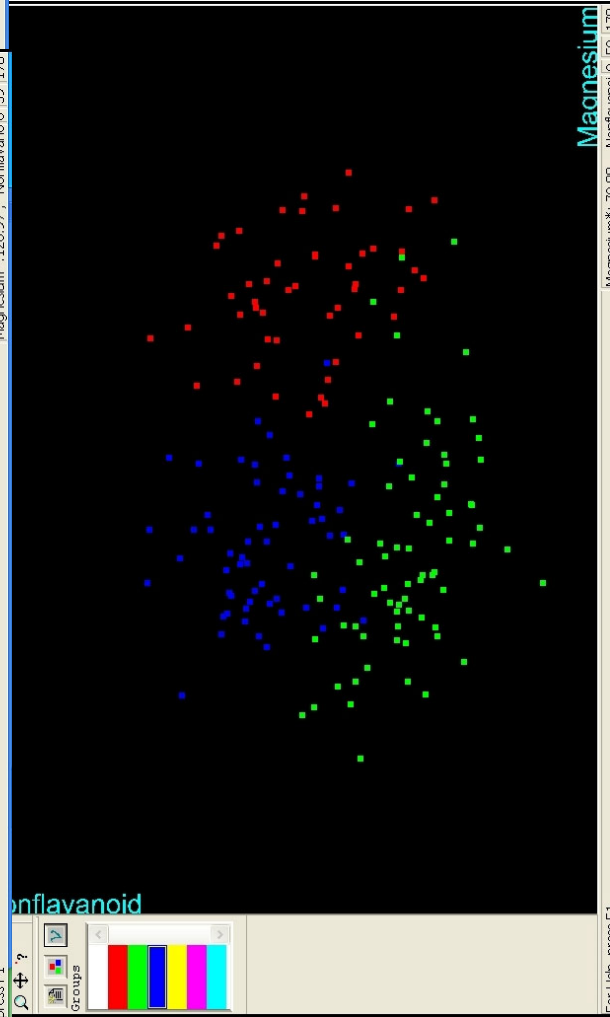
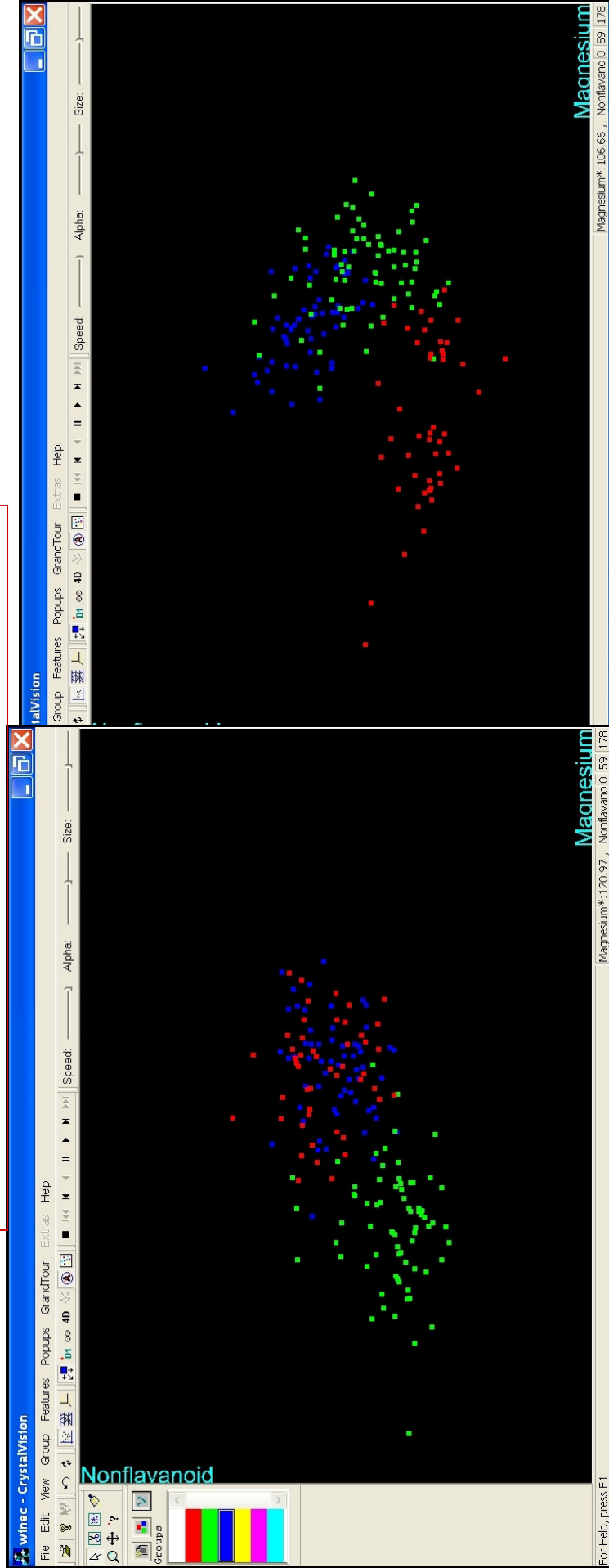
Invented by Asimov

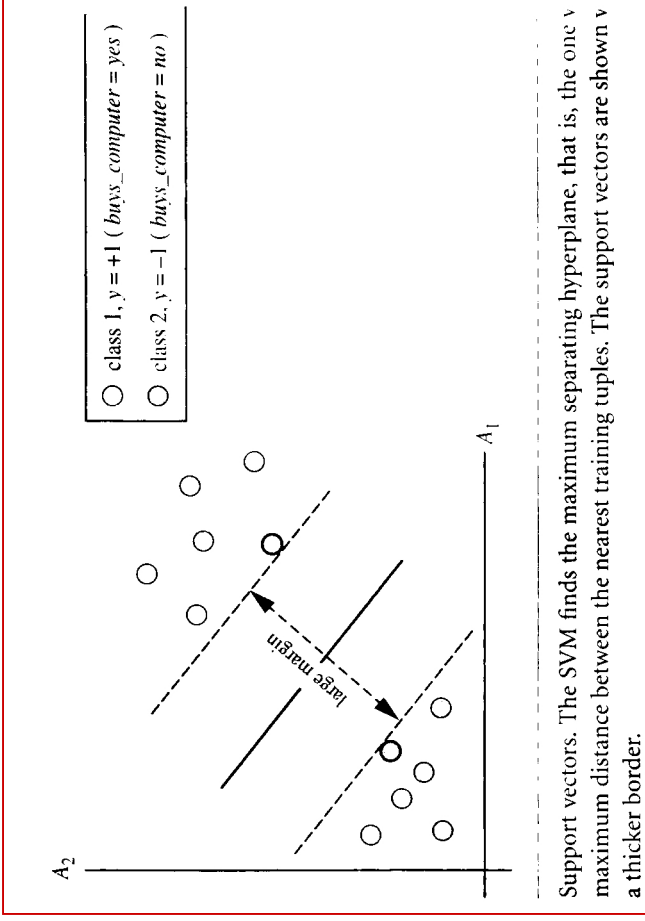


Grand Tour of the wine dataset 2



Grand Tour of the wine dataset 3



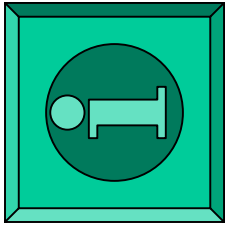


Find hyperplane that separates clusters

Use RBF when plane will not work.

Support Vector Machine - rather confusing name.

For math. details see books referenced earlier.



<http://www.csie.ntu.edu.tw/~cjlin/libsvm/>

SVM-toy is a good introduction

SVM works well on this dataset - Grand Tour agrees

The screenshot shows the Weka Explorer interface with the SVM classifier selected. The classifier output window displays the following results:

Time taken to build model: 0.11 seconds

=== Stratified cross-validation ===
 === Summary ===

| | | |
|----------------------------------|-----------|-----------|
| Correctly Classified Instances | 175 | 98.3146 % |
| Incorrectly Classified Instances | 3 | 1.6854 % |
| Kappa statistic | 0.9745 | |
| Mean absolute error | 0.226 | |
| Root mean squared error | 0.279 | |
| Relative absolute error | 51.4678 % | |
| Root relative squared error | 59.5404 % | |
| Total Number of Instances | 178 | |

=== Detailed Accuracy By Class ===

| TP Rate | FP Rate | Precision | Recall | F-Measure | Class |
|---------|---------|-----------|--------|-----------|-------|
| 1 | 0.008 | 0.983 | 1 | 0.992 | W1 |
| 0.958 | 0 | 1 | 0.958 | 0.978 | W2 |
| 1 | 0.015 | 0.96 | 1 | 0.98 | W3 |

=== Confusion Matrix ===

```

a b c <-- classified as
59 0 0 | a = W1
1 68 2 | b = W2
0 0 48 | c = W3
  
```

The interface also shows the classifier options: Use training set (unchecked), Supplied test set (unchecked), Cross-validation (checked) with 10 folds and 66% split, and Percentage split (unchecked). The result list shows the model path: 23:45:17 - functions.SMO and 23:46:04 - functions.SMO.

J. Platt (1998). "Fast Training of Support Vector Machines using Sequential Minimal Optimization".

Advances in Kernel Methods - Support Vector Learning, B. Schoelkopf, C. Burges, and A. Smola, eds., MIT Press.

Now lets try some other machine learning algorithms on the particle physics dataset...

- Decision Tree C4.5
- VizRank
- SVM
- Neural Net with back propagation

**SVM DOES NOT WORK WELL
GRAND TOUR EXPLAINS WHY.**

Weka Explorer

Preprocess | Classify | Cluster | Associate | Select attributes | Visualize

Classifier: Choose **J48 - C 0.25 - M 2**

Test options:
 Use training set
 Supplied test set
 Cross-validation Folds: **10**
 Percentage split %: **66**
 More options...

(Nom) wine
 Start Stop

Result list (right-click for options):
 23:45:17 - functions.SMO
 23:46:04 - functions.SMO
 00:01:03 - trees.J48

Classifier output:

Time taken to build model: 0.02 seconds

=== Stratified cross-validation ===
 === Summary ===

| | | |
|----------------------------------|-----------|-----------|
| Correctly Classified Instances | 167 | 93.8202 % |
| Incorrectly Classified Instances | 11 | 6.1798 % |
| Kappa statistic | 0.9058 | |
| Mean absolute error | 0.0486 | |
| Root mean squared error | 0.2019 | |
| Relative absolute error | 11.0723 % | |
| Root relative squared error | 43.0865 % | |
| Total Number of Instances | 178 | |

=== Detailed Accuracy By Class ===

| TP Rate | FP Rate | Precision | Recall | F-Measure | Class |
|---------|---------|-----------|--------|-----------|-------|
| 0.983 | 0.034 | 0.935 | 0.983 | 0.959 | W1 |
| 0.944 | 0.056 | 0.918 | 0.944 | 0.931 | W2 |
| 0.875 | 0.008 | 0.977 | 0.875 | 0.923 | W3 |

=== Confusion Matrix ===

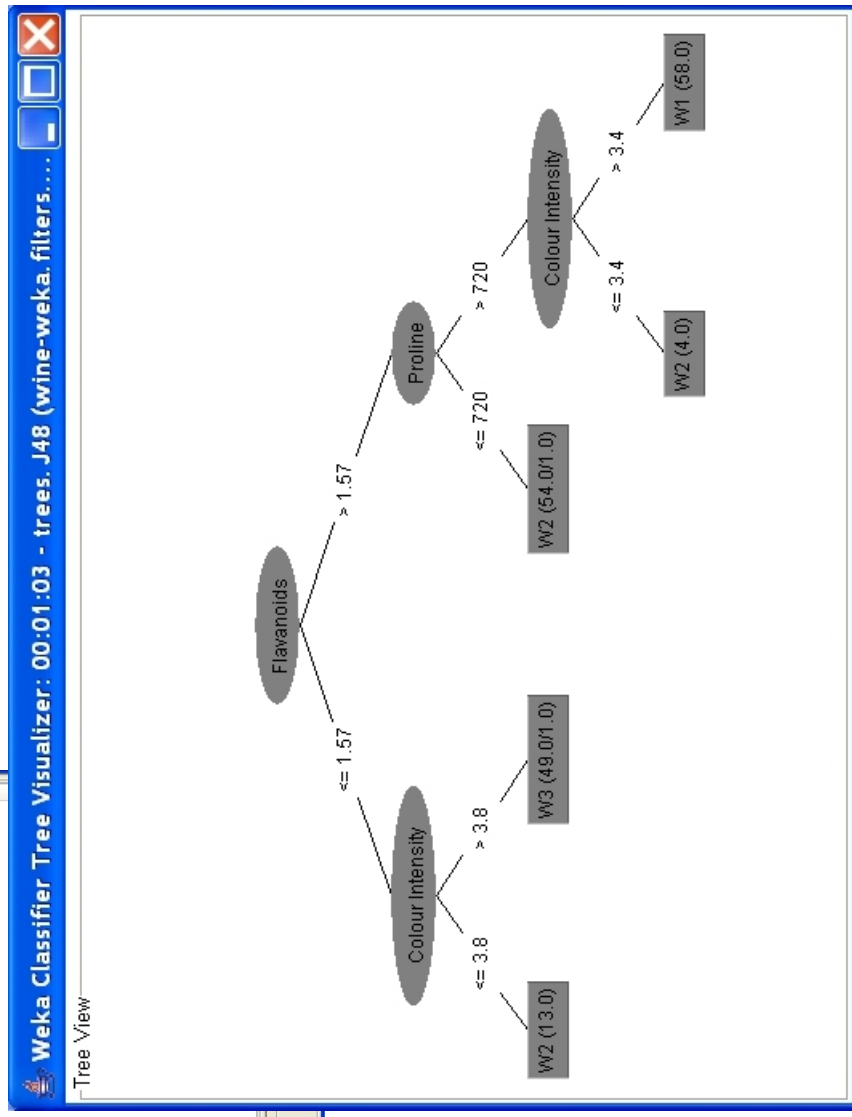
| a | b | c | <-- classified as |
|----|----|----|-------------------|
| 58 | 1 | 0 | a = W1 |
| 3 | 67 | 1 | b = W2 |
| 1 | 5 | 42 | c = W3 |

Status: OK

DECISION TREES

BIG SUBJECT

FOR WINE DATASET

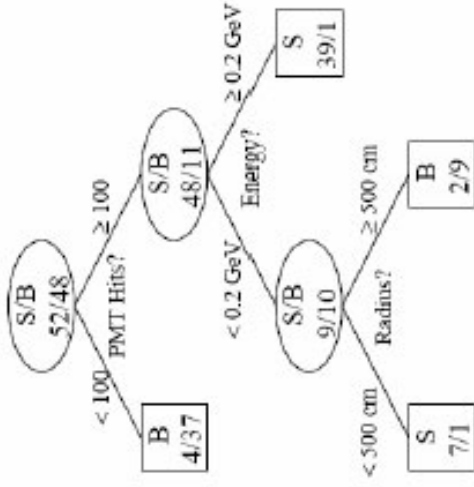


Flavonoids
 Colour
 Proline

94% selection

Decision Trees

Decision trees emerged in mid 80's:
 CART (Breiman, Friedman etc), C4.5
 (Quinlan) etc



Criteria used for commercial trees

(p = fraction of correctly classified events)

$$Q(p) = p$$

$$Q(p) = -2p(1 - p)$$

$$Q(p) = p \log p + (1 - p) \log(1 - p)$$

Gini index

cross - entropy

Split nodes recursively until a stopping criterion is satisfied.

Parent node with W events and correctly classified p^*W events is split into two daughters nodes iff

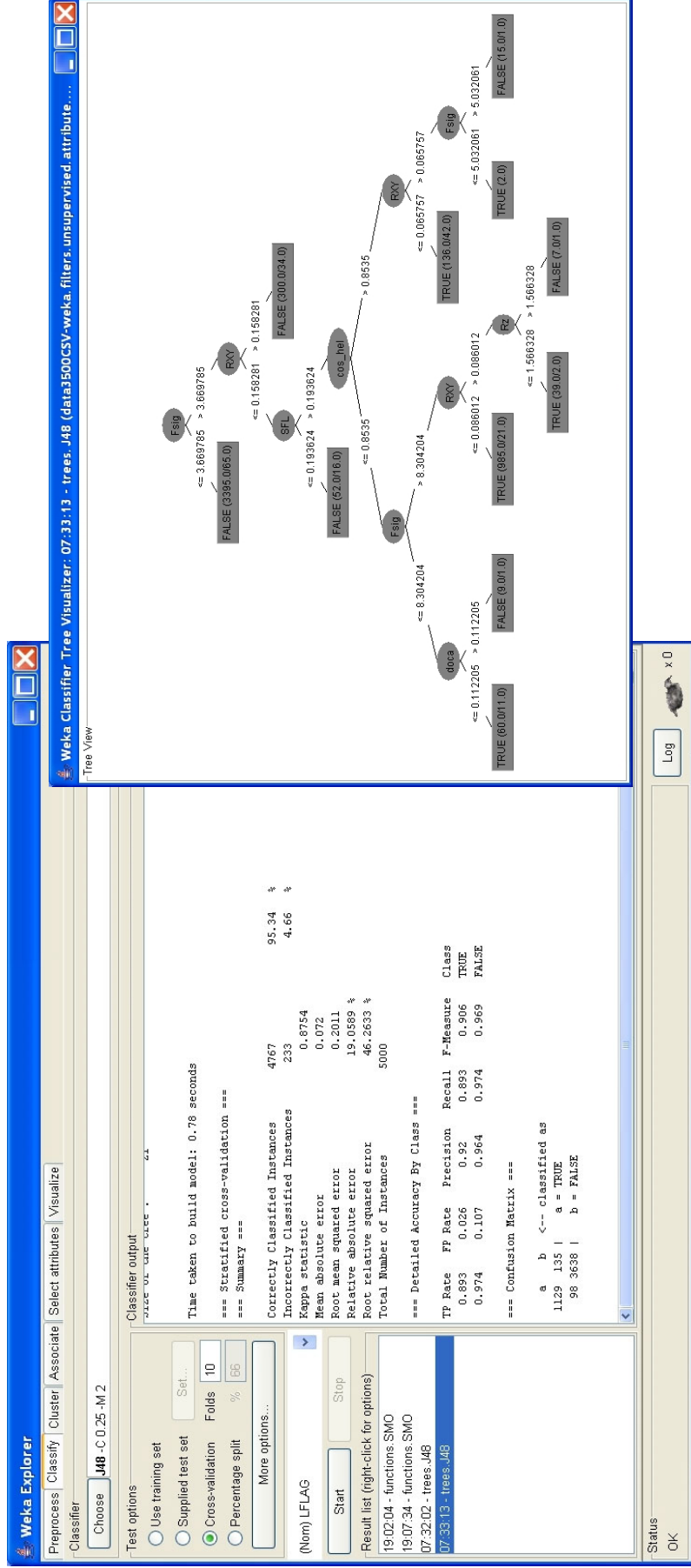
$$WQ(p) < W_1Q(p_1) + W_2Q(p_2)$$

Stopping criteria:

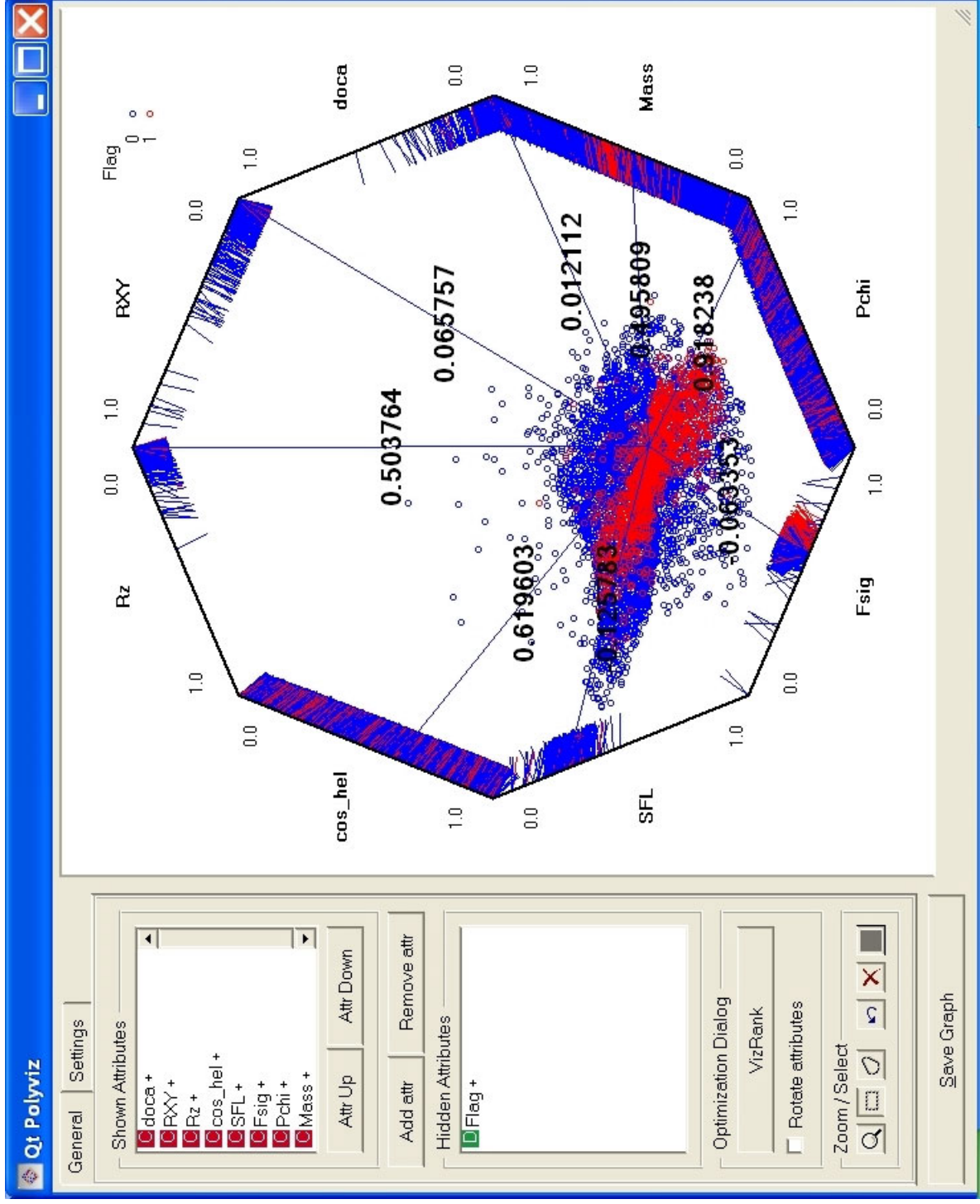
- unable to find a split that satisfies the split criterion
- maximal number of terminal nodes in the tree
- minimal number of events per node

Output of a decision tree is discrete: 1 if an event falls into a signal node, 0 otherwise.

Ilya Narsky Caltech Seminar Oct 2005.

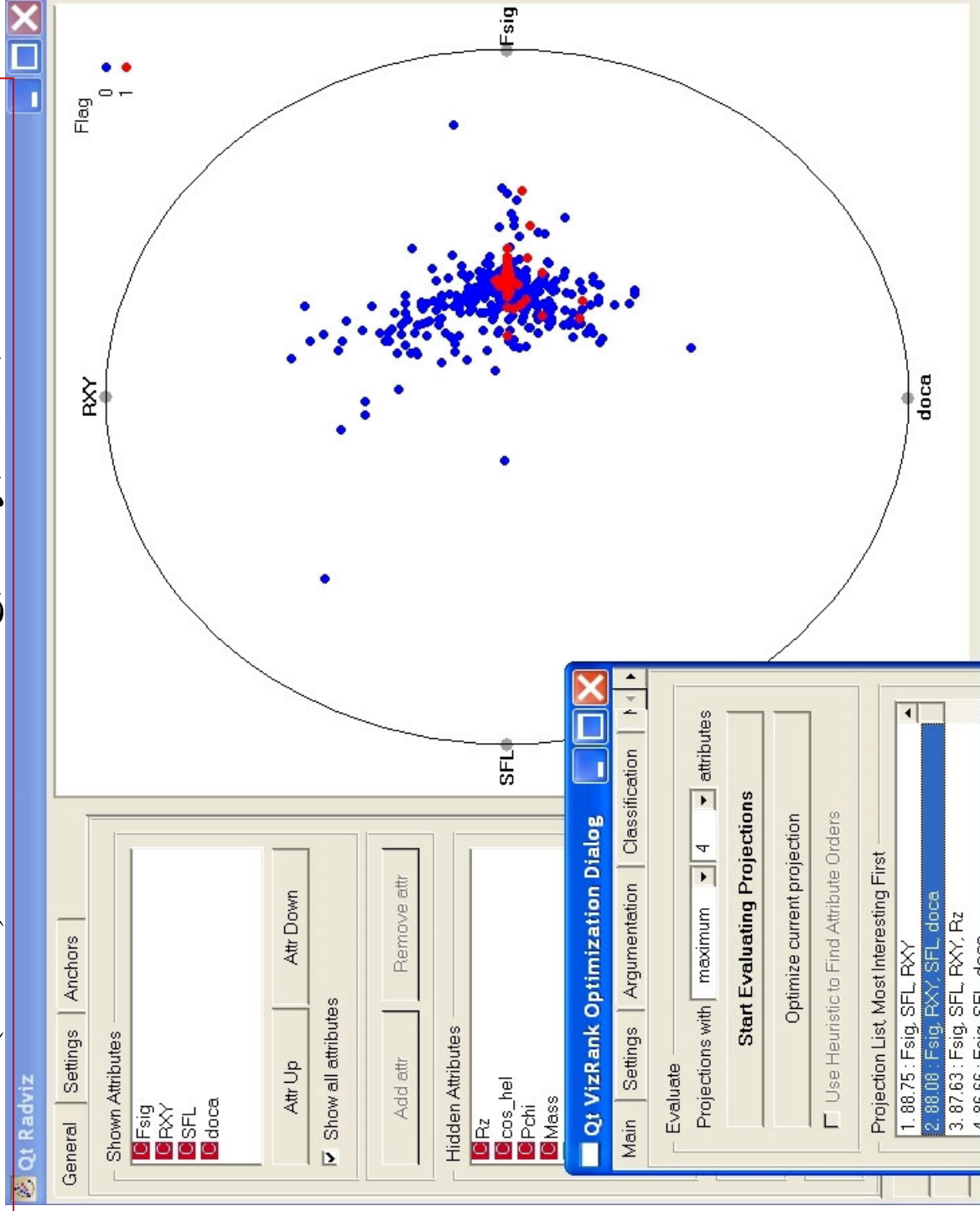


Key variables are: Fsig, Rxy, SFL, cos-hel, doca 95% selection
Remember the parallel coords analysis....



Useful way to see what variables matter.....

VizRank (kNN) Selects Fsig, Rxy, SFL, doxa 88%



Weka Explorer

Preprocess | Classify | Cluster | Associate | Select attributes | Visualize

Classifier
Choose **SMO-C 1.0-E 1.0-G 0.01 -A 250007-L 0.0010-P 1.0E-12-N 0-V 1-W 1**

Test options
 Use training set
 Supplied test set Set...
 Cross-validation Folds **10**
 Percentage split % **66**
 More options...

(Nom) LFLAG
Start Stop

Result list (right-click for options)
 19:02:04 - functions.SMO
 19:07:34 - functions.SMO
 07:32:02 - trees.J48
 07:33:13 - trees.J48
07:43:28 - functions.SMO

Classifier output

Time taken to build model: 31.01 seconds

=== Stratified cross-validation ===
 === Summary ===

| | | |
|----------------------------------|------------|---------|
| Correctly Classified Instances | 3813 | 76.26 % |
| Incorrectly Classified Instances | 1187 | 23.74 % |
| Kappa statistic | 0.0966 | |
| Mean absolute error | 0.2374 | |
| Root mean squared error | 0.4872 | |
| Relative absolute error | 62.831 % | |
| Root relative squared error | 112.1071 % | |
| Total Number of Instances | 5000 | |

=== Detailed Accuracy By Class ===

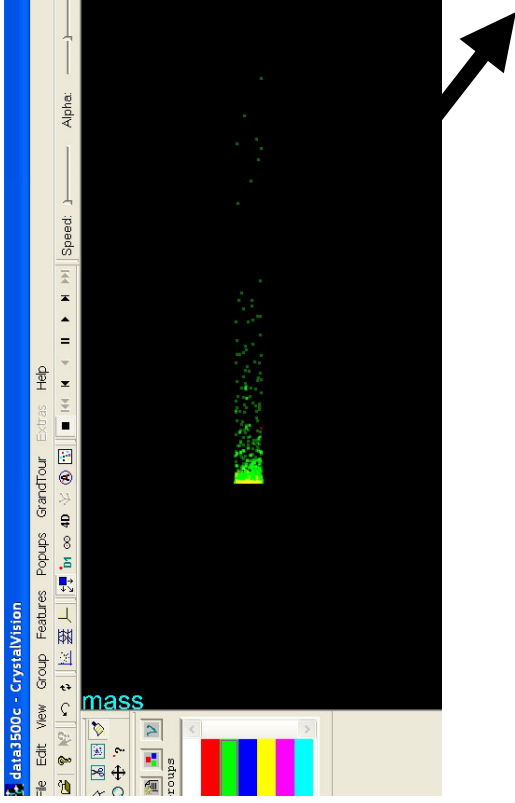
| TP Rate | FP Rate | Precision | Recall | F-Measure | Class |
|---------|---------|-----------|--------|-----------|-------|
| 0.07 | 0.003 | 0.881 | 0.07 | 0.13 | TRUE |
| 0.997 | 0.93 | 0.76 | 0.997 | 0.863 | FALSE |

=== Confusion Matrix ===

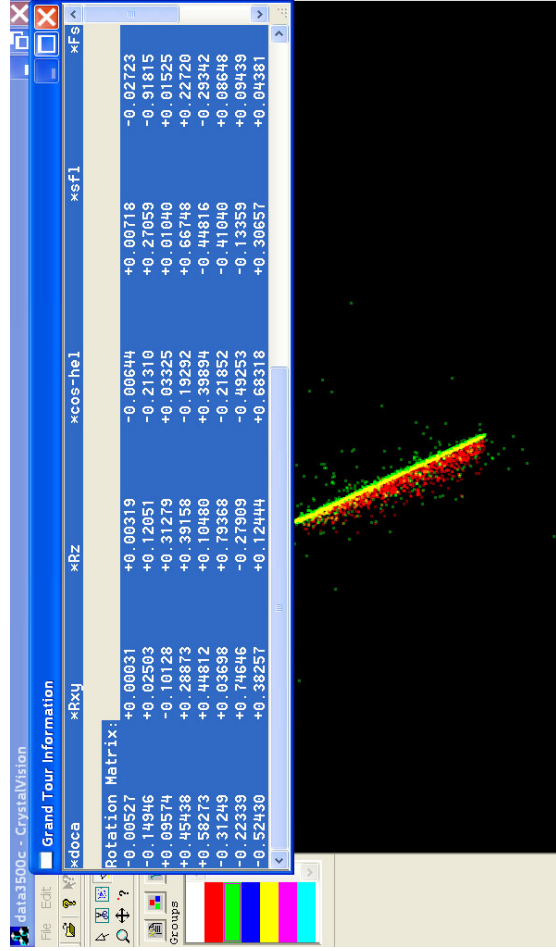
| a | b | <-- classified as |
|----|------|-------------------|
| 89 | 1175 | a = TRUE |
| 12 | 3724 | b = FALSE |

Status OK

SVM (RBF not used) works very badly on this data
 Grand Tour backs this conclusion up.....



Mass v Rxy
Standard Projection



CrystalVision
GrandTour
Cannot separate signal

SUMMARY

C4.5 1129 135
 98 3638

95%

SF BF

S
B

SVM 89 1175
 12 3724

76%

VizRANK 88%

NN with backpropagation

927 337
157 3579

90%

Bagging

1145 119
96 3640

96%

Exploratory data analysis with crystalvision 968 S 44 B !!

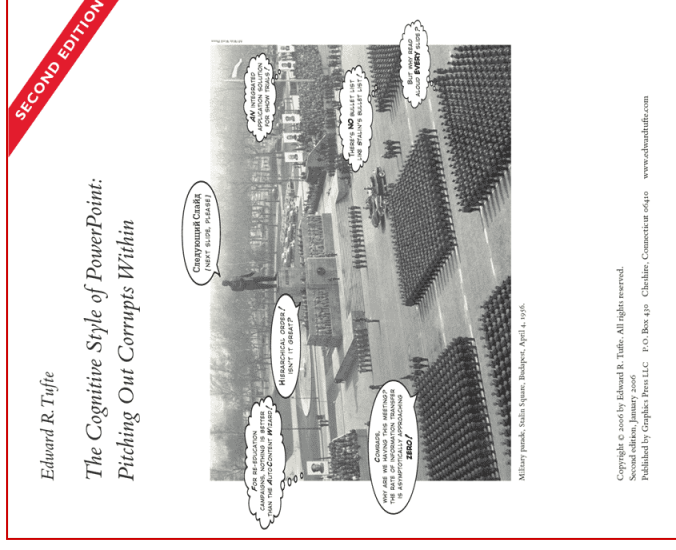
VISUAL DATA ANALYSIS HELPS ONE TO UNDERSTAND THESE RESULTS

SOME OTHER USEFUL DATA VISUALISATIONS

How can you display the data in a way that it can be easily understood ?



<https://www.edwardtufte.com/tufte/>



Should be read by all graduate students !

For last 100 years mathematicians have been suspicious of pictures and visual proofs.....perhaps this is changing.....
Synthese Lib Vol 327, 2005



Visualisations of some mathematical surfaces

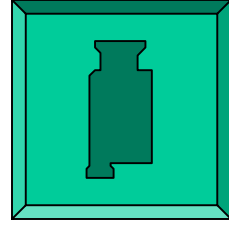
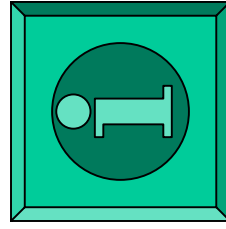
<http://vmm.math.uci.edu/3D-XplorMath/Surface/gallery.html>

Sphere Does Elegant Gymnastics in New Video, Dana Mackenzie. Science 281:5377 (July 1998) 634-635.

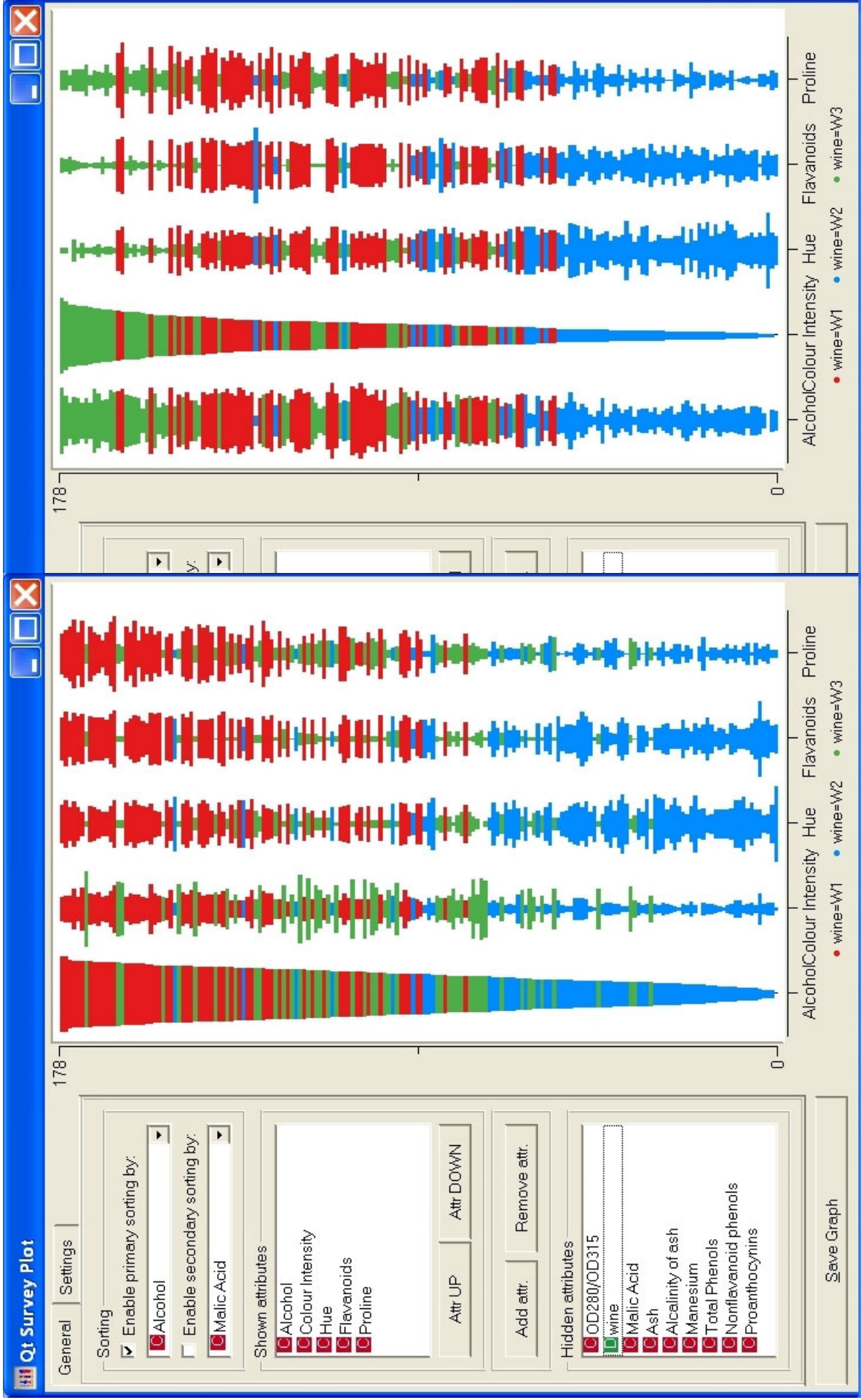
Is it possible to turn a sphere inside out without tearing or creasing it? The answer is yes.

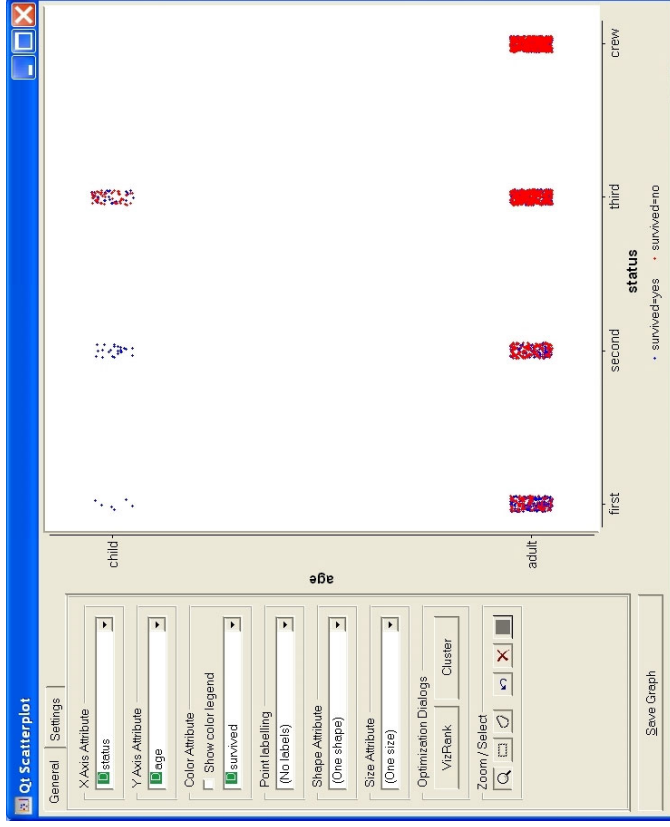
The proof, by Stephen Smale, is over forty years old but until now there has not been a satisfying demonstration. In this interesting article, the author explains how George Francis and John Sullivan at the University of Illinois were able to use a surface created by Robert Kusner in 1983 to create a 6/2 minute computer animation of the eversion process. During the process, it is necessary to keep the energy level (defined so that the energy increases as more bending takes place) at a minimum at each stage. It was noted that the surface Kusner created had an energy level that would make it a candidate for the halfway point of the eversion process. Once the halfway point was known, it seemed possible to go backward to the sphere and forward to the sphere turned inside out. Francis and Sullivan showed with their animation that this is indeed the case. Their video has been shown recently at the Siggraph 98 convention in Orlando and the International Congress of Mathematicians in Berlin.

<http://new.math.uiuc.edu/optiverse/>



SURVEY PLOT - WINE DATA





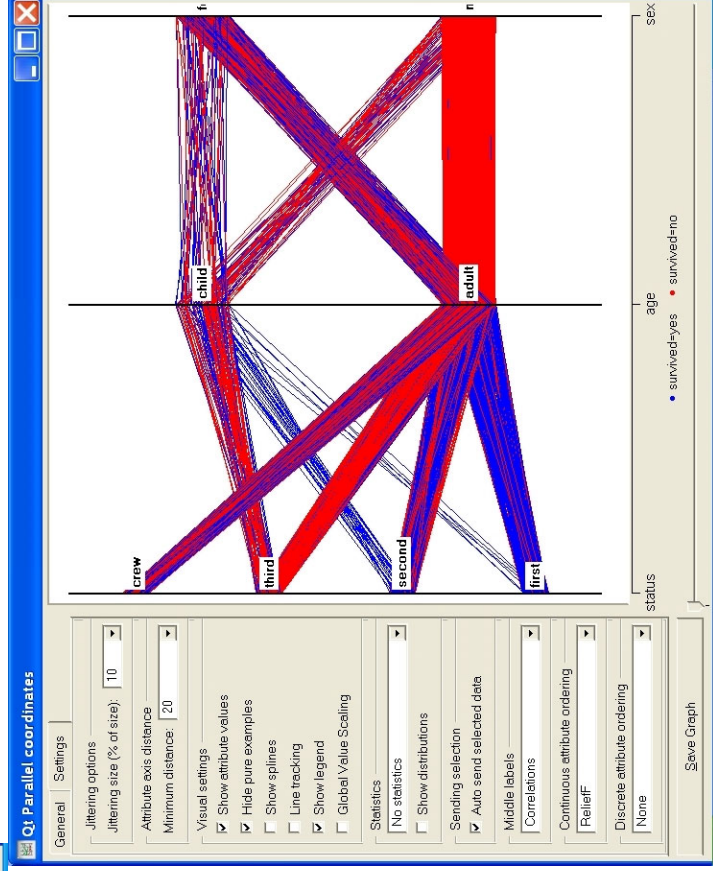
SURVIVED

RED = NO

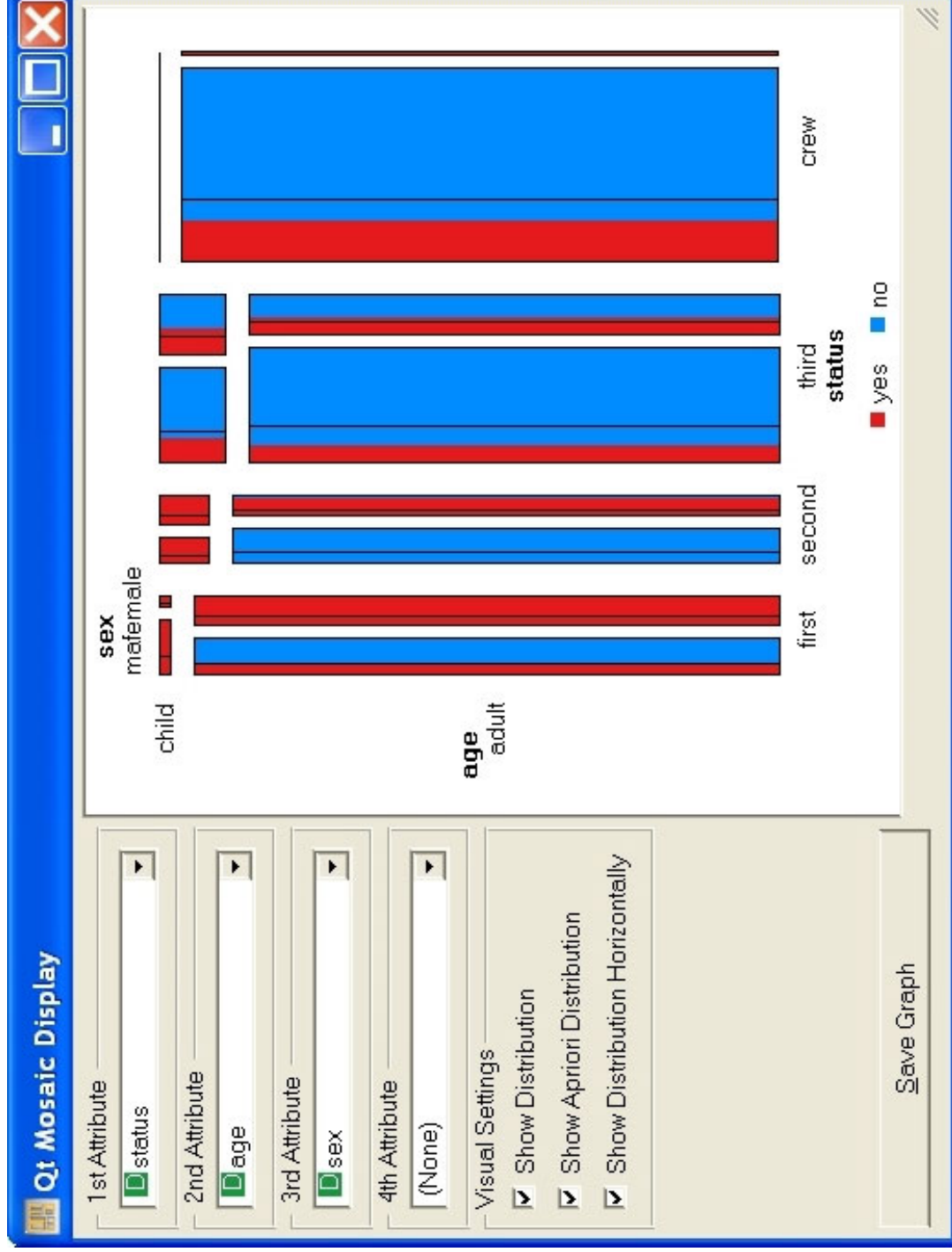
BLUE = YES

Data on Titanic Disaster

Scatterplot and parallel coords do not immediately tell you who and who did not survive

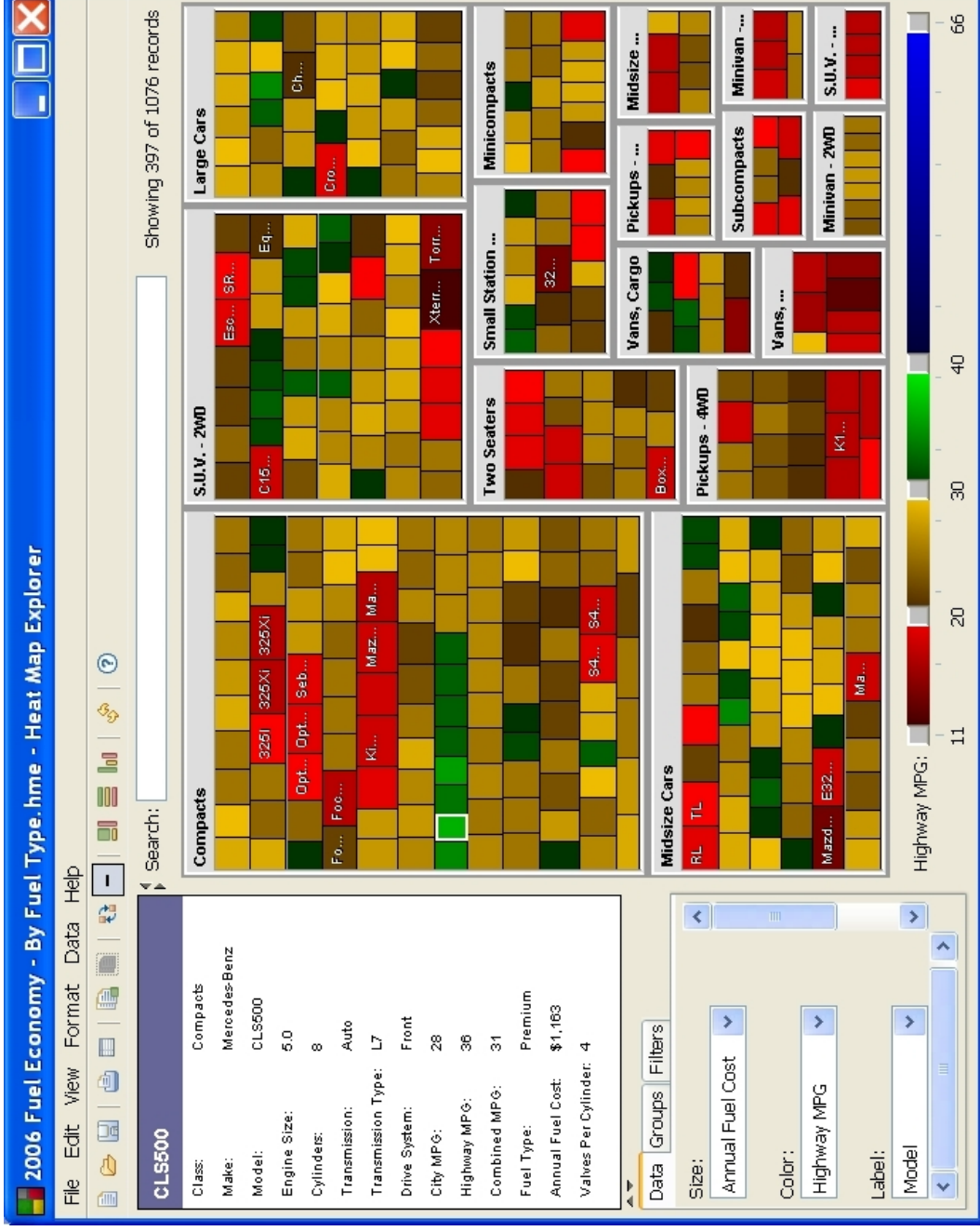


MOSAIC DISPLAY WORKS VERY WELL WITH THIS DATA

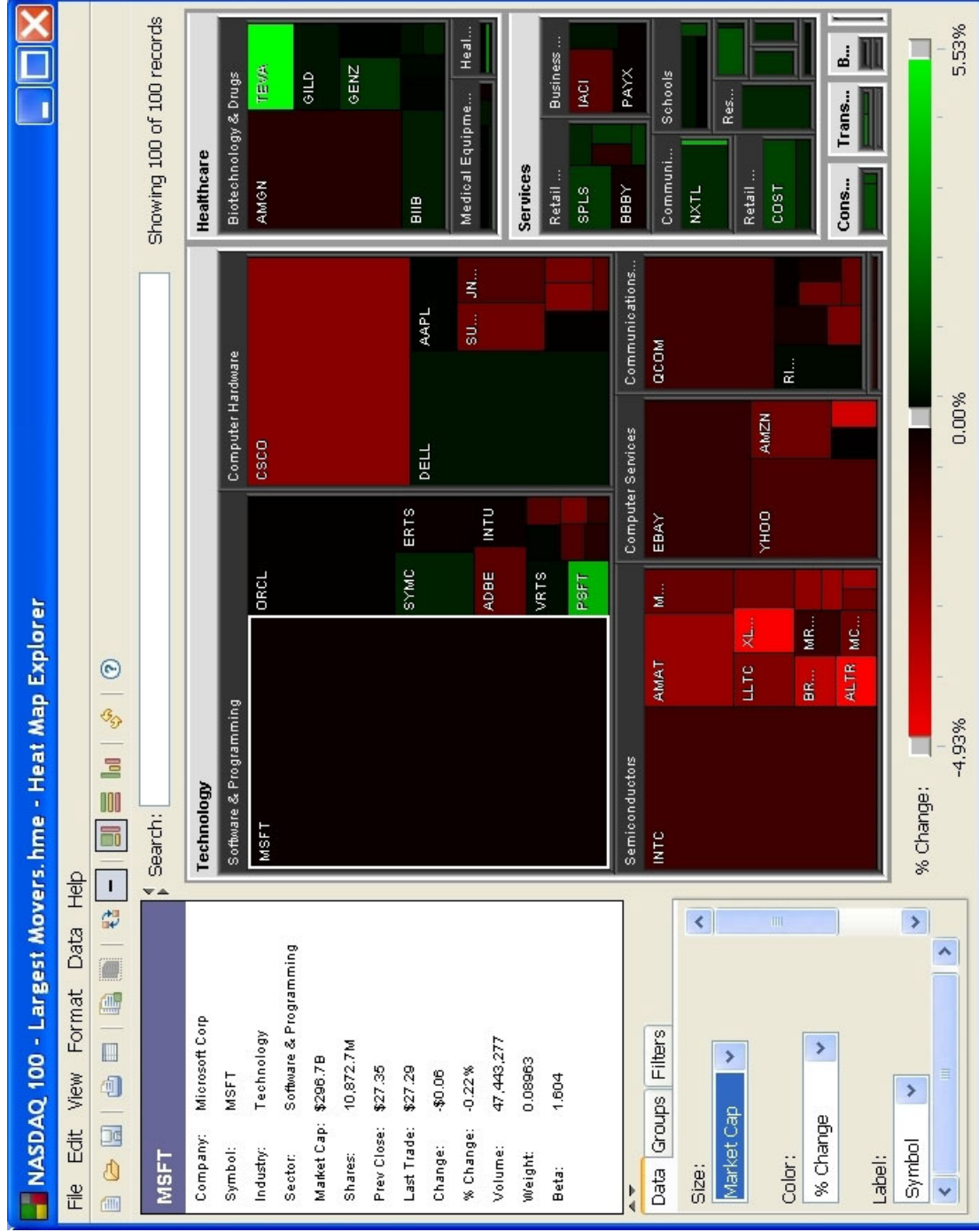


HEAT MAPS - invented by USA professor who wanted to visualise the data on his hard disk

Has drill down procedure



Excellent for looking at a large amount of data quickly – online histograms ?



Useful for stock brokers.....

NOW ITS YOUR TURN....

- **WHERE TO START**
- **PRACTICAL ADVICE**

| Software | Site | Comment |
|-----------------------|---|--|
| CrystalVision | ftp://www.galaxy.gmu.edu/pub/ | Windows. ExplorN Unix α -channel. GT, PC Needs development. |
| GGobi | www.ggobi.org | No α -channel.GT, PC All Platforms. Access to R. |
| Mondrian | http://stats.math.uni-augsburg.de/Mondrian/ | Java. α -channel. |
| Visulab | http://www.inf.ethz.ch/personal/hinterbe/Visulab/ | Excel plugin. PC only |
| Orange | http://www.ailab.si/orange | Component based data mining. C++ and python scripting. PC. |
| WEKA | http://www.cs.waikato.ac.nz/ml/weka/ | Java based data mining package Large no of algorithms included. |
| Datadesk | http://www.datadesk.com/ | Commercial. Linked plots. Stats. |
| Statistica | http://www.statsoft.com/ | Commercial. Very powerful. Not evaluated yet. Graphics + Stats. |
| VisualExplorer | www.curvaceous.com | Commercial. PC for process control Excel PlugIn. |

When to use a particular visualisation ???

**Benchmark Development for the Evaluation of
Visualization for Data Mining**

Georges G. Grinstein¹, Patrick Hoffman¹, Sharon J. Laskowski², Ronald M. Pickett¹

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²The National Institute of Standards and Technology, Gaithersburg, MD 20899
sharon.laskowski@nist.gov

Table 8 Scatter Plot Matrix

| TASK | See Outliers | See Clusters | Find Class Clusters | See All Important Features | See Some Important Features | See Possible Rule/Model | See Exact Rule/Model |
|--------------------|--------------|--------------|---------------------|----------------------------|-----------------------------|-------------------------|----------------------|
| DATA SET | | | | | | | |
| Balloons | | | | | | | |
| Balloons-flattened | | | | | | | |
| Lenses | | | | | | | |
| Lenses-flattened | | | | | | | |
| Corrings | Y | Y | Y | Y | Y | Y | |
| Monks 1-training | | | | | | | |
| Iris | Y | Y | Y | | Y | Y | |
| Congress | | | | | | | |
| Liver | Y | Y | Y | | | | |
| Cars | Y | Y | Y | | Y | Y | |
| Wine | Y | Y | Y | | Y | Y | |

Table 6 Survey Plot

| TASK | See Outliers | See Clusters | Find Class Clusters | See All Important Features | See Some Important Features | See Possible Rule/Model | See Exact Rule/Model |
|--------------------|--------------|--------------|---------------------|----------------------------|-----------------------------|-------------------------|----------------------|
| DATA SET | | | | | | | |
| Balloons | | | | Y | Y | | Y |
| Balloons-flattened | | | | Y | Y | | Y |
| Lenses | | | | | Y | Y | |
| Lenses-flattened | | | | | Y | Y | |
| Corrings | Y | | | Y | Y | Y | |
| Monks 1-training | | | | Y | Y | Y | Y |
| Iris | Y | Y | Y | Y | Y | Y | |
| Congress | | | | Y | Y | | |
| Liver | | | | | | | |
| Cars | | | | Y | Y | Y | |
| Wine | | | | Y | Y | Y | |

Table 4 Parallel Coordinates

| TASK | See Outliers | See Clusters | Find Class Clusters | See All Important Features | See Some Important Features | See Possible Rule/Model | See Exact Rule/Model |
|--------------------|--------------|--------------|---------------------|----------------------------|-----------------------------|-------------------------|----------------------|
| DATA SET | | | | | | | |
| Balloons | | | | | | | |
| Balloons-flattened | | | | | | | |
| Lenses | | | | | | | |
| Lenses-flattened | | | | | | | |
| O-rings | Y | Y | Y | Y | Y | Y | |
| Monks1-training | | Y | | Y | Y | Y | Y |
| Iris | Y | Y | Y | Y | Y | Y | |
| Congress | | | | | | | |
| Liver | Y | Y | | | | | |
| Cars | Y | Y | Y | | Y | Y | |
| Wine | Y | Y | Y | | Y | Y | |

Table 5 Radviz

| TASK | See Outliers | See Clusters | Find Class Clusters | See All Important Features | See Some Important Features | See Possible Rule/Model | See Exact Rule/Model |
|--------------------|--------------|--------------|---------------------|----------------------------|-----------------------------|-------------------------|----------------------|
| DATA SET | | | | | | | |
| Balloons | | Y | Y | | | Y | |
| Balloons-flattened | | Y | Y | | Y | Y | |
| Lenses | | Y | Y | | Y | | |
| Lenses-flattened | | Y | Y | | Y | | |
| O-rings | Y | Y | Y | Y | Y | Y | |
| Monks1-training | | Y | | | | | |
| Iris | Y | Y | Y | | | Y | |
| Congress | Y | Y | Y | | Y | | |
| Liver | Y | Y | | | | | |
| Cars | Y | Y | Y | | Y | Y | |
| Wine | Y | Y | Y | | Y | Y | |

WITH THE RIGHT TOOLKIT

(WEKA/ORANGE/CRYSTAL VISION
ARE VERY POWERFUL STARTING
POINTS)

Visualise the data

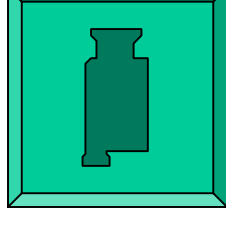
Apply various data mining techniques to your data

Compare the results and then

use your own judgement on how to proceed

OCCAMS RAZOR is a good principle

WARNING ... VIZ-O-Matic
The dangers of Glitziness



CONCLUSIONS

How was this seminar researched ????
Google – data mined the Internet
Books and papers !! The book is not dead yet.

There are powerful visualisation and machine learning techniques available. This field is rapidly growing.

USE THEM IN YOUR RESEARCH !!!!!!!

WE SHOULD BUILD THEM INTO OUR
DATA ANALYSIS SOFTWARE

STANDARD HEP REPOSITORY OF DATA SAMPLES
TO EVALUATE NEW METHODS

Can we data mine particle physics data without a priori ideas
of the physics we wish to see ????????????

FINAL THOUGHT.....

**IDEAS GUIDE YOU WHEN
YOU CANNOT SEE.**