Data Mining and Visualization

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Overview

- Data mining components
  - Functionality
  - Example application
    - Quality control
- Visualization
  - Use of 3D
  - Example application
    - Market research
- Statistics and visualization in Excel
  - What's the problem?

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NAG Data Mining Components (DMC)

Data Cleaning

- *Data imputation* adding missing values
- *Outlier detection* finding suspect data records

Data Transformation

- *Scaling Data* before distance computation
- *Principal Component Analysis* reducing # of variables

Cluster Analysis

- *k-means* analyst decides # of clusters in data
- *Hierarchical* stepwise agglomeration of data

DMC: Classification techniques

- *Classification Trees* Two types of decision tree:
  - binary (Gini index)
  - n-ary (entropy-based)
- *Generalized Linear Models* Fitting of
  - Binomial distribution (for binary classification tasks)
  - Poisson distribution (for count data)
- *k-Nearest Neighbours*
  - Predict values using k most similar records in a training dataset
  - Set prior probabilities for data classes
  - Also used for regression (see below)

DMC: Regression techniques

- Regression Trees
  - Minimise sum of squares about mean
    - robust estimate of the mean, or sample average
- Linear Regression
  - Automatic selection of model variables
- Multi-Layer Perceptron Neural Networks
  - Flexible non-linear models
    - Free parameters in MLP optimised using conjugate gradients
- Nearest Neighbours (see above)
- Radial Basis Function Models
  - function of distance from centre location to data records

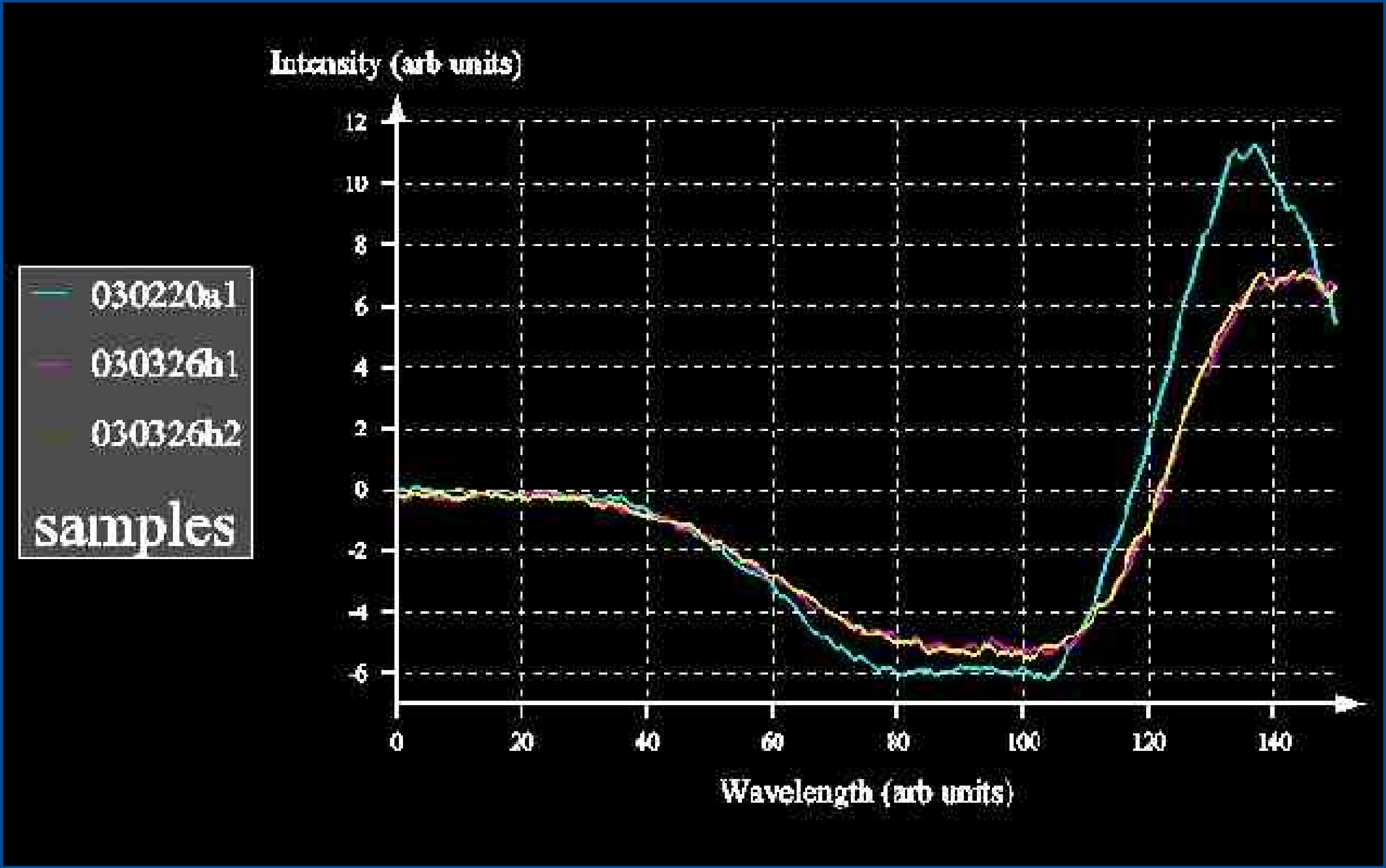
DMC: other techniques

- Association rules
  - Determine relationships between nominal data values
- Utility functions
  - Random number generators
  - Rank ordering
  - Sorting
  - Mean and sum of squares updates
  - Two-way classification comparison
  - Save and load models

Example application: Quality control

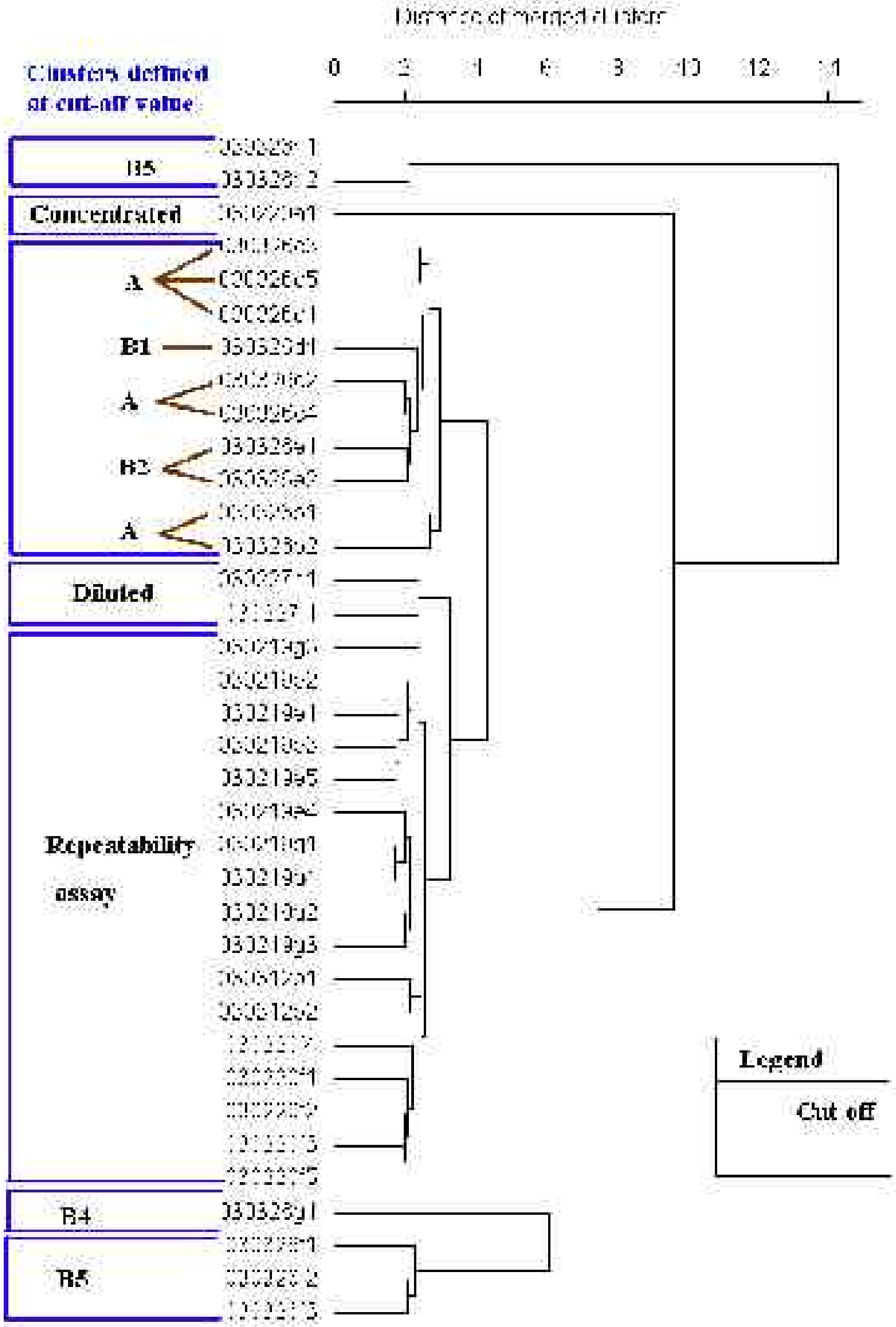
- Detection of changes in sample
  - due to e.g. heating
- Use circular dichroism spectroscopy
  - measures difference in absorbance by left & right polarized light
- Generates spectrum for each sample
  - Intensity vs wavelength
- Some spectra look similar, others don’t
- How to classify them?

Spectra display



Classification

- 36 spectra, 152 intensity values each
- Read into 36 x 152 matrix
- Passed to hierarchical cluster analysis routines
  - Euclidean distances between data points
  - Average link distances between clusters
- Output displayed as dendogram
  - tree plot showing merging of clusters with distance
- Introduce a cut-off to define “natural” clusters


Distance of merged clusters
0
2
4
6
8
10
12
14
Clusters defined at cut-off value
B5
Concentrated
A
B1
A
B2
A
Diluted
Repeatability assay
B4
B5
Legend
Cut off

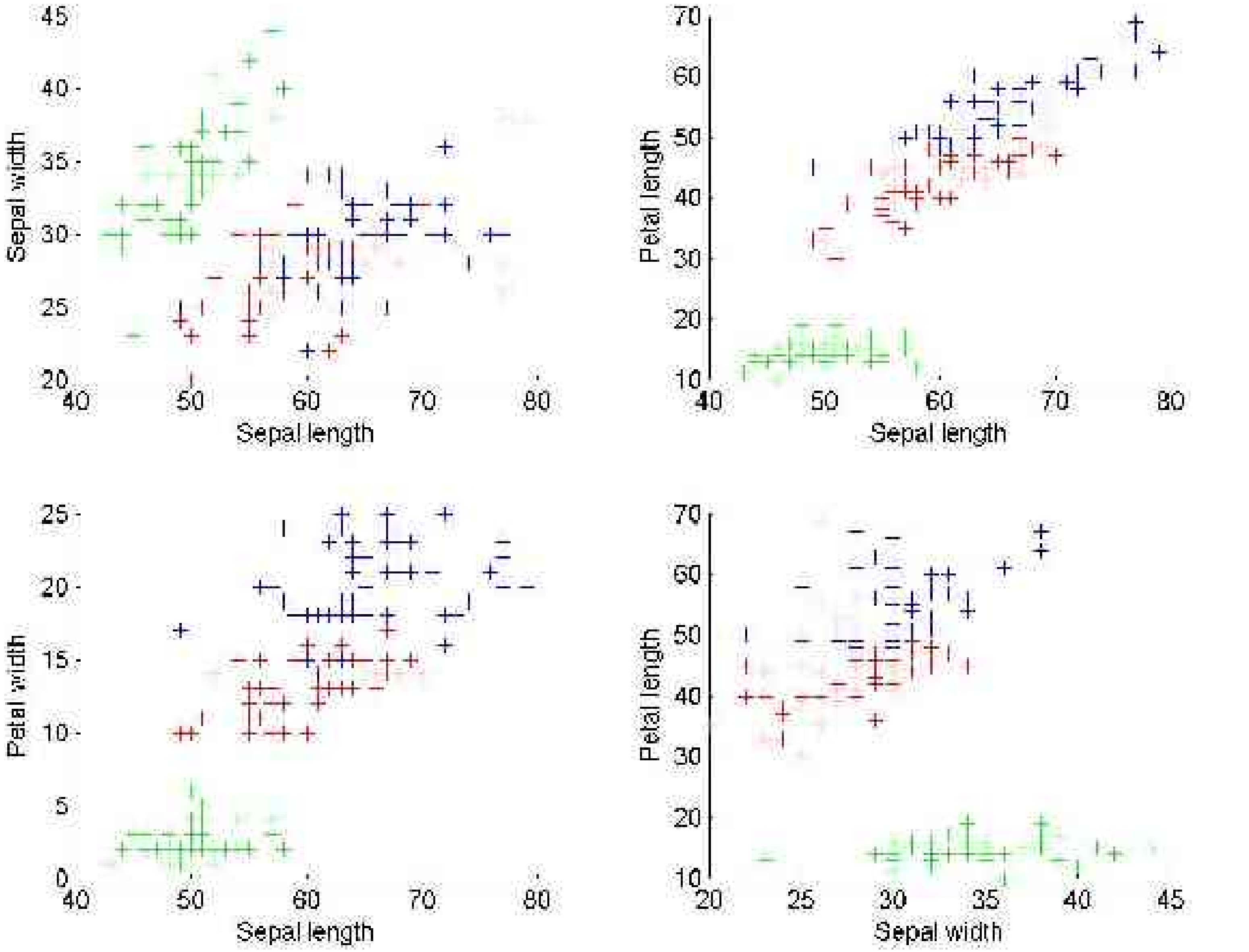
Analysis

- Cut off gives seven natural clusters
  - not v. sensitive to distance functions
- Some of the results can be understood w.r.t experimental conditions
  - e.g. 030220a1 - concentrated sample (evaporation)
  - e.g. 030319g5 to 030330f5 - repeatable experiment
- But there are some outliers
  - e.g. 030326e1, 030326e2 in normals
  - needs consultation with domain experts

Example application: Classification

- Fisher’s iris dataset
  - 4 measurements made on 50 iris specimens from each of three species
  - petal length, petal width, sepal length, sepal width
  - How to classify the species?
- 150 data points
- Each point
  - has 4 independent variables
  - belongs in one of three classes
    - red, green, blue
- How to display dataset?

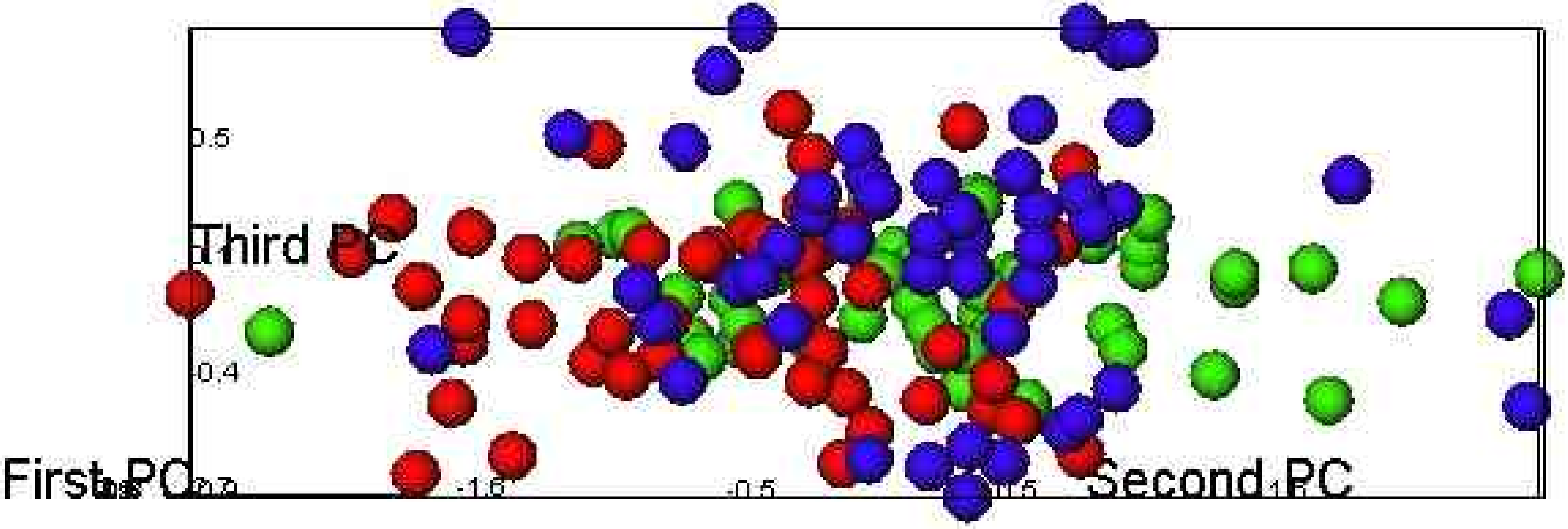
2D scatterplots



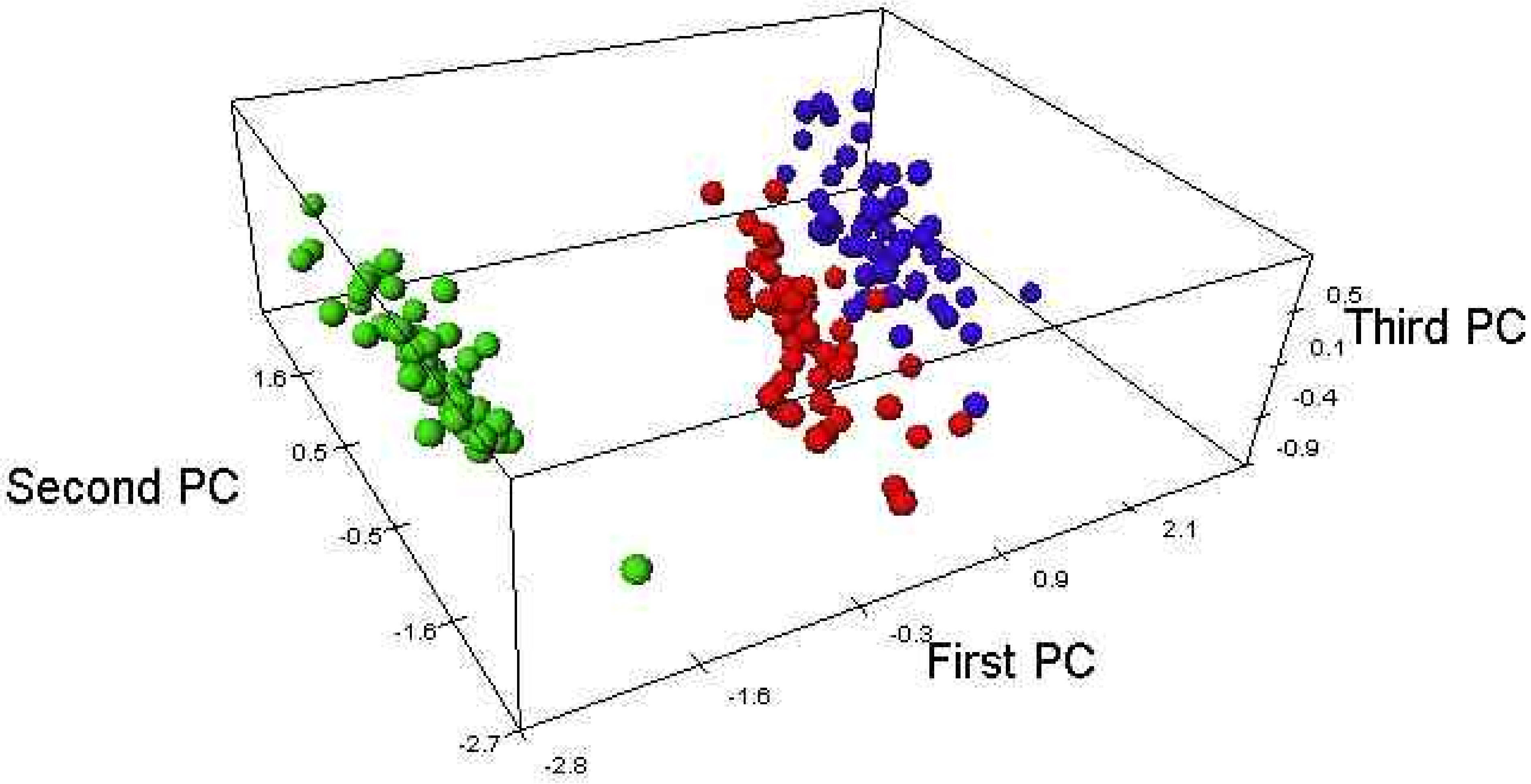
Scatterplots?

- In 2D, need 6 plots
  - to show each variable vs every other one
- Need to consider them all at the same time
- Can reduce the number of variables
  - using principal components analysis
  - first three explain ~95% of the variance
- Scatterplot in 3D

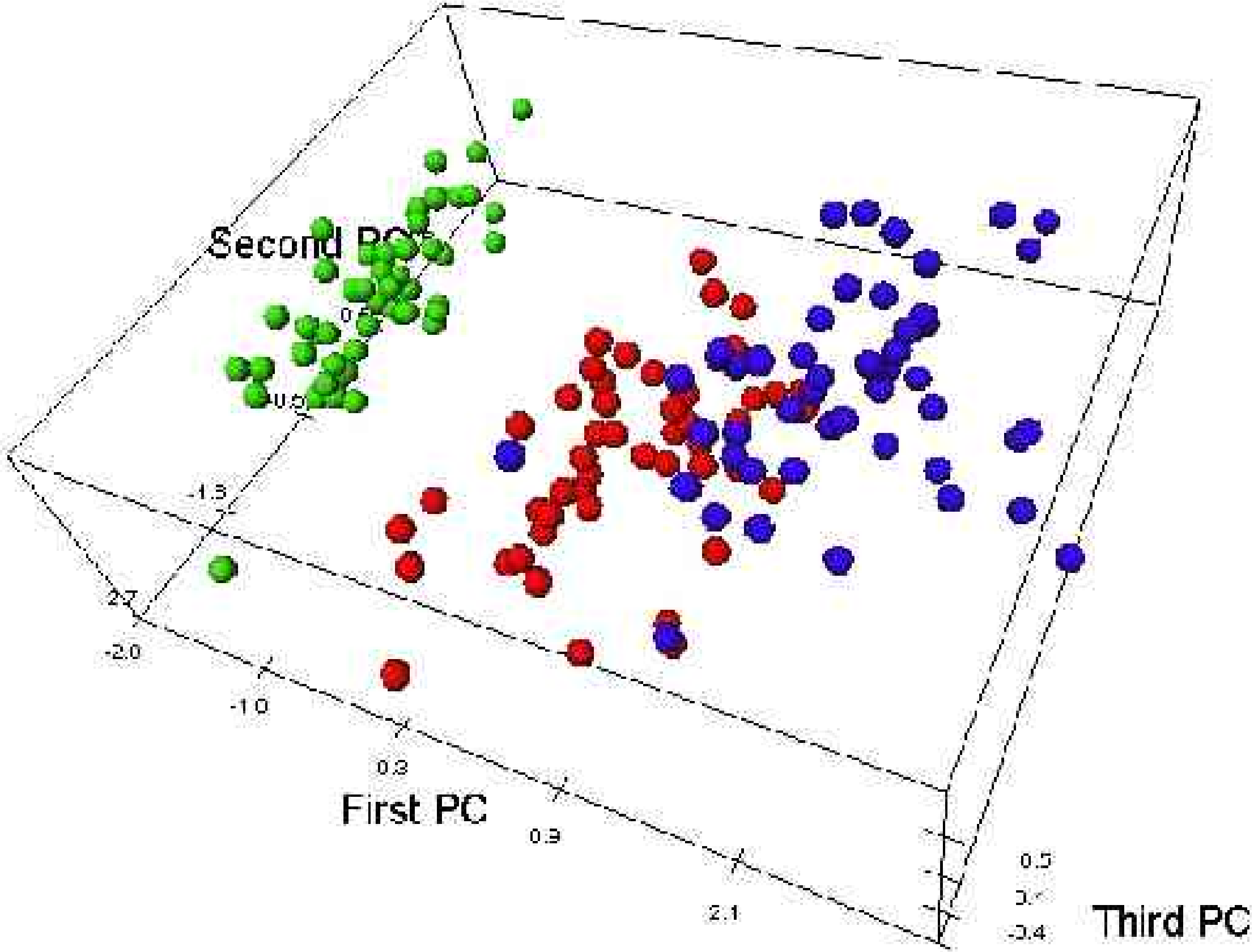
3D scatterplot



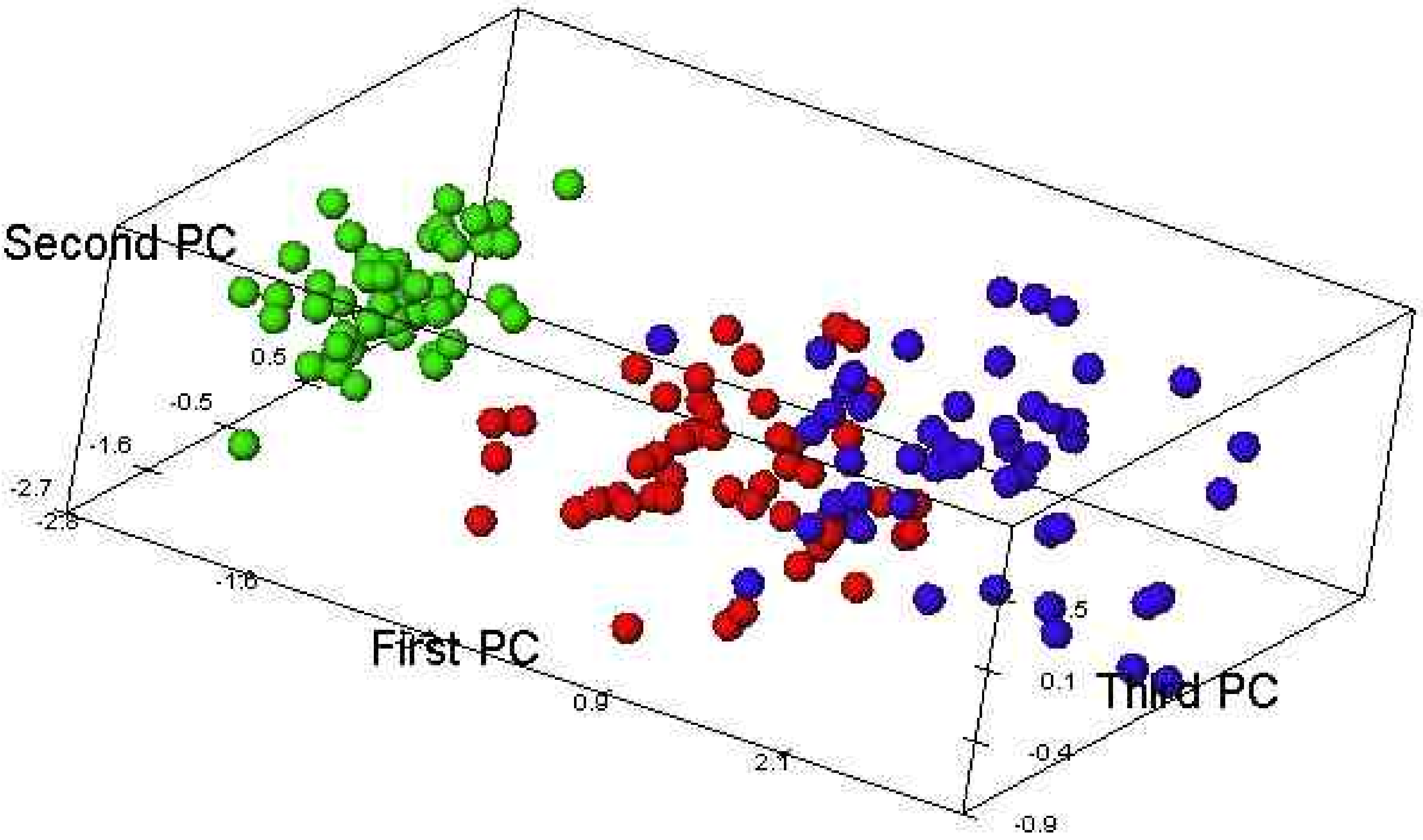
3D scatterplot



3D scatterplot



3D scatterplot



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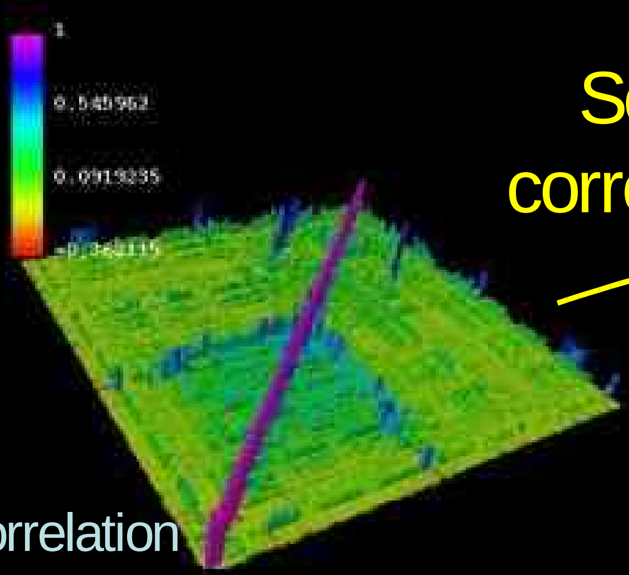
Example: Visual datamining

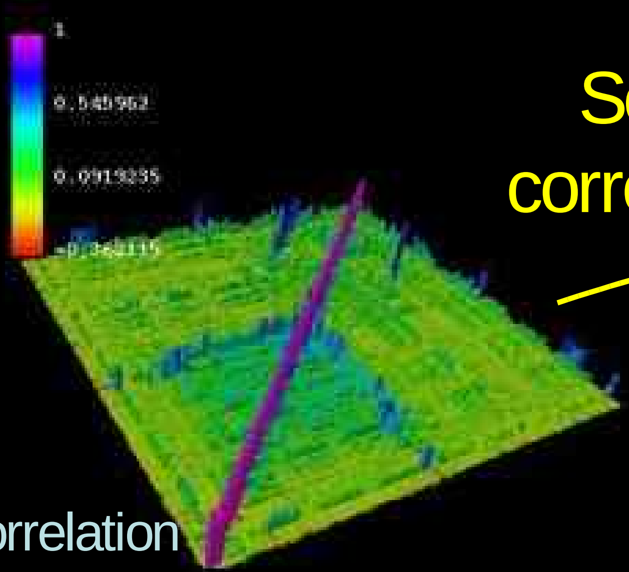
- Dutch financial asset management company
  - Keen to target products at entrepreneurs
  - How does entrepreneurship relate to other customer characteristics?
- Marketing dataset
  - 25,000 customers (sampled from full customer base)
  - Each characterised by values for 100 variables
    - Investment history = “entrepreneurship”
    - Income
    - Age
    - …



Correlation matrix

Select strongly correlated variables

Select strongly correlated variables



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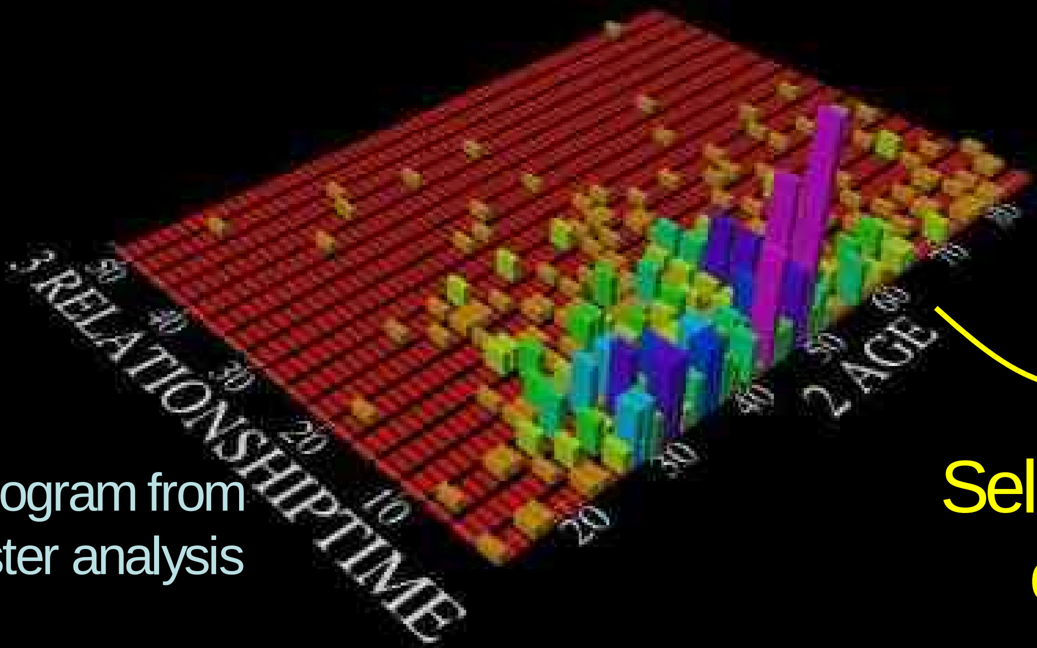
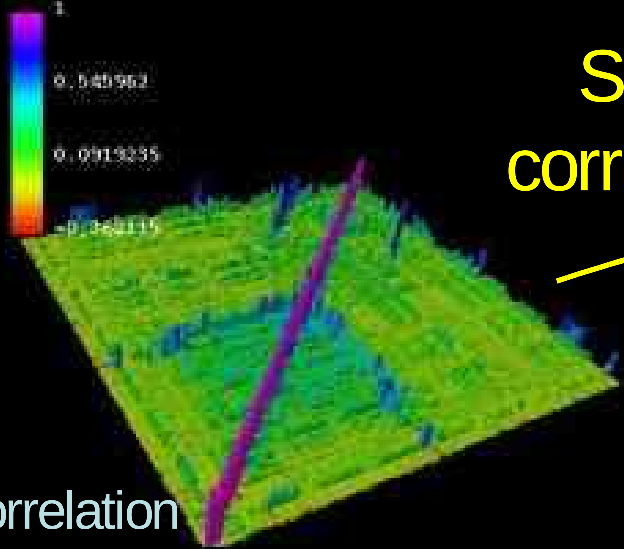


Histogram from cluster analysis

Select variables of interest



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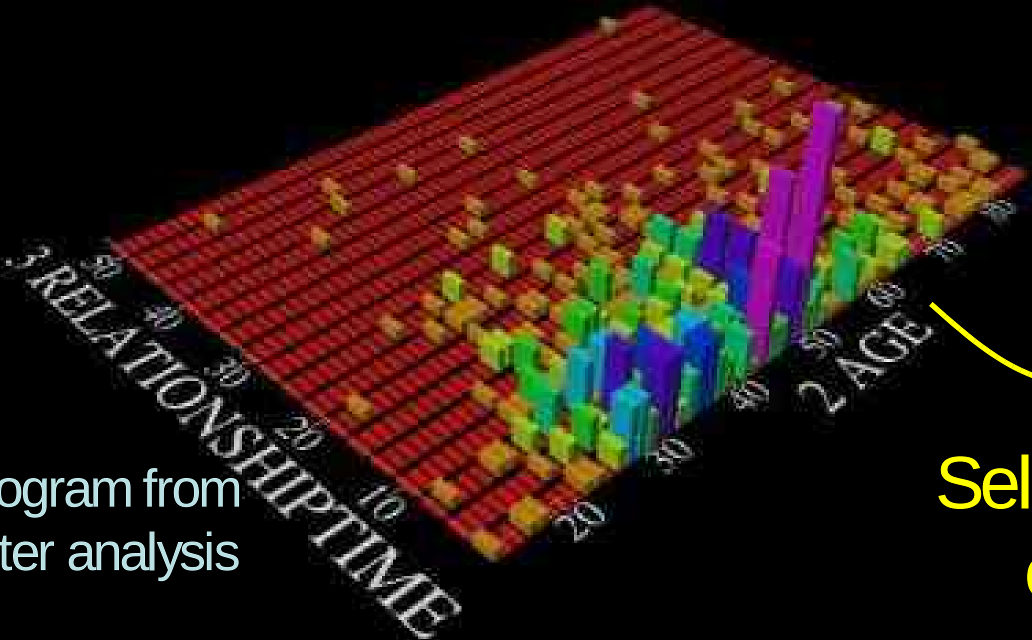

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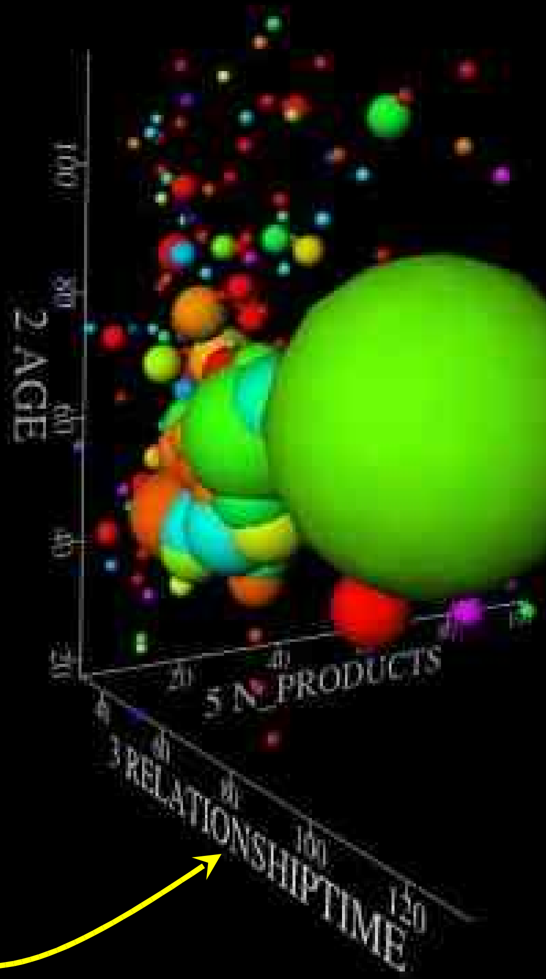

Scatter plot

Lessons learnt

- 3D correlation landscape useful
  - Identifying significant variables
  - Focus on data distributions
  - Select appropriate ranges for cluster analysis
- Cluster visualization helpful
  - Non-linear relationships in data revealed
- 3D visualization combined with direct interaction
  - Selection of correlated variables
  - Binning and sorting
- Done with IRIS Explorer

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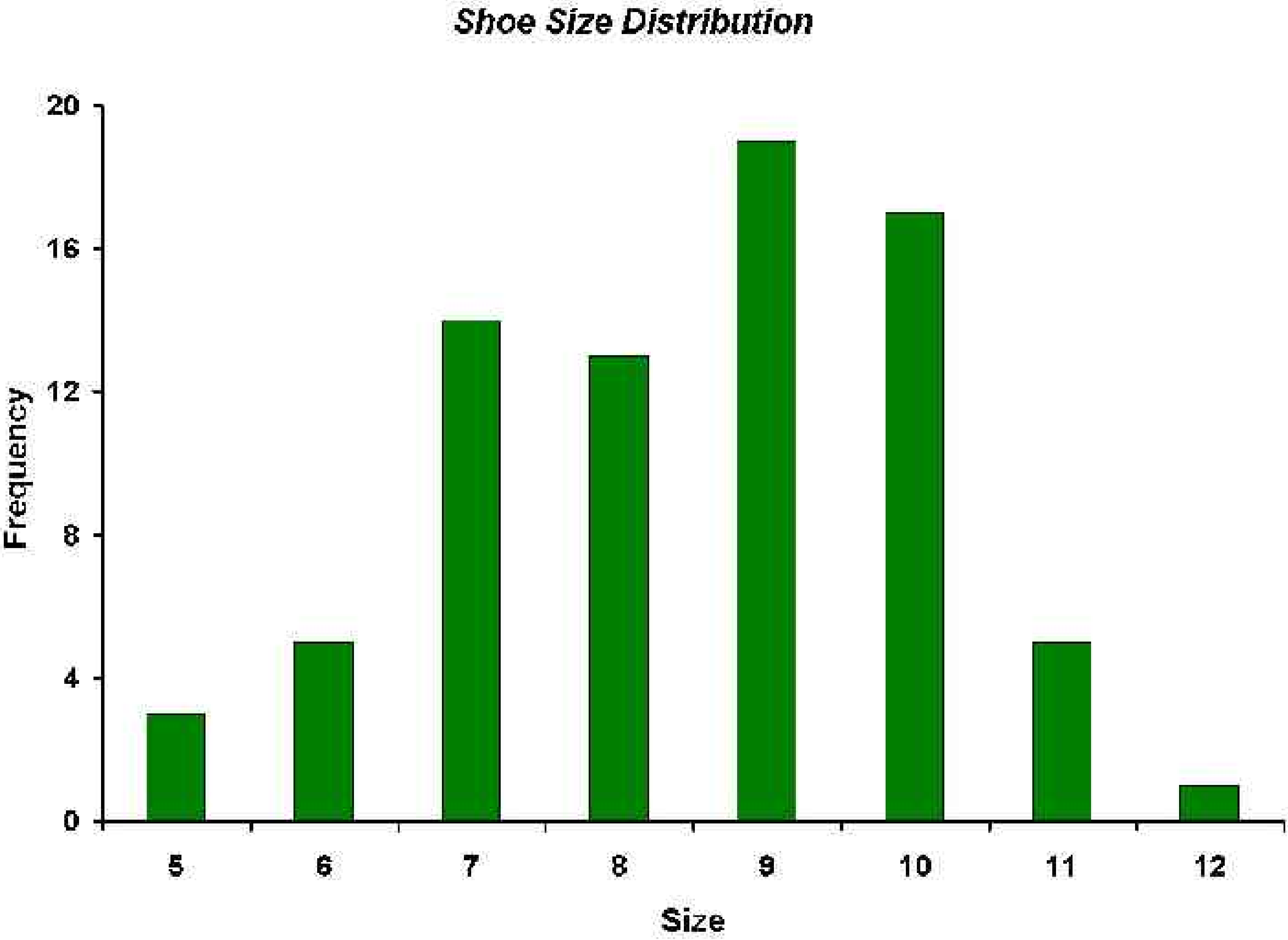
Simple visualization: shoe size survey

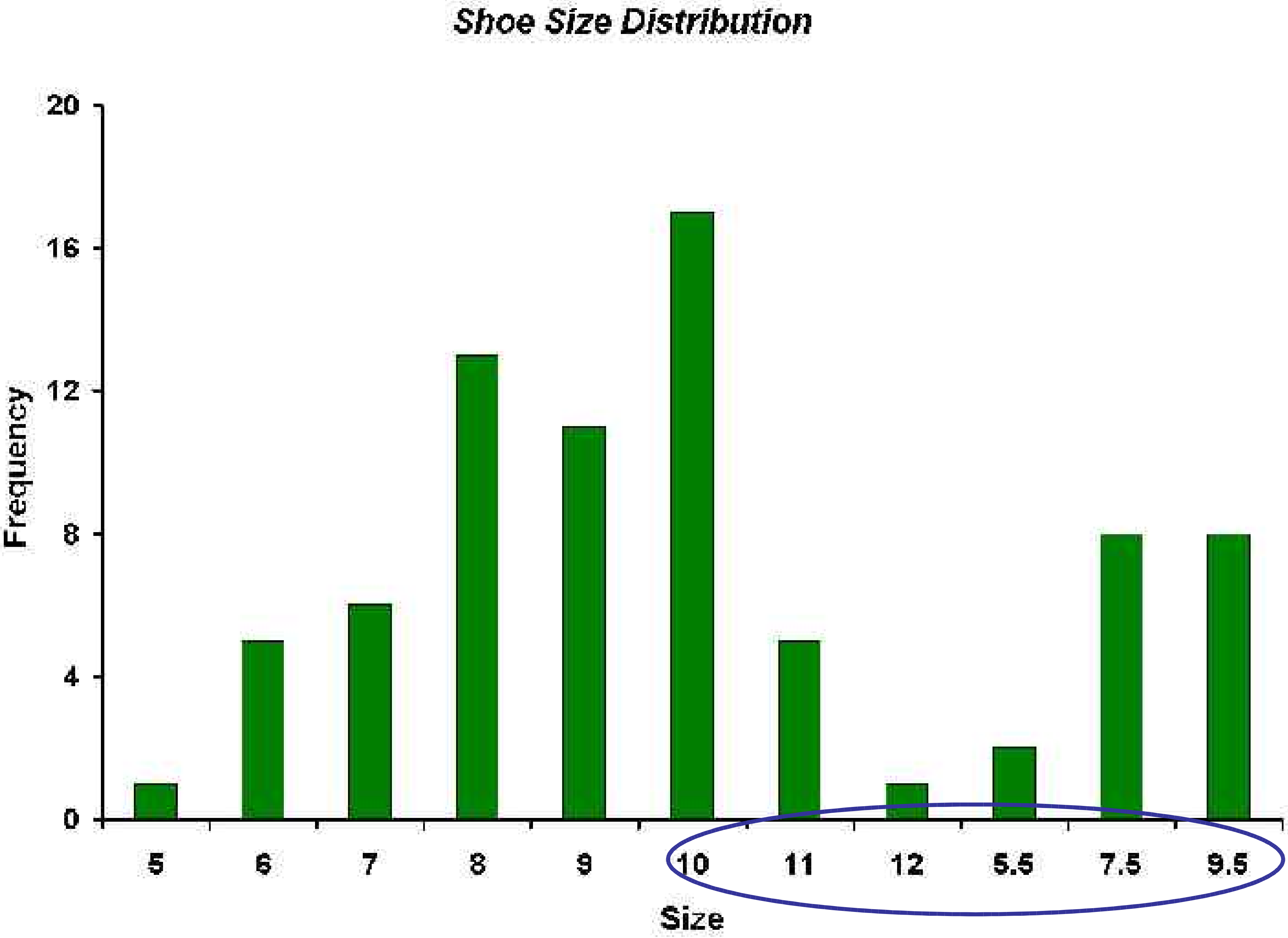
Shoe size	5	6	7	8	9	10	11	12
Frequency	3	5	14	13	19	17	5	1

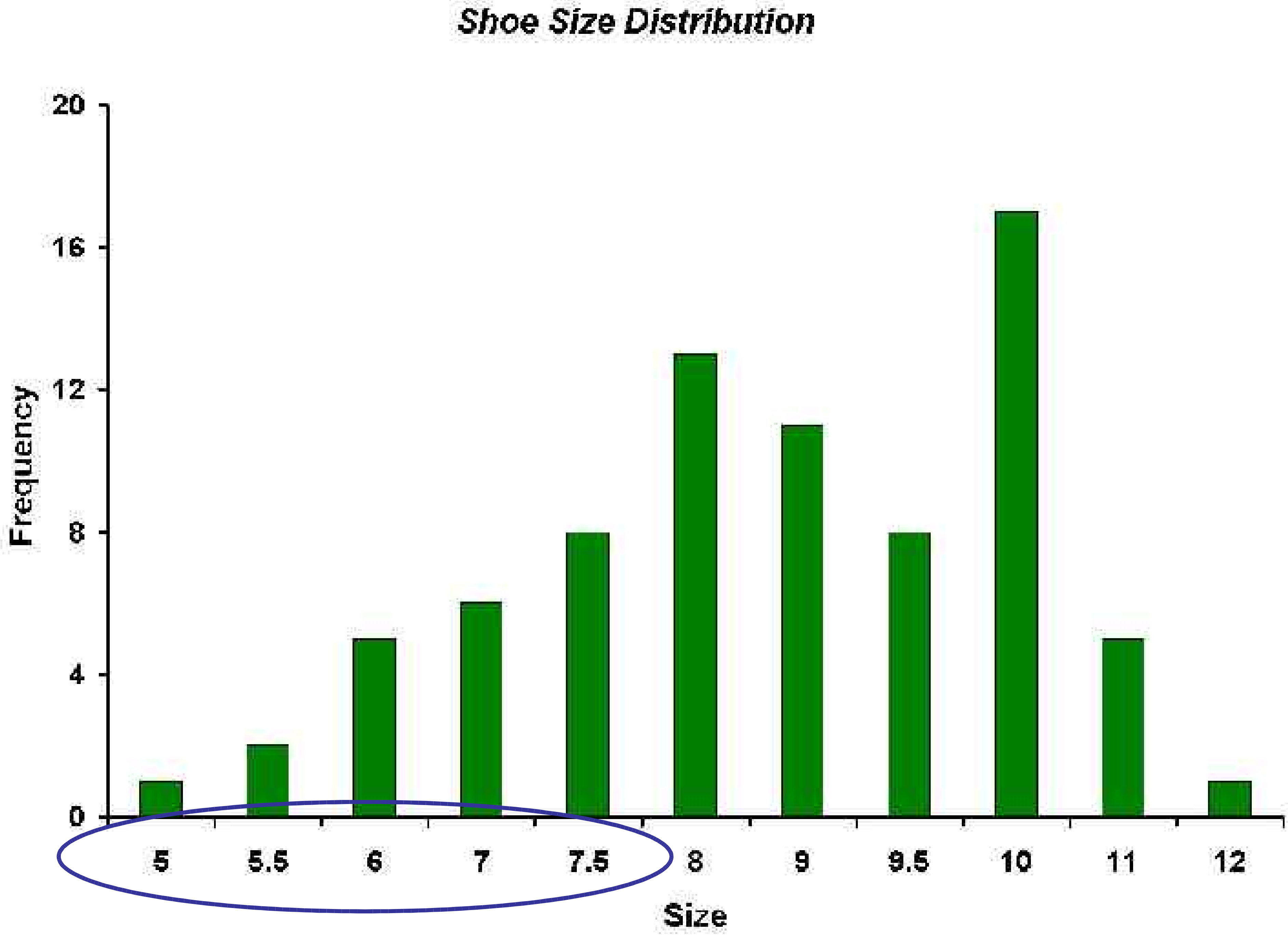
- Visualize using Excel
  - Chart wizard creates visualization easily
  - Interactive control over appearance
    - Colours, line width, text, fonts, placement
  - Data and visualization linked together


Shoe Size Distribution
Frequency
20
16
12
8
4
0
5
6
7
8
9
10
11
12
Size

Second survey (now with half-sizes)

Shoe size	5	6	7	8	9	10	11	12	5.5	7.5	9.5
Frequency	3	5	14	13	19	17	5	1	2	8	8


Shoe Size Distribution
Frequency
20
16
12
8
4
0
5
6
7
8
9
10
11
12
5.5
7.5
9.5
Size


Shoe Size Distribution
Frequency
0
4
8
12
16
20
5
5.5
6
7
7.5
8
9
9.5
10
11
12
Size

What’s wrong with this picture?

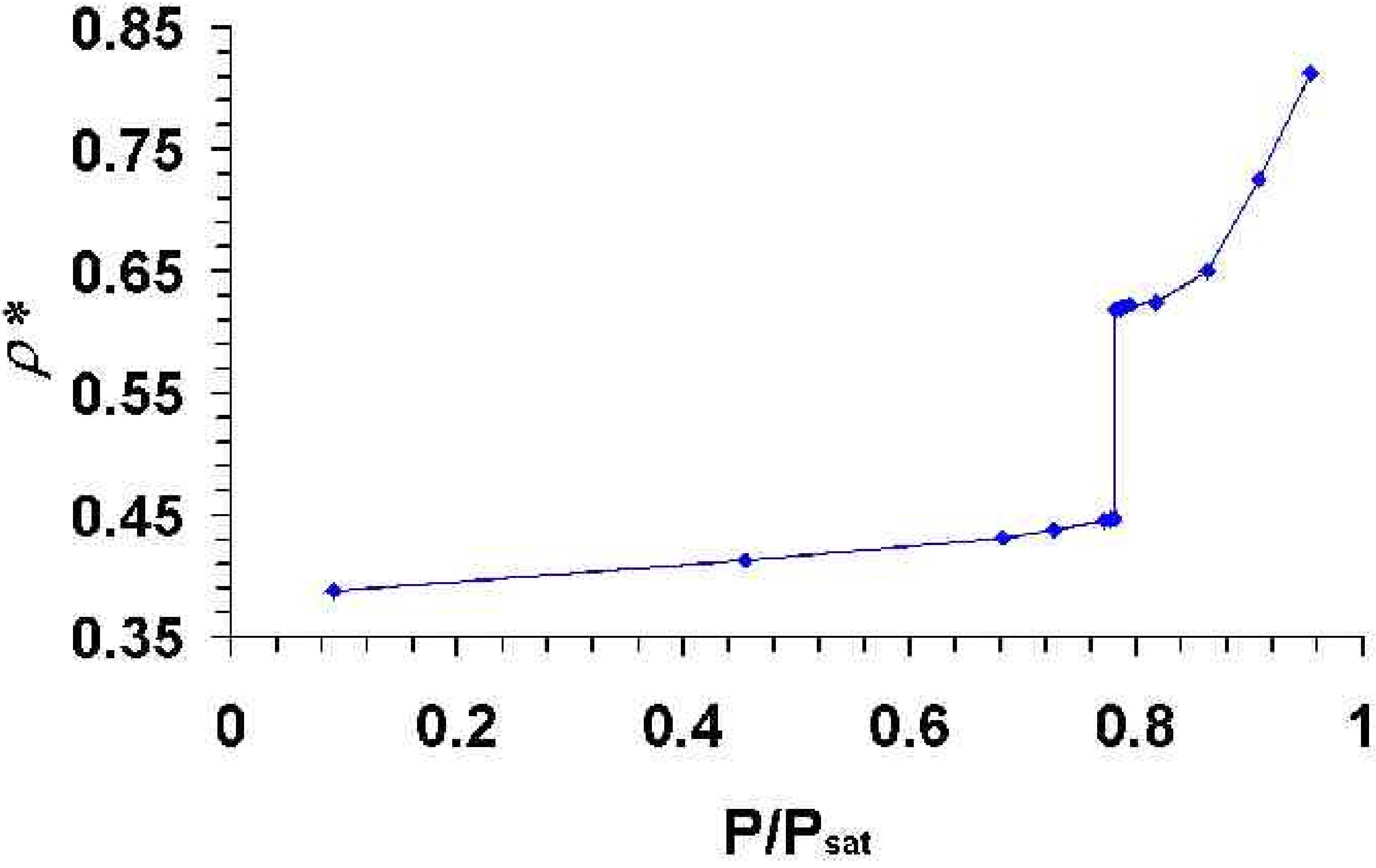
- Ordering of values on X axis reflects order in spreadsheet
  - not numerical order
- Spacing on X axis doesn’t reflect difference between values
  - spacing is everywhere the same
- Could pay close attention to labels
  - But might be harder for more complex data
  - Obscures missing data

Another example – adsorption isotherm

- Measurement of fluid density inside porous solid as a function of fluid pressure
- Confined fluid can condense before saturation
  - Capillary condensation
  - Vertical jump in isotherm
- Plot data using
  - Scatter plot
  - Line graph

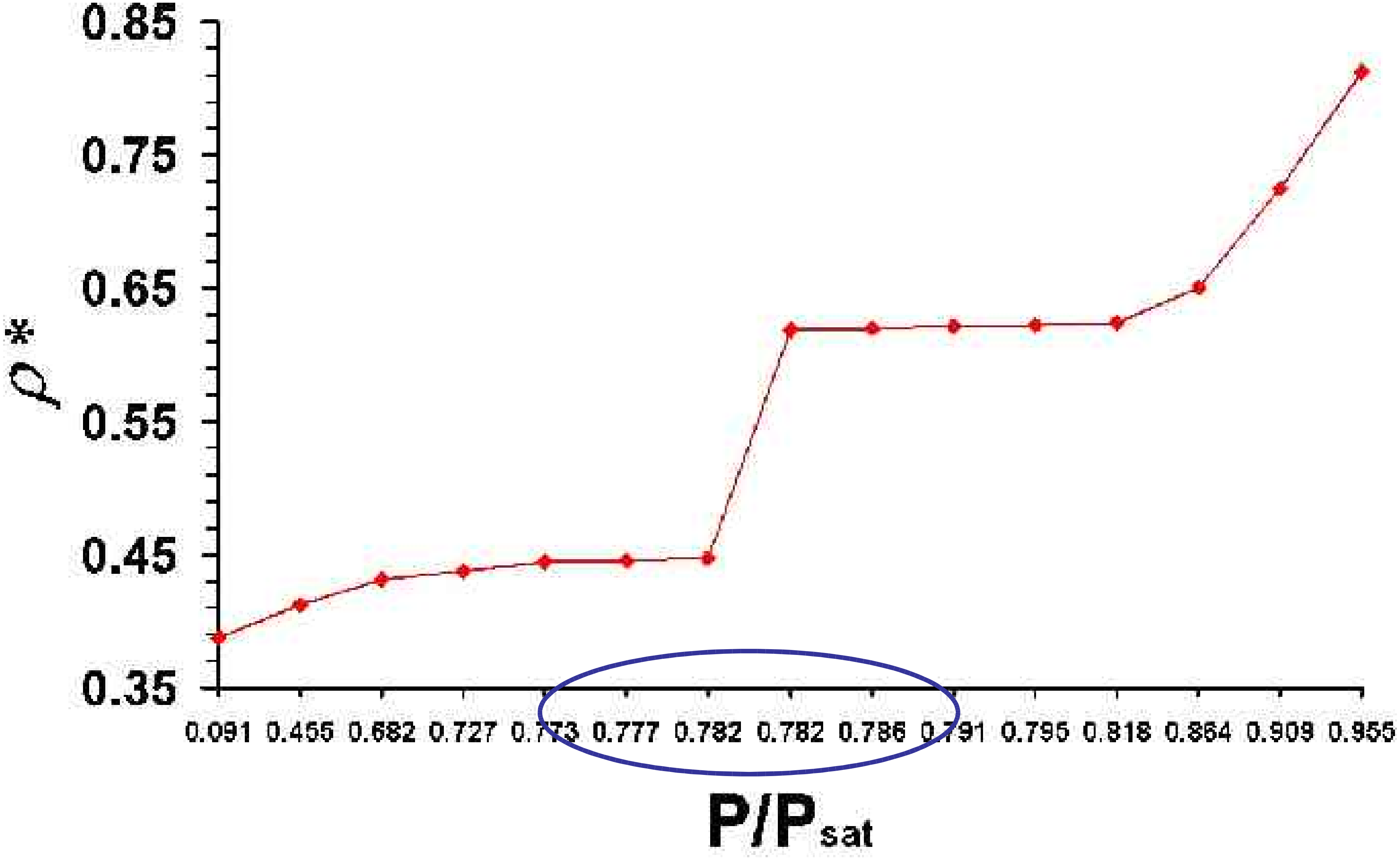
Scatter plot

Adsorption isotherm



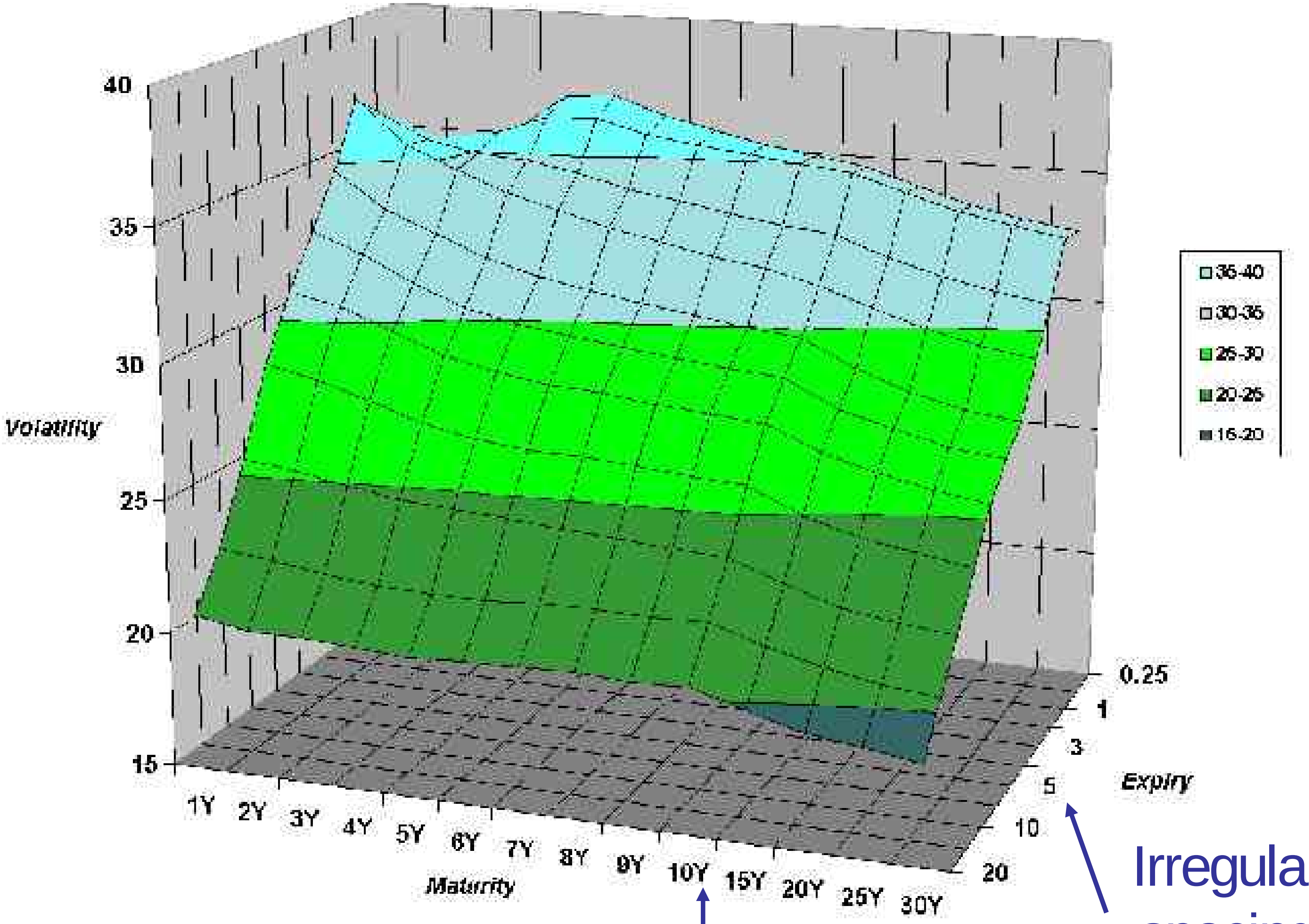
Line graph

Adsorption isotherm



Another example – derivative calculation

- Black-Scholes modelling of options on swap agreements (“swaptions”)
  - Option volatility as a function of
    - Swap maturity
    - Option expiry time
- Display in Excel as a surface plot

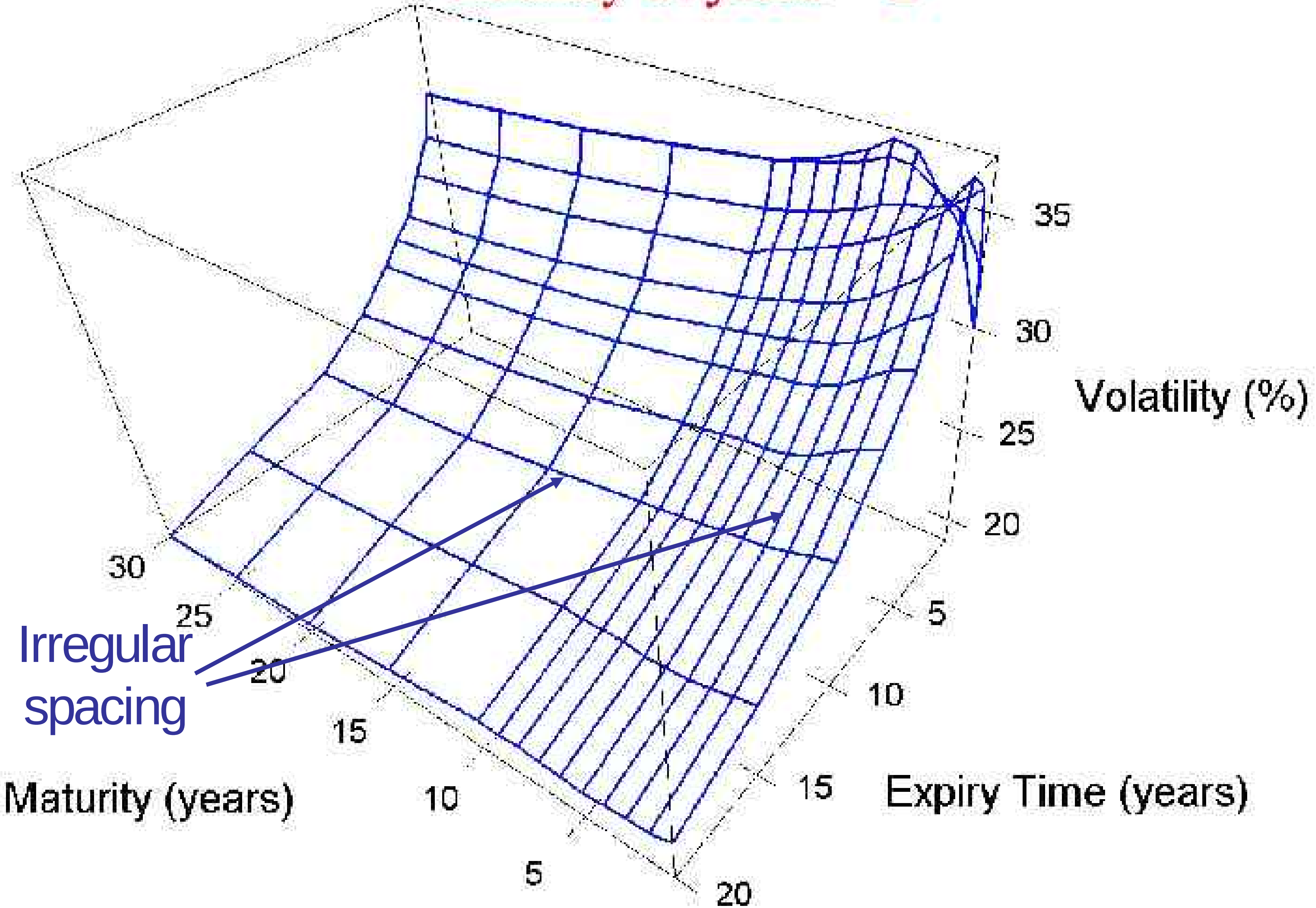


Irregular spacing

What’s wrong with this picture?

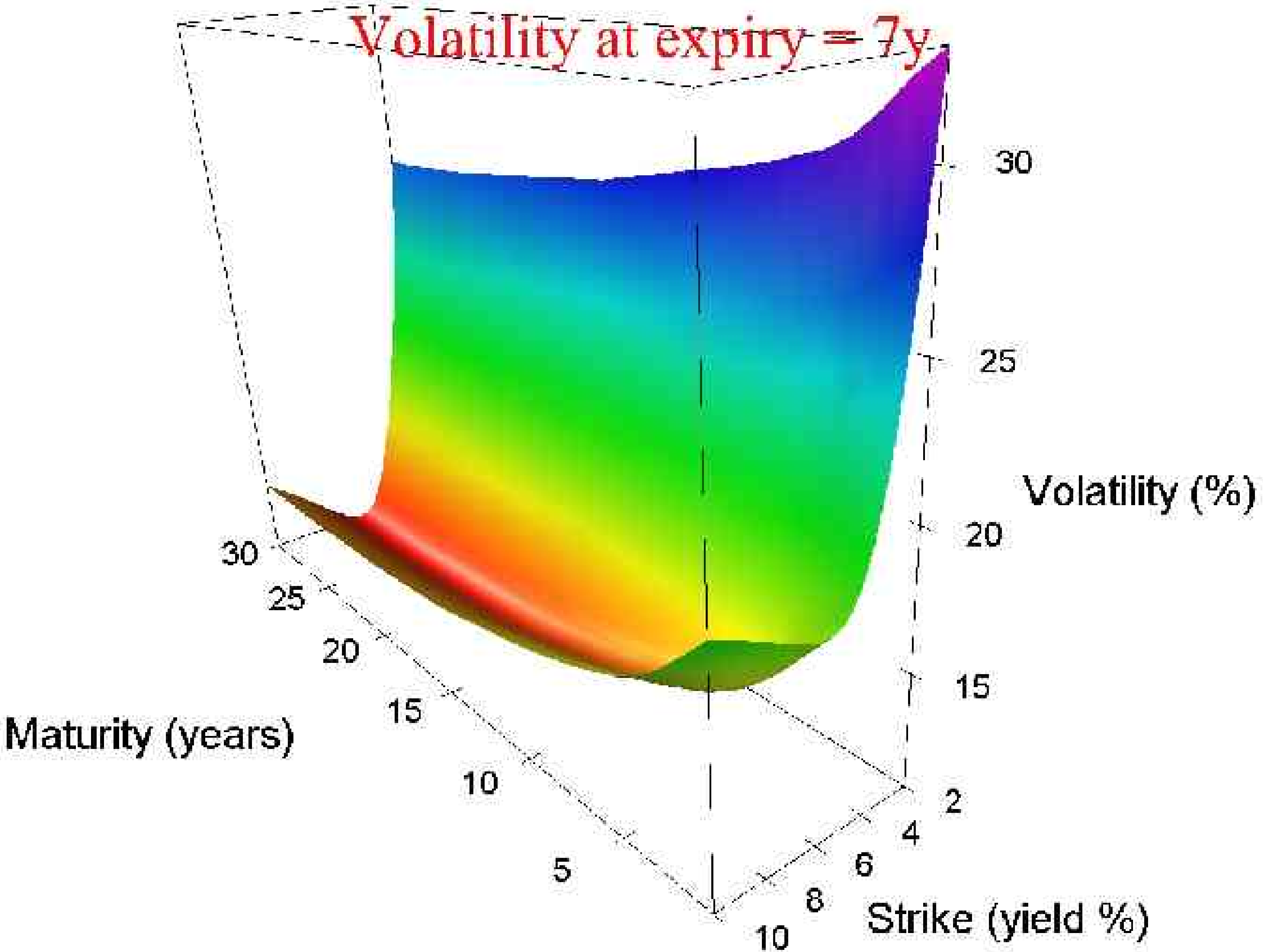
- See above
  - Irregular spacing, discontinuities
- This is only one part of the dataset
  - Volatility also depends on strike value
  - Want plots at other strike values
  - Want to see other relationships
    - e.g. volatility (strike) = “volatility smile”
- Use IRIS Explorer

Volatility at yield = 2

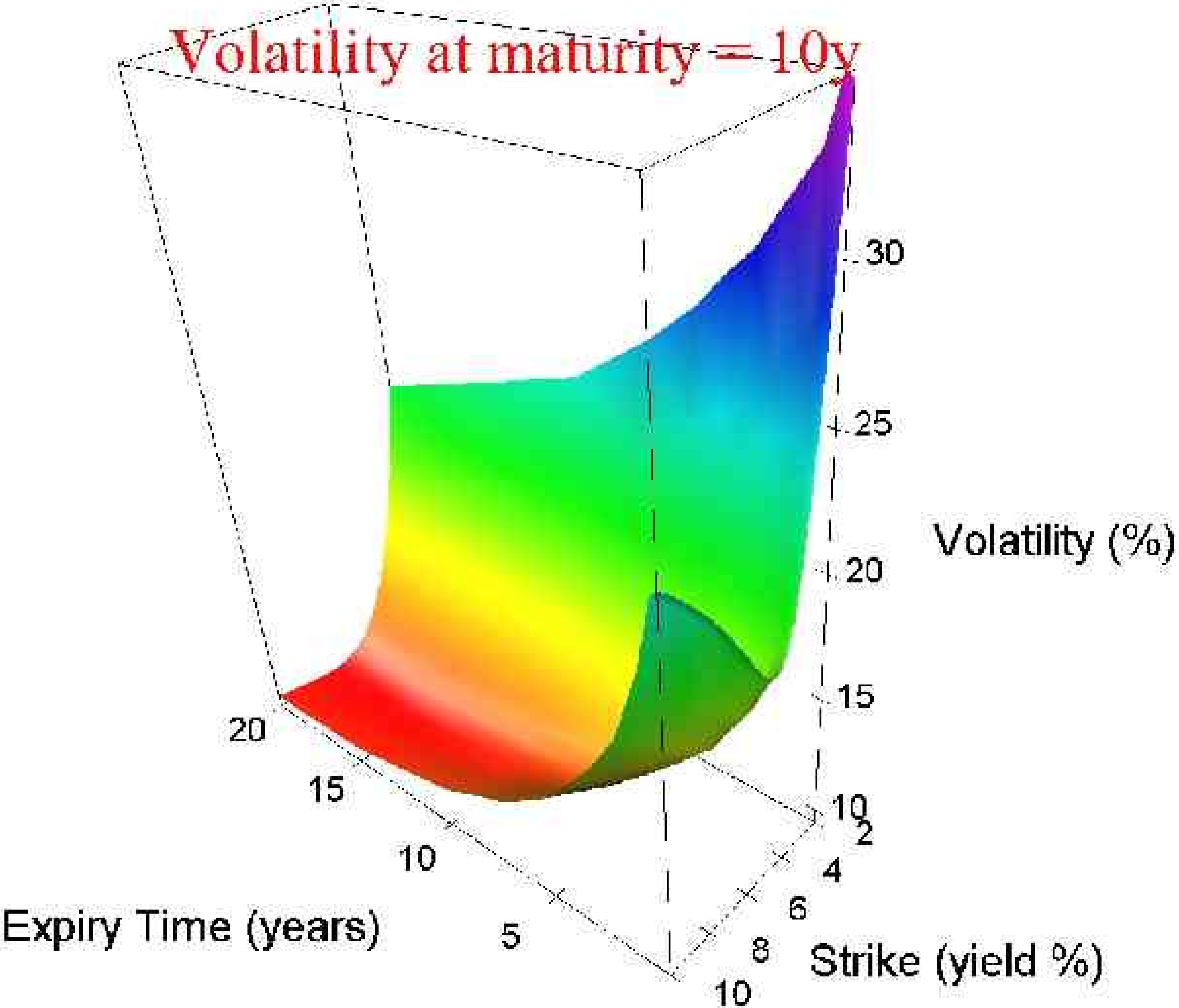


Irregular spacing

Volatility at expiry = 7y



Volatility at maturity = 10y



Two types of axis in Excel charts

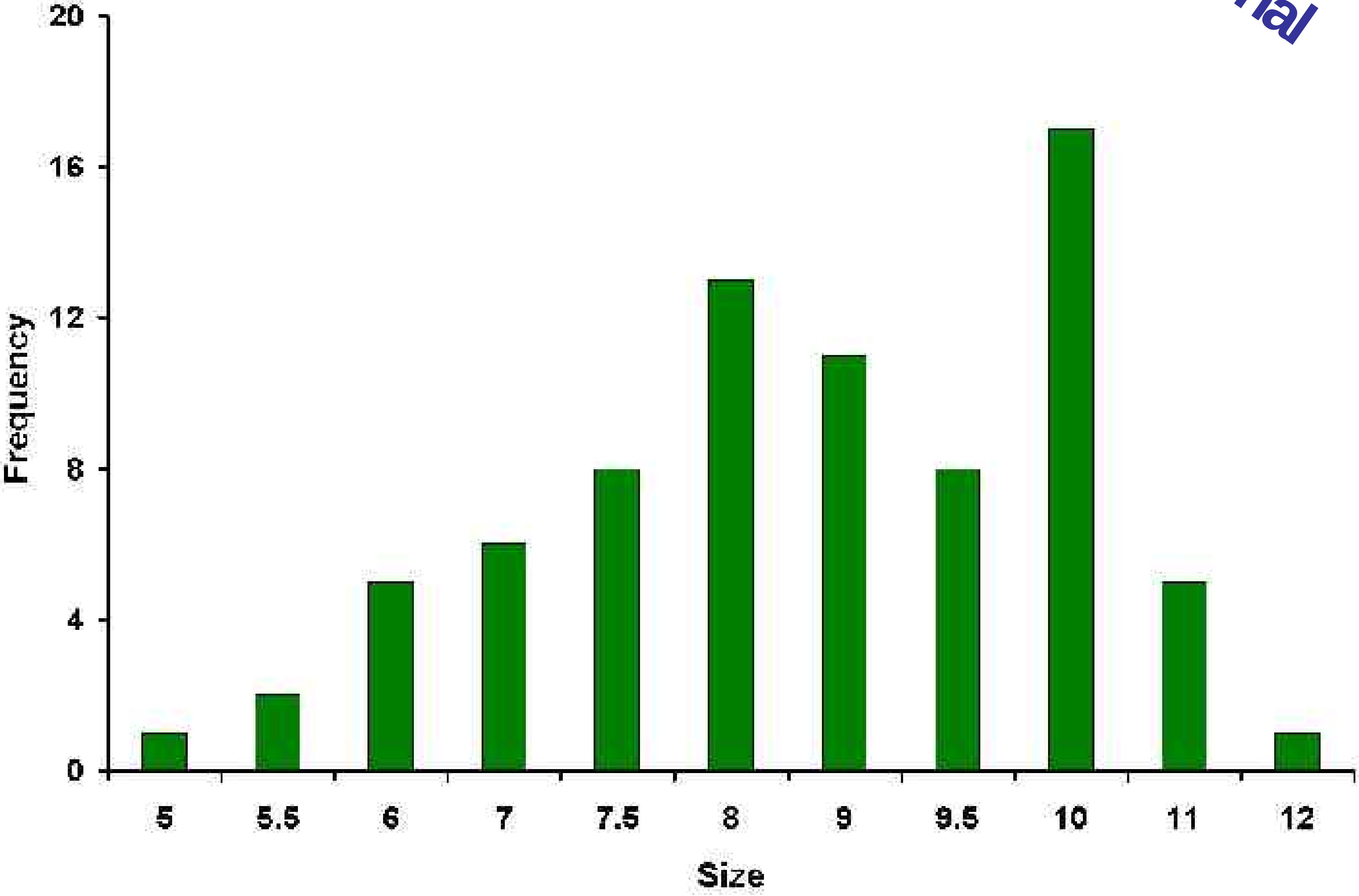
- Value
  - Data treated as continuously varying numerical values
  - Marker placed at location reflecting its value
  - Used in Excel Scatter plots
- Category
  - Data treated as sequence of non-numerical text labels
  - Marker location reflects position in sequence
  - Points distributed evenly along axis
  - Used in Excel Bar chart, Line chart, Surface plot…

NAG Schools Excel Add-in (N-SEA)

- Supports instruction in statistics
- Functionality for
  - Data sampling
  - Frequency plots
  - Box and whisker plots
  - Histograms
  - Continuous bar charts
- Allows (X/Y) ordering of data points in plotting
  - and inclusion of points with zero Y values

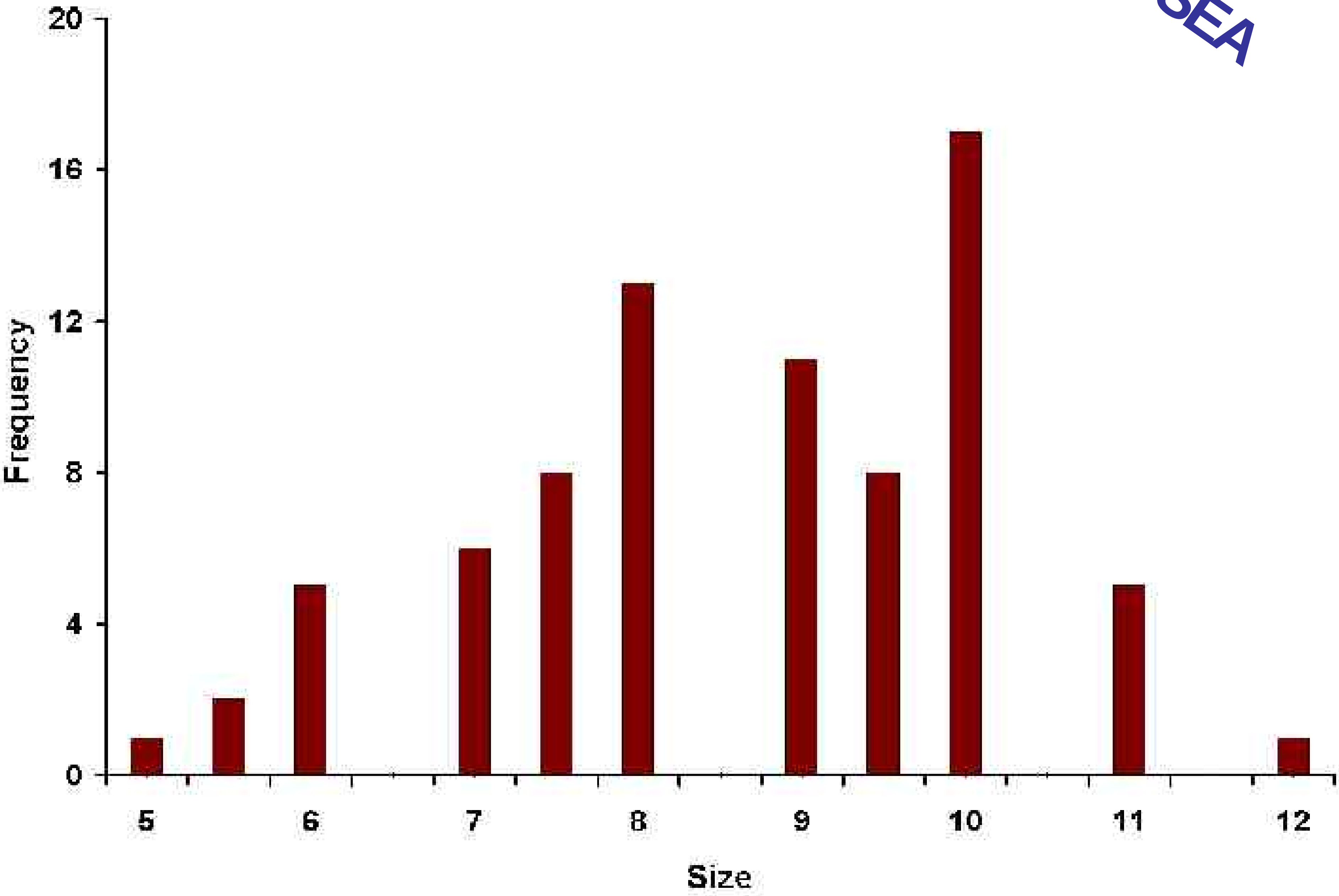
Original

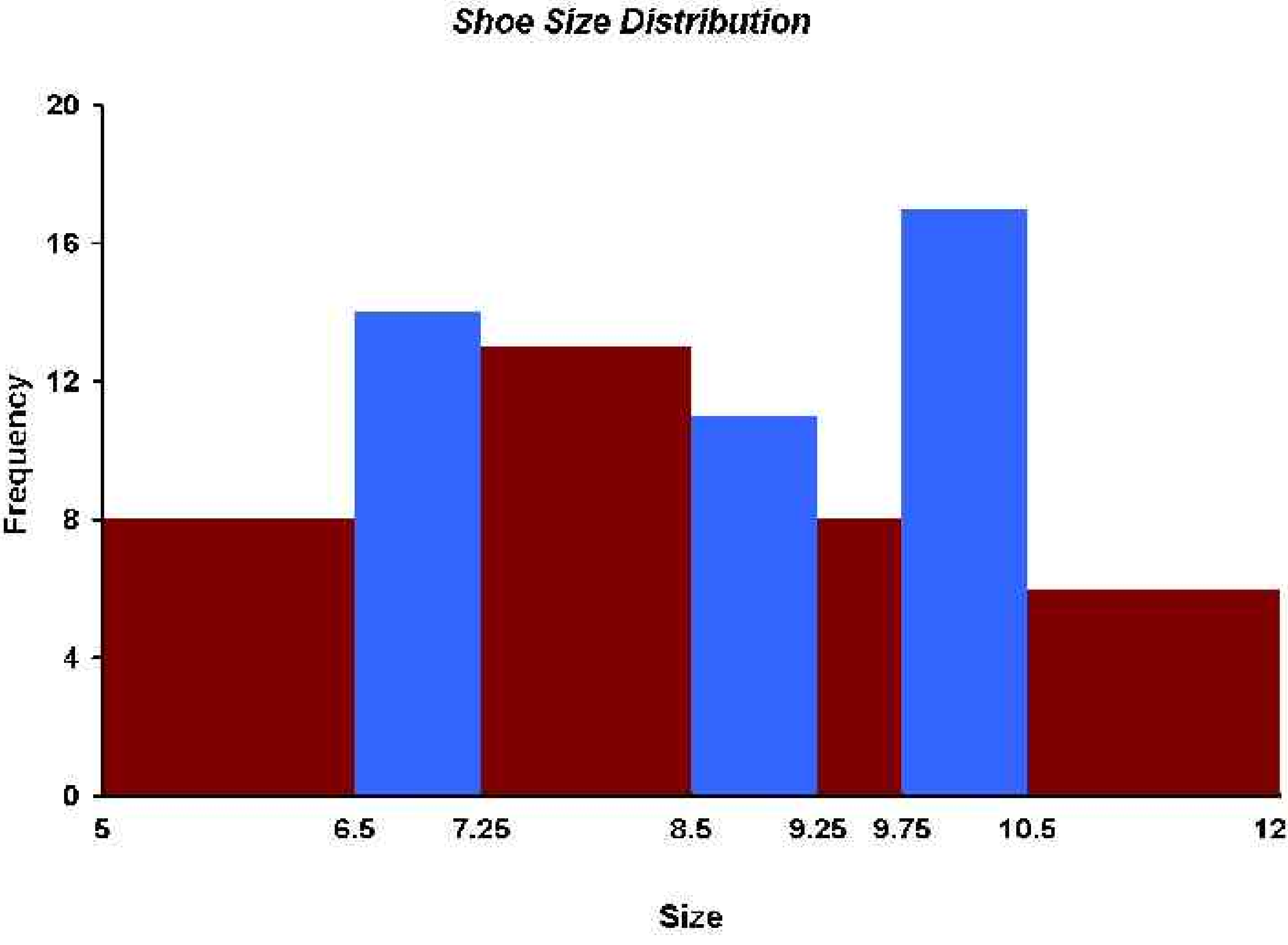
Shoe Size Distribution



Shoe Size Distribution

N-SEA




Shoe Size Distribution
Frequency
20
16
12
8
4
0
5
6.5
7.25
8.5
9.25
9.75
10.5
12
Size

Conclusions

- Data mining components offer basic routines
  - Developers can incorporate them into applications
  - No wheel-reinvention, stone canoes, chocolate teapots
    - cf NAG numerical library
- Visualization is crucial for analysis
  - Integration of data mining & visualization is application-dependent
  - Interactivity important
- Problems with (even) well-known tools
  - Be aware
  - Work around