Master of Technology in Knowledge/Software Engineering

KE5107: Data Mining Methodology and Methods

Data Exploration and Visualisation

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Module Objectives

- To learn how to examine the underlying structure of the data.
- To learn how to examine data for any systematic relationship among the variables through workshops.
- To be familiar with some descriptive and graphic tools for exploring data visually in order to discover and confirm patterns and trends.

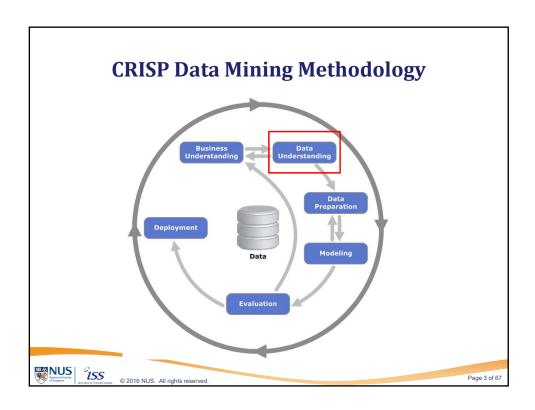
Agenda

- Data exploration goals
- Basic data visualisation methods
- Multi-dimensional visualisation
- Advanced visualisation techniques









Data Exploration Goals

1. Data Quality Assessment

Before attempting to build a prediction model or do any data mining it is good practice to explore and profile the data to become familiar with it, determine its quality, identify missing values, inconsistencies, outliers etc

 Data errors should be fixed in the data cleaning and preparation phase.

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Goals for Exploratory Data Analysis

2. Knowledge Discovery

Visualisation provides a powerful means of finding patterns, trends, relationships, structure and exceptions in the data

- No specific goal is needed
- Very interactive and exploratory







Goals for Exploratory Data Analysis

3. Find ways to improve the data set for modeling

Feature Selection

- Look for variables related to the target (useful for prediction)
- Look for variables that are "duplicates" of others (can delete)

Data Transformations

- Look for patterns and correlations that may suggest valuable transformations, e.g.

> chemical_ratio = Na/K weight_ratio = brain weight/body weight





Goals for Exploratory Data Analysis

4. Data Profiling

Characterise a set of records in terms of their attributes. The characterisation will be a generalisation (i.e. need not be 100% correct)

Common task is customer profiling, e.g.

- Most people who buy sports cars are young, rich & single!
- diabetes type2 patients are typically older & overweight
- Bank Y's investment account holders are usually married with children and a well paid job





Data Exploration Principles

- · Let the data speak for itself
 - Be open, make no prior assumptions
- Interpret what you see
 - Develop and explore hunches, then pursue this line of analysis until you confirm/disown it
 - Be interactive, pro-active



During data exploration you lead the way!





Agenda

- Data Exploration Goals
- → Basic Data Visualisation methods
 - Advanced Visualisation Techniques

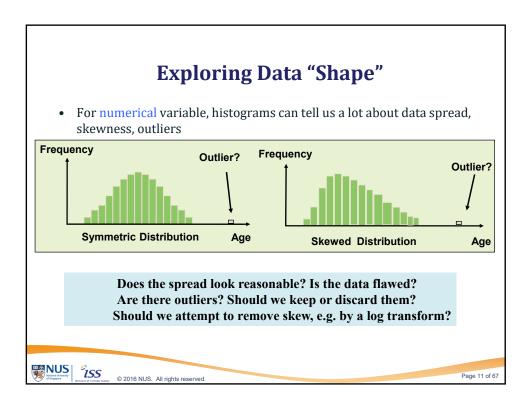


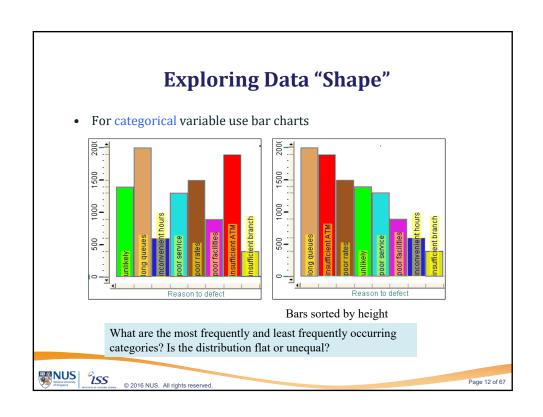
Data Exploration Basic Steps

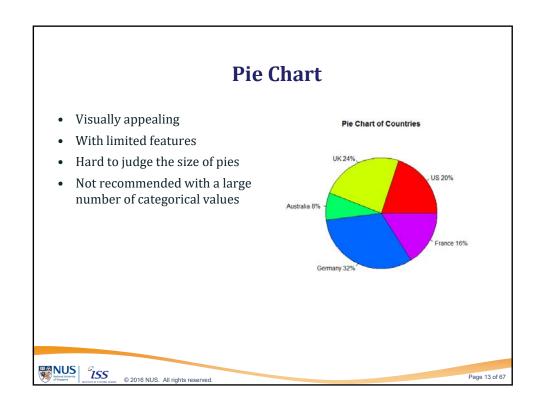
- 1. Discover the "shape" & quality of the data
- 2. Look for outliers, extreme & unusual values
- 3. Look for relationships between variables
- 4. Build profiles of important subsets of the data

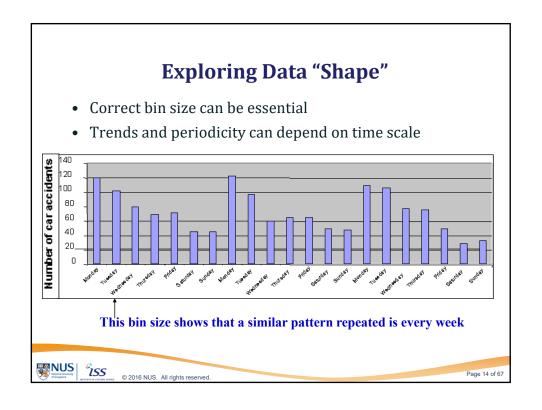


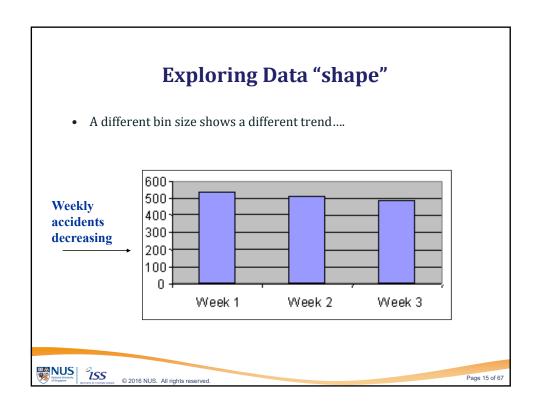
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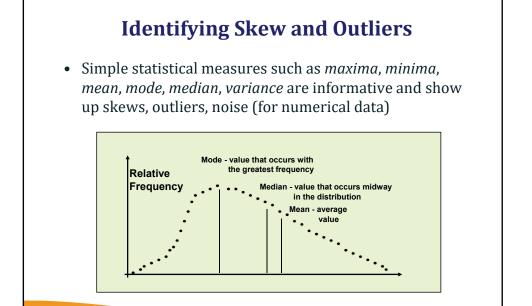












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Data Summary

• Summary of these simple statistical measures can be presented as numbers, which are not easy to interpret.

MinTemp	MaxTemp	Rainfall	Evaporation
Min. :-5.300	Min. : 8.40	Min. : 0.000	Min. : 0.600
1st Qu.: 1.925	1st Qu.:14.70	1st Qu.: 0.000	1st Qu.: 2.200
Median : 7.100	Median :19.20	Median: 0.000	Median : 4.000
Mean : 7.011	Mean :20.29	Mean : 1.386	Mean : 4.509
3rd Qu.:12.400	3rd Qu.:24.95	3rd Qu.: 0.200	3rd Qu.: 6.400
Max. :20.900	Max. :35.80	Max. :25.800	Max. :13.800

Skewness:

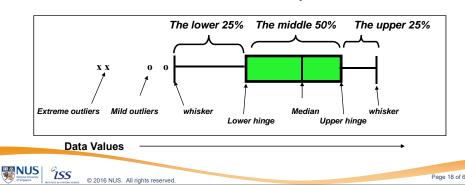
MinTemp MaxTemp Rainfall Evaporation 0.05347228 0.38465167 3.63725482 0.70497219

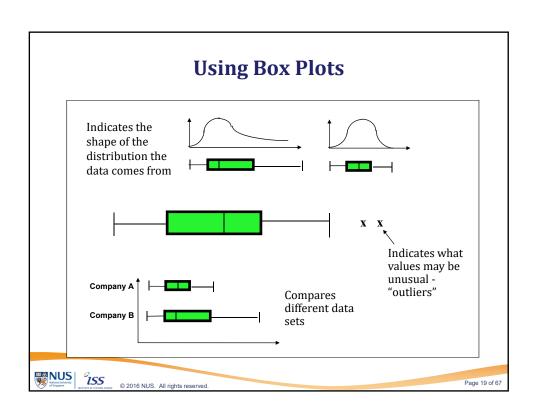
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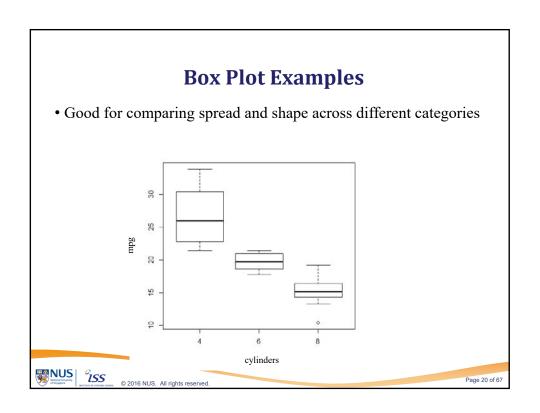
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Box Plots (Box & Whisker)

- Show key statistical measures in a single picture!
 - Box shows the middle 50% of the data
 - The whiskers show the end points (excluding outliers)
 - Mild outliers lie between 1.5 to 3 times the box length on either side of the box, extreme outliers are beyond this

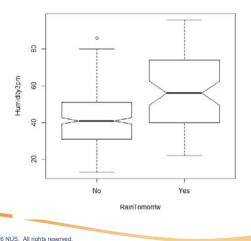






Box Plot Examples

 \bullet The notches around the median indicate an approximate 95% confidence level for the differences between the medians

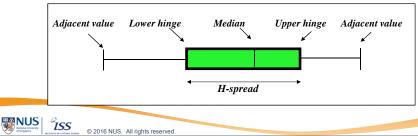


How Box-Plots Work

- 1. Calculate the Median and "Hinges"
 - The median splits the data sample into two parts
 - The hinges are the middle values of each part
 - The Upper and lower Hinges form the sides of the box
 - The difference between the hinges called the H-spread
- 2. Define inner fences

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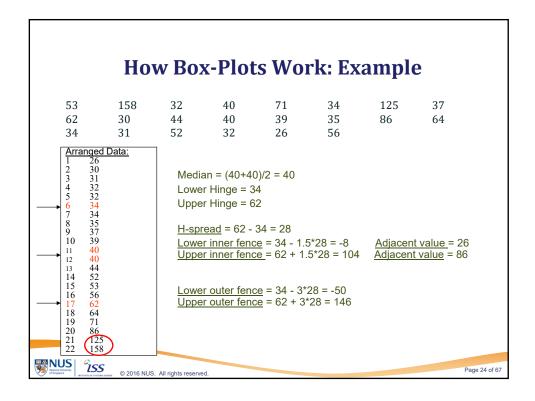
- Lower inner fence = lower hinge 1.5* (H-spread)
- Upper inner fence = Upper hinge + 1.5* (H-spread)
- The data values that are closest to, but still inside the inner fences are called adjacent values, these form the whiskers

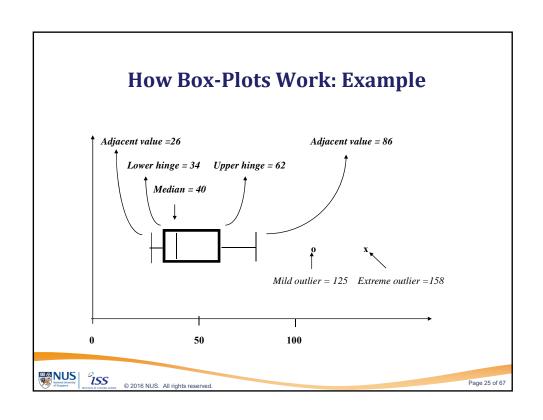


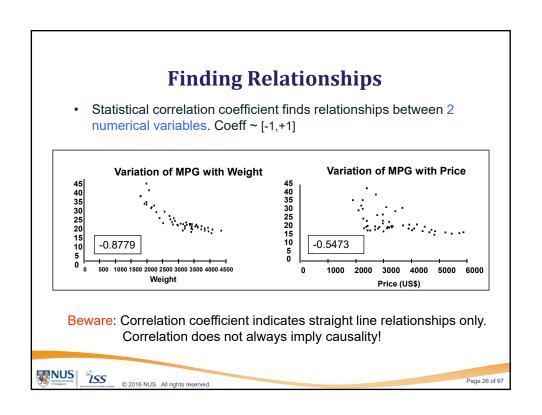
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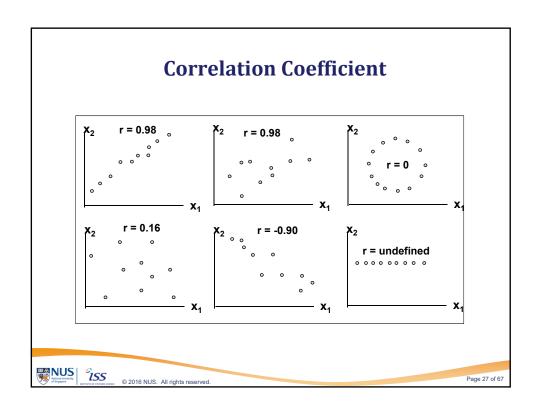
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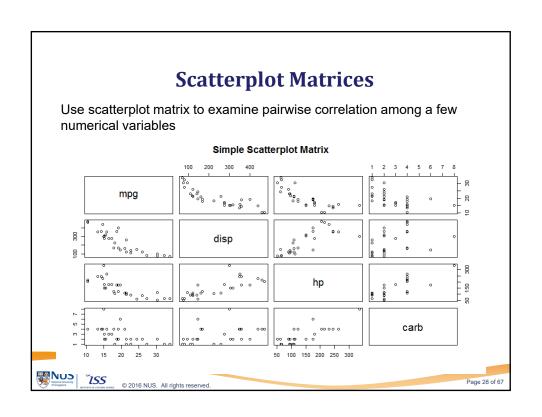
How Box-Plots Work Define outer fences Lower outer fence = Lower hinge - 3* (H-spread) Upper outer fence = Upper hinge + 3* (H-spread) 5. Data values that are between the inner and outer fences are called *mild outliers* 6. Data values that are beyond the outer fence are called *extreme outliers* Adjacent value Lower hinge Median Upper hinge Adjacent value Mild outliers Extreme outliers NUS ZSS Page 23 of 67











Multi-Dimensional Visualisation

How can we find relationships between 3+ variables?

Basic

- Scatter plots

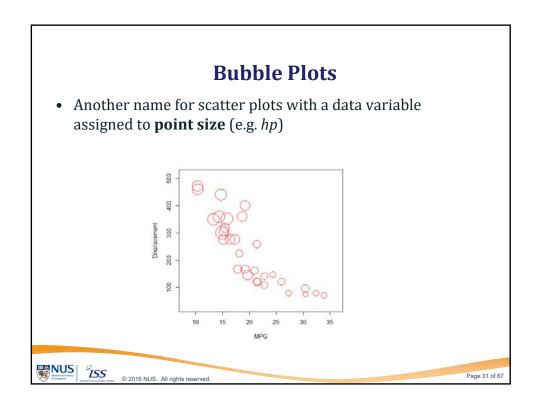
- Overlays
- Co-Plots
- 3-D Graphics
- Many more....

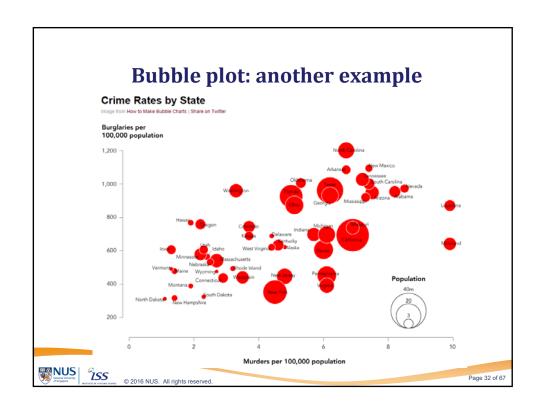
More advanced

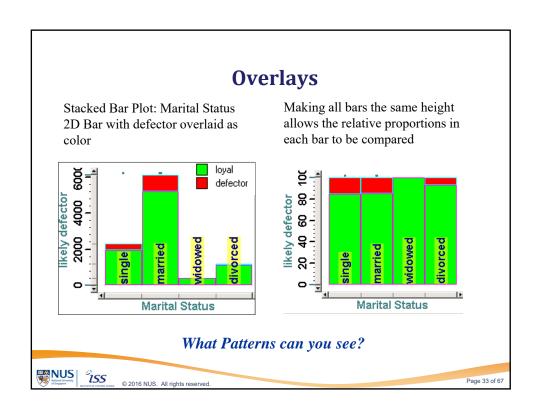
- Principle Component Analysis
- Multi-Dimensional Scaling
- Parallel Coordinates
- Star Plots
- Chernoff faces
- Many more....

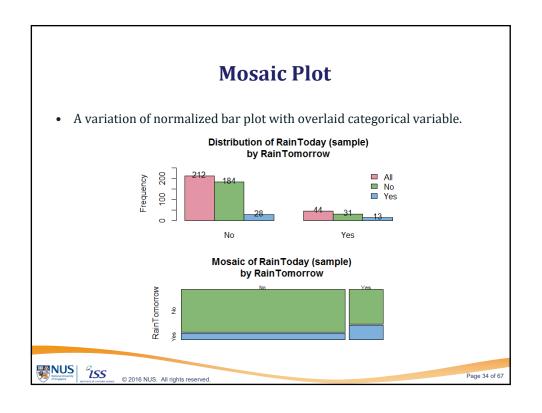


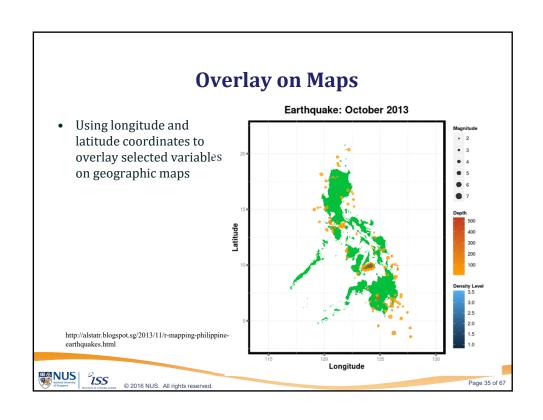
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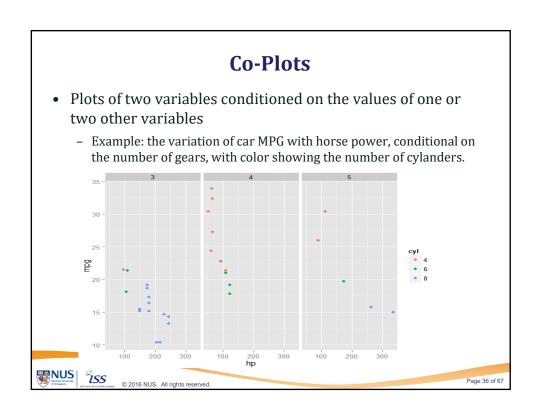






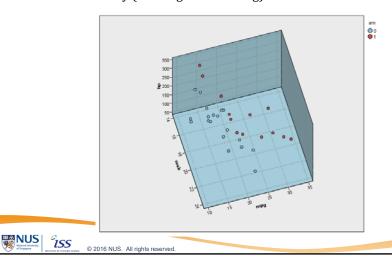






3-D Data Visualisation

- 3-D offers more scope for viewing multiple dimensions
- Need interactivity (rotating and zooming) to make best use of 3D visualisation

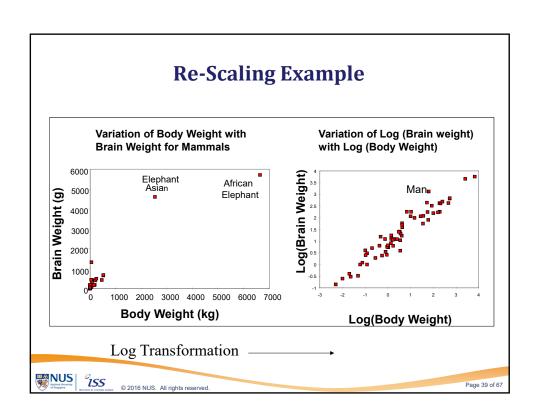


Data Transformations for More Visible Patterns

- Can make patterns easier to see
- Examples
 - Rescaling
 Log() ~ reduce effects of large variables
 Square() ~ exaggerate effect of large variables
 - Derived variables
 profit = units sold * unit cost
 int.call rate = number international calls/total calls
 activity rate = average monthly transactions/ avg. balance
 Odds of an event = p / (1-p)



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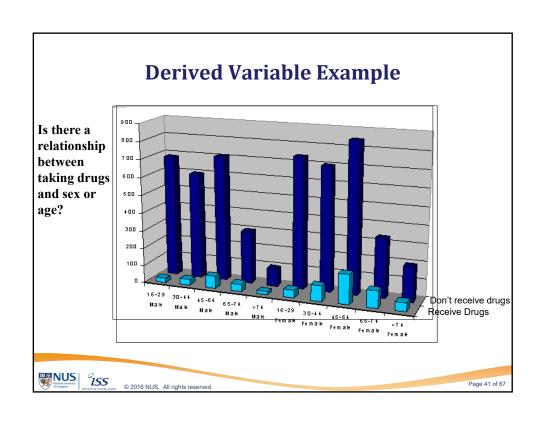
Derived Variable Example

The following data describes the number of people who take psychotropic drugs from randomly taken samples classed by age and sex

Sex	age group	Mean age	Receiving drugs	Not receiving drugs
Male	16-29	23.2	21	683
Male	30-44	36.5	32	596
Male	45-64	54.3	70	705
Male	65-74	69.2	43	295
Male	>74	79.5	19	99
Female	16-29	23.2	46	738
Female	30-44	36.5	89	700
Female	45-64	54.3	169	847
Female	65-74	69.2	98	336
Female	>74	79.5	51	196

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Derived Variable Example

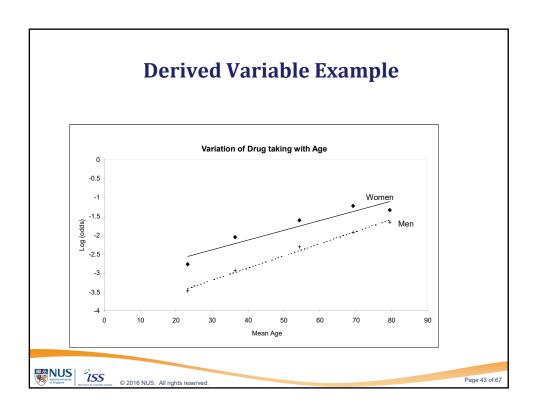
Use Log Odds transformation

- Log (odds) = Log(No. receive/No. not receiving)
[Odds of an event = p / (1-p)]

Sex	Age group	Mean age	Receiving drugs	Not receiving drugs	Odds	Log(odds)
Male	16-29	23.2	21	683	0.0307	-3.48197
Male	30-44	36.5	32	596	0.0537	-2.9245
Male	45-64	54.3	70	705	0.0993	-2.3097
Male	65-74	69.2	43	295	0.1458	-1.92578
Male	>74	79.5	19	99	0.1919	-1.65068
Female	16-29	23.2	46	738	0.0623	-2.7753
Female	30-44	36.5	89	700	0.1271	-2.06244
Female	45-64	54.3	169	847	0.1995	-1.6118
Female	65-74	69.2	98	336	0.2917	-1.23214
Female	>74	79.5	51	196	0.2602	-1.34629



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Agenda

- Data Exploration Goals
- Basic Data Visualisation methods
- → Advanced Visualisation Techniques



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Visualisation for Multivariate Data

- Visualising data with a large number of variables can be very challenging.
- One major approach is to simplify the problem by
 - Reducing the number of variables describing the data Principal Component Analysis
 - Reducing the number of dimensions of the problem Multidimensional Scaling
- Or find innovative ways to visualise many variables in one graph by
 - Showing links between many different categories Link Analysis
 - Using parallel vertical axes Parallel Coordinates
 - Using axes starting from one central point Radar Chart
 - Using icons e.g. Star Plot, Chernoff Faces



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Principle Component Analysis

- Used when some of the variables in a data set are correlated (there is some redundancy)
- We can find a smaller set of <u>uncorrelated</u> variables which are linear combinations of the original variables

$$Z_1 = a_{11} * X_1 + a_{12} * X_2 + \dots$$

 $Z_i = a_{i1} * X_1 + a_{i2} * X_2 + \dots$

- These are the Principle Components (sometimes called factors), derived in decreasing order of importance - the earlier ones account for greater variations in the data
- PCA is performed to help:
 - Visually analyse and explore the data
 - Identify natural groupings or summaries of data
 - Create a set of factors that can later be used to create predictive models

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PCA Example

- Data describing the % of people employed in nine different industries in countries in Europe:
- · Industries are
 - AGR (agriculture)
 - MIN (Mining)
 - MAN (Manufacture)
 - PS (Power Supplies)
 - CON (Construction)
 - SER (Service Industries)
 - FIN (Finance)
 - SPS (Social and Personal services)
 - TC (Transport & Communications)



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PCA Example

	AGR	MIN	MAN	PS	CON	SER	FIN	SPS	TC
Be lg iu m	3.3	0.9	27.6	0.9	8.2	19.1	6.2	26.6	7.2
Denmark	9.2	0.1	21.8	0.6	8.3	14.6	6.5	32.2	7.1
Fra n c e	10.8	0.8	27.5	0.9	8.9	16.8	6	22.6	5.7
W.G e rm a	6.7	1.3	35.8	0.9	7.3	14.4	5	22.3	6.1
Ire la n d	23.2	1	20.7	1.3	7.5	16.8	2.8	20.8	6.1
Ita ly	15.9	0.6	27.6	0.5	10	18.1	1.6	20.1	5.7
Luxe mb ur	7.7	3.1	30.8	0.8	9.2	18.5	4.6	19.2	6.2
Ne the rla n	6.3	0.1	22.5	1	9.9	18	6.8	28.5	6.8
UK	2.7	1.4	30.2	1.4	6.9	16.9	5.7	28.3	6.4
Austria	12.7	1.1	30.2	1.4	9	16.8	4.9	16.8	7
Fin la n d	13	0.4	25.9	1.3	7.4	14.7	5.5	24.3	7.6
Greece	41.4	0.6	17.6	0.6	8.1	11.5	2.4	11	6.7
Norway	9	0.5	22.4	0.8	8.6	16.9	4.7	27.6	9.4
Portuga1	27.8	0.3	24.5	0.6	8.4	13.3	2.7	16.7	5.7
Sp a in	22.9	0.8	28.5	0.7	11.5	9.7	8.5	11.8	5.5
Sweden	6.1	0.4	25.9	0.8	7.2	14.4	6	32.4	6.8
Sw itze rla n	7.7	0.2	37.8	0.8	9.5	17.5	5.3	15.4	5.7
Turke y	66.8	0.7	7.9	0.1	2.8	5.2	1.1	11.9	3.2
Bu lg a ria	23.6	1.9	32.3	0.6	7.9	8	0.7	18.2	6.7
C ze c h o slo	16.5	2.9	35.5	1.2	8.7	9.2	0.9	17.9	7
E.G e rm a n		2.9	41.2	1.3	7.6	11.2	1.2	22.1	8.4
Hungary	21.7	3.1	29.6	1.9	8.2	9.4	0.9	17.2	8
Poland	31.1	2.5	25.7	0.9	8.4	7.5	0.9	16.1	6.9
Romania	34.7	2.1	30.1	0.6	8.7	5.9	1.3	11.7	5
USSR	23.7	1.4	25.8	0.6	9.2	6.1	0.5	23.6	9.3
Yugoslavia	48.7	1.5	16.8	1.1	4.9	6.4	11.3	5.3	4

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PCA Example

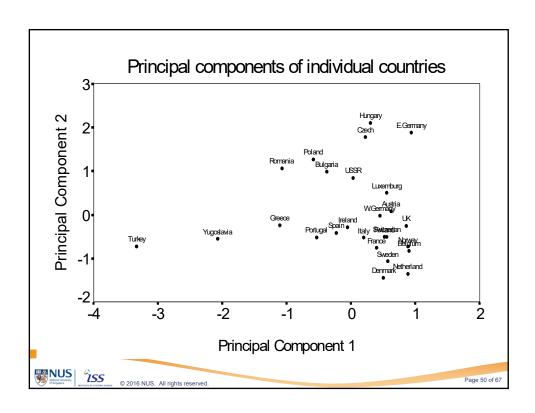
 Looking at the first two PC's can show groupings in the data

Coeffic	Coefficients of Principal components:					
	Princ.Comp.1	Princ.Comp. 2				
AGR	-0.97812	0.07822				
MIN	-0.00247	0.9017				
MAN	0.64891	0.5182				
PS	0.47752	0.38107				
CON	0.60724	0.07486				
SER	0.70759	-0.51108				
FIN	0.13888	-0.66218				
SPS	0.72344	-0.32331				
TC	0.685	0.29569				

But we must plot them in a scatter plot first!



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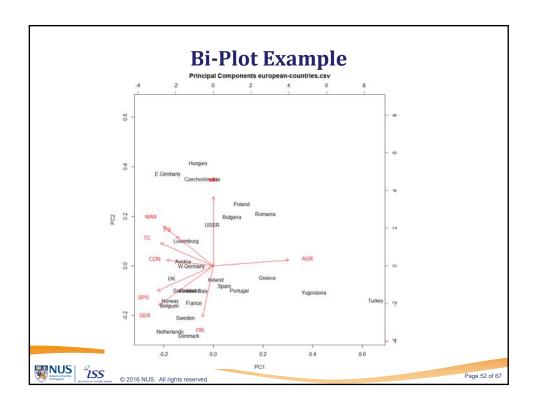


Bi-Plots

- To allow display of both the observations and variables of a matrix of multivariate data on the same plot.
- Associated with PCA and MDS, or other dimension reduction techniques
- Observations represented as points
- Variables represented as vectors
- Interpretation:
 - Angle between vectors ~ correlation between fields
 - Cosine of the angle between a vector and an axis ∼ its importance contribution to the axis dimension
 - Points close to each other ~ observations with similar values

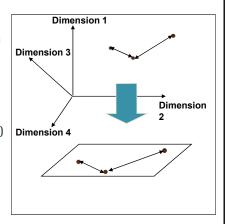


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Multi-Dimensional Scaling

- Alternative to PCA
- Maps objects from N-dimensional space to Mdimensional space while preserving distances between them (M<N)
- Not an exact procedure moves objects around in the smaller M-dimensional space and checks how well the real distances between them are reproduced in the new configuration (maximizes the goodness-of-fit)
- Good when relationships between objects (variables) are not known but a distance matrix can be estimated from similarities / differences between objects (PCA relies on the correlation matrix to indicate distances between objects)







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Analysis of Breakfast Cereals (1)

Consider twenty three breakfast cereals:

- All Bran (AllB)
- All Bran with extra fibre (AllF)
- AppleJacks(AppJ)
- Cornflakes(CorF)
 Corn Pops (CorP)
- Cracklin' Oat Bran (Crac)
- Crispix (Cris)
- Froot Loops (Froo)
- Frosted Flakes (FroF) Frosted Mini-Wheats (FrMW)
- Fruitful Bran (FruB)
- Just Right Crunch Nuggets (JRCN)
- Just Right Fruit & Nut (JRFN)
- Meusliz Crispy blend (MuCB)
- Nut & Honey Crunch (Nut&) Nutri Grain Almond Raisin (NGAR)
- Nutri Grain Wheat (NutW) Product 18 (prod)
- Raisin Bran (RaBr) Raisin Squares (RaiS)
- Rice Krispies (RiKr)
- Sugar Smacks (Smac)
- Special K (Spec)

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Data collected:

- Number of calories
- Amount of protein (g)
- Amount of fat (g)
- Amount of sodium (mg)
- Amount of dietary fibre (g)
- Amount of complex carbohydrates (g)
- Amount of sugars (g)
- Display shelf position (shelf 1, 2, or 3)
- Vitamin & mineral content (0, 25 or 100)
- Type of cereal (Hot or cold)

Analysis of Breakfast Cereals (2)

The raw data....

AIIB	0.1818	0.6	0.3333	0.8125	0.6429	0	0.3333	3	0.9677	0
AllF	0	0.6	0	0.4375	1	0.0667	0	3	1	0
AppJ	0.5455	0.2	0	0.3906	0.0714	0.2667	0.9333	2	0.0323	0
CorF	0.4545	0.2	0	0.9063	0.0714	0.9333	0.1333	1	0.0484	0
CorP	0.5455	0	0	0.2813	0.0714	0.4	0.8	2	0	0
Crac	0.5455	0.4	1	0.4375	0.2857	0.2	0.4667	3	0.4516	0
Cris	0.5455	0.2	0	0.6875	0.0714	0.9333	0.2	3	0.0323	0
Froo	0.5455	0.2	0.3333	0.3906	0.0714	0.2667	0.8667	2	0.0323	0
FroF	0.5455	0	0	0.625	0.0714	0.4667	0.7333	2	0.0161	0
FrMW	0.4545	0.4	0	0	0.2143	0.4667	0.4667	2	0.2581	0
FruB	0.6364	0.4	0	0.75	0.3571	0.4667	0.8	3	0.5484	0
JRCN	0.5455	0.2	0.3333	0.5313	0.0714	0.6667	0.4	3	0.129	1
JRFN	0.8182	0.4	0.3333	0.5313	0.1429	0.8667	0.6	3	0.2419	1
MuCB	1	0.4	0.6667	0.4688	0.2143	0.6667	0.8667	3	0.4516	0
Nut&	0.6364	0.2	0.3333	0.5938	0	0.5333	0.6	2	0.0645	0
NGAR	0.8182	0.4	0.6667	0.6875	0.2143	0.9333	0.4667	3	0.3548	0
NutW	0.3636	0.4	0	0.5313	0.2143	0.7333	0.1333	3	0.2258	0
Prod	0.4545	0.4	0	1	0.0714	0.8667	0.2	3	0.0806	1
RaBr	0.6364	0.4	0.3333	0.6563	0.3571	0.4667	0.8	2	0.7097	0
Rais	0.3636	0.2	0	0	0.1429	0.5333	0.4	3	0.2903	0
RiKr	0.5455	0.2	0	0.9063	0	1	0.2	1	0.0484	0
Smac	0.5455	0.2	0.3333	0.2188	0.0714	0.1333	1	2	0.0645	0
Spec	0.5455	1	0	0.7188	0.0714	0.6	0.2	1	0.1129	0
Opec	0.0400	'		0.7 100	0.07 14	0.0	0.2		0.1123	





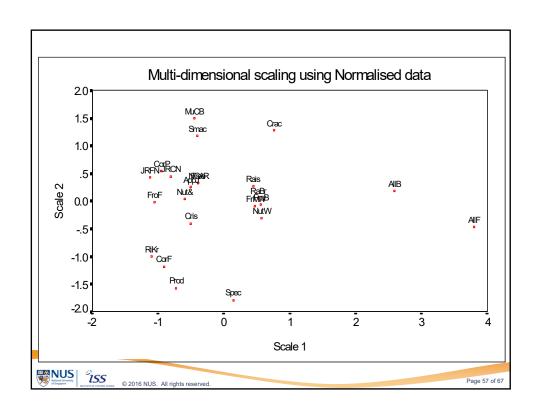
Analysis of Breakfast Cereals (3)

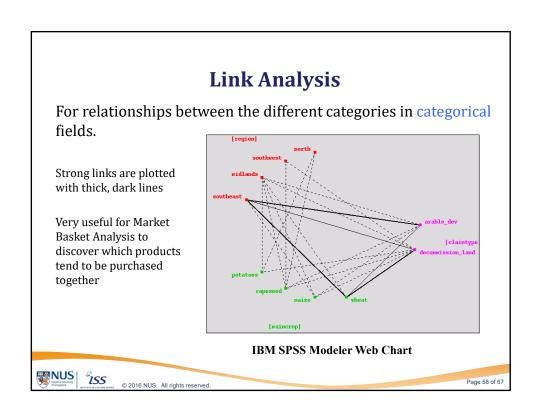
After MDS....

Cereal	x	<u>y</u>	Cereal	x	<u>y</u>
AllB	-1.94950	.96880	JRFN	09340	-1.85250
AllF	-2.54750	1.89990	MuCB	75230	57030
AppJ	.50930	.52080	Nut&	.36060	.00250
CorF	1.74630	06280	NGAR	49820	79920
CorP	.62080	.43560	NutW	26060	12870
Crac	-1.50940	.26850	Prod	.29640	-2.10090
Cris	.19300	76100	RaBr	25810	.52940
Froo	.36430	.39810	Rais	55240	.15500
FroF	1.48990	.23990	RiKr	1.83320	29600
FrMW	.06770	.64070	Smac	.25140	1.04770
FruB	65360	.08110	Spec	1.33440	1.00080
JRCN	.00790	-1.61720	1		



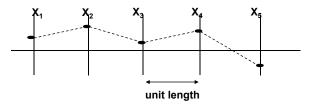
Source | Sou





Parallel Coordinates

- 2-D Visualisation of multi-dimensional data, *Inselberg (IBM, early '80s)*
- Map N-dimensions to a series of parallel vertical axes, one per variable
- A line joining a point on each axis ~ a point in the Ndimensional space



Good for generally numerical datasets with a moderate number of dimensions and no more than a few thousand records.

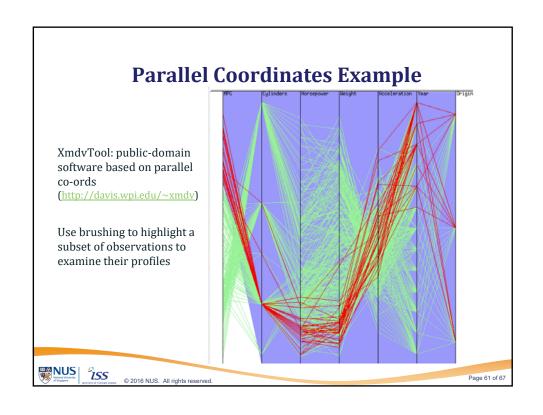




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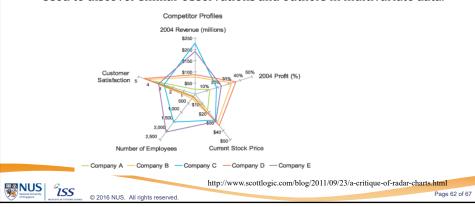
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Parallel Coordinates Similar to profile TABLE 2: STANDARDIZED VALUES ID# ROR5 SALESGR5 EPS5 P/E plots -0.47 -0.58 -0.77 -0.55 1.79 3.00 2.91 1.39 2.77 0.67 2.54 1.23 1.36 1.04 2.22 2.42 1.81 1.81 -0.14 -1.99 -0.85 -0.84 0.67 1.07 0.27 0.76 0.37 0.93 0.74 0.00 -0.93 Can help identify similar records, -0.19 -0.23 useful variables Standardized Value Profile Plot 21 NUS SESSE © 2016 NUS. All rights reserved.



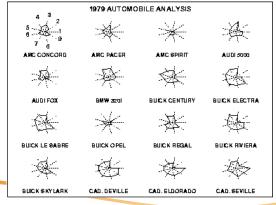
Radar Chart

- Displaying multivariate data in the form of a two-dimensional chart of three or more quantitative variables represented on axes starting from the same point
- Also known as spider chart, cobweb chart, etc.
- Used to discover similar observations and outliers in multivariate data.



Icon-based Multi-Dimensional Visualization

- Using icons like stars, stick figures, shape coding, color icons, etc. to discover similar or dissimilar observations.
- **Star Plot**: Each star represents a single observation.
- Helpful for small dataset



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Icon-based Multi-Dimensional Visualization

- Chernoff Faces: Each multi-dimensional observation is represented as a face with facial features determined by the component values. These features are
 - Upper hair
 - Chin curve
 - Lower hair
 - Eye size
 - Lip size
 - Eye space
 - Eye slant
 - Lip curve
 - Face size (eyes to mouth)





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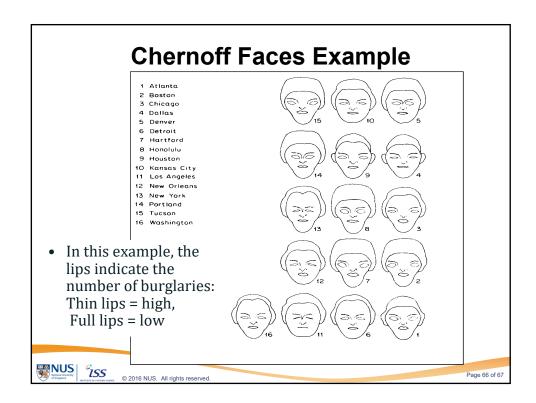
Chernoff Faces Example

• Data below gives the number of crimes per 100,000 population in several American cities

	Murder	Rape	Robbery	Assault	Burglary	Largency	Auto
	Man-slaughter						Theft
Atlanta	16.5	24.8	106	147	1112	905	494
Boston	4.2	13.3	122	90	982	669	954
Chicago	11.6	24.7	340	242	808	609	645
Dallas	18.1	34.2	184	293	1668	901	602
Denver	6.9	41.5	173	191	1534	1368	780
Detroit	13	35.7	477	220	1566	1183	788
Hartford	2.5	8.8	68	103	1017	724	468
Honolulu	3.6	12.7	42	28	1457	1102	637
Houston	16.8	26.6	289	186	1509	787	697
Kansas City	10.8	43.2	255	226	1494	955	765
Los Angeles	9.7	51.8	286	355	1902	1386	862
New Orleans	10.3	39.7	266	283	1056	1036	776



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Summary: Understanding your Data

- Establish Data Quality
 - Rubbish in rubbish out!
- Knowledge Discovery
 - Look for useful patterns, relationships, trends
 - Be open, don't be limited by preconceived ideas!
- Identify Data Enhancements
 - Identify what has to be done in data preparation



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