

07

Visualization Techniques Multivariate Data

Notice

- **Author**

- ◆ **João Moura Pires (jmp@fct.unl.pt)**

- **This material can be freely used for personal or academic purposes without any previous authorization from the author, provided that this notice is kept with.**
- **For commercial purposes the use of any part of this material requires the previous authorisation from the author.**

Multivariate Data

- Data that does not generally have an explicit spatial attribute
- **Point-Based Techniques**
 - Project records from an n -dimensional data space to an arbitrary k -dimensional display space, such that data records map to k -dimensional points. (e.g. Scatterplots)
- **Line-Based Techniques**
 - ◆ Points corresponding to a particular record or dimension are linked together with straight or curved lines. (e.g. Line Graphs, Parallel Coordinates)
- **Region-Based Techniques**
 - ◆ Filled polygons are used to convey values, based on their size, shape, color, or other attributes. (e.g. Bar Charts/Histograms)

Table of Contents

- **Introduction**
- **Point-Based Techniques**
- **Line-Based Techniques**
- **Region-Based Techniques**
- **Combinations of Techniques**

Introduction

Multivariate Data

- **Data that does not generally have an explicit spatial attribute**

Multivariate Data

- Data that does not generally have an explicit spatial attribute
- **Point-Based Techniques**
 - Project records from an **n-dimensional data** space to an arbitrary **k-dimensional display space**, such that data records map to k-dimensional points. (e.g. **Scatterplots**)

Multivariate Data

- Data that does not generally have an explicit spatial attribute
- **Point-Based Techniques**
 - Project records from an **n-dimensional data** space to an arbitrary **k-dimensional display space**, such that data records map to k-dimensional points. (e.g. **Scatterplots**)
- **Line-Based Techniques**
 - ◆ Points corresponding to a particular record or dimension are linked together with **straight or curved lines**. (e.g. **Line Graphs, Parallel Coordinates**)

Multivariate Data

- Data that does not generally have an explicit spatial attribute
- **Point-Based Techniques**
 - Project records from an **n-dimensional data** space to an arbitrary **k-dimensional display space**, such that data records map to k-dimensional points. (e.g. **Scatterplots**)
- **Line-Based Techniques**
 - ◆ Points corresponding to a particular record or dimension are linked together with **straight or curved lines**. (e.g. **Line Graphs, Parallel Coordinates**)
- **Region-Based Techniques**
 - ◆ Filled polygons are used to convey values, based on their size, shape, color, or other attributes. (e.g. **Bar Charts/Histograms**)

Point-Based Techniques

Multivariate Data: Point-Based Techniques

- **Scatterplots and Scatterplot Matrices**
 - Their **success** stems from our innate **abilities to judge relative position within a bounded space**

Multivariate Data: Point-Based Techniques

- **Scatterplots and Scatterplot Matrices**
 - Their **success** stems from our innate **abilities to judge relative position within a bounded space**
- As the **dimensionality** of the data increases, the choices for visual analysis consist of:
 - **dimension **subsetting**** (user selection or algorithm based suggestion);

Multivariate Data: Point-Based Techniques

- **Scatterplots and Scatterplot Matrices**

- Their **success** stems from our innate **abilities to judge relative position within a bounded space**

- As the **dimensionality** of the data increases, the choices for visual analysis consist of:

- **dimension **subsetting**** (user selection or algorithm based suggestion);

- **dimension **embedding**** (mapping dimensions to other graphical attributes besides position, such as color, size, and shape);

Multivariate Data: Point-Based Techniques

- **Scatterplots and Scatterplot Matrices**

- Their **success** stems from our innate **abilities to judge relative position within a bounded space**

- As the **dimensionality** of the data increases, the choices for visual analysis consist of:

- **dimension *subsetting*** (user selection or algorithm based suggestion);

- **dimension *embedding*** (mapping dimensions to other graphical attributes besides position, such as color, size, and shape);

- **multiple displays** (either superimposed or juxtaposed - e. g. scatterplot matrix);

Multivariate Data: Point-Based Techniques

- **Scatterplots and Scatterplot Matrices**

- Their **success** stems from our innate **abilities to judge relative position within a bounded space**

- As the **dimensionality** of the data increases, the choices for visual analysis consist of:

- **dimension **subsetting**** (user selection or algorithm based suggestion);

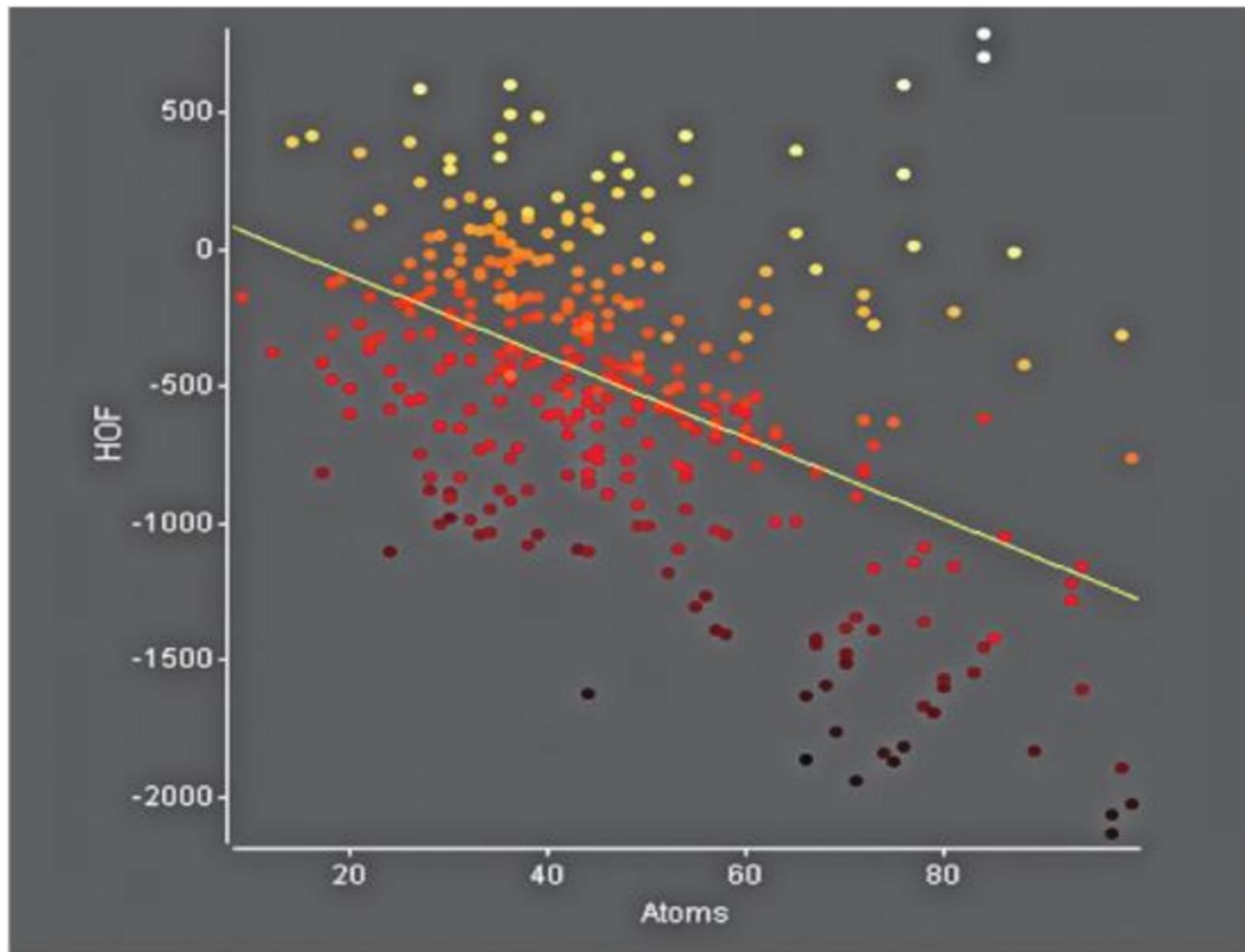
- **dimension **embedding**** (mapping dimensions to other graphical attributes besides position, such as color, size, and shape);

- **multiple displays** (either superimposed or juxtaposed - e. g. scatterplot matrix);

- **dimension **reduction**** (to transform the high-dimensional data to data of lower dimension).

Multivariate Data: Point-Based Techniques

■ Scatterplots



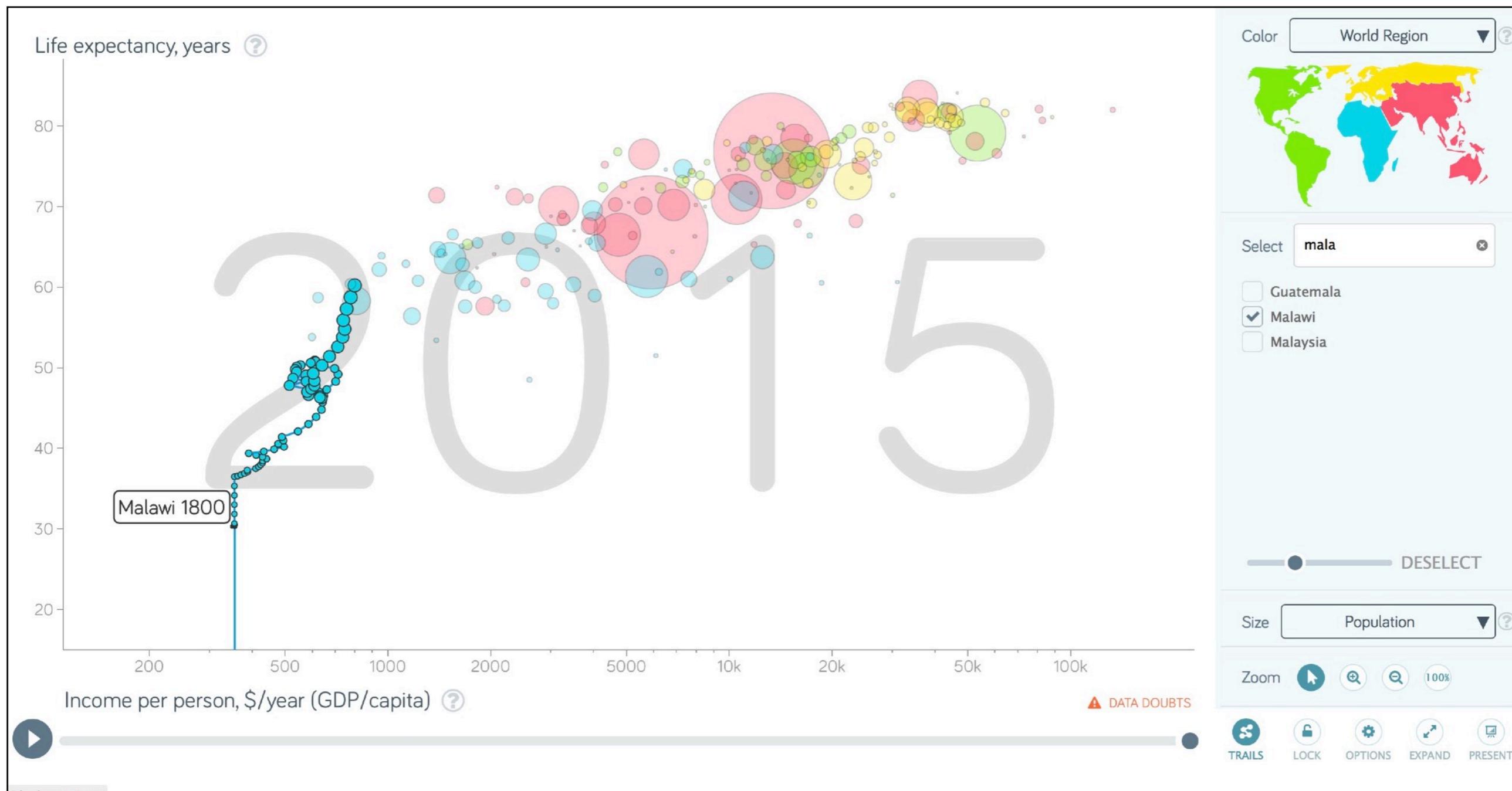
x -coordinate: number of atoms;
 y -coordinate: heat information;

$$y = mx + b; m = -12.5 \text{ and } b = 50$$

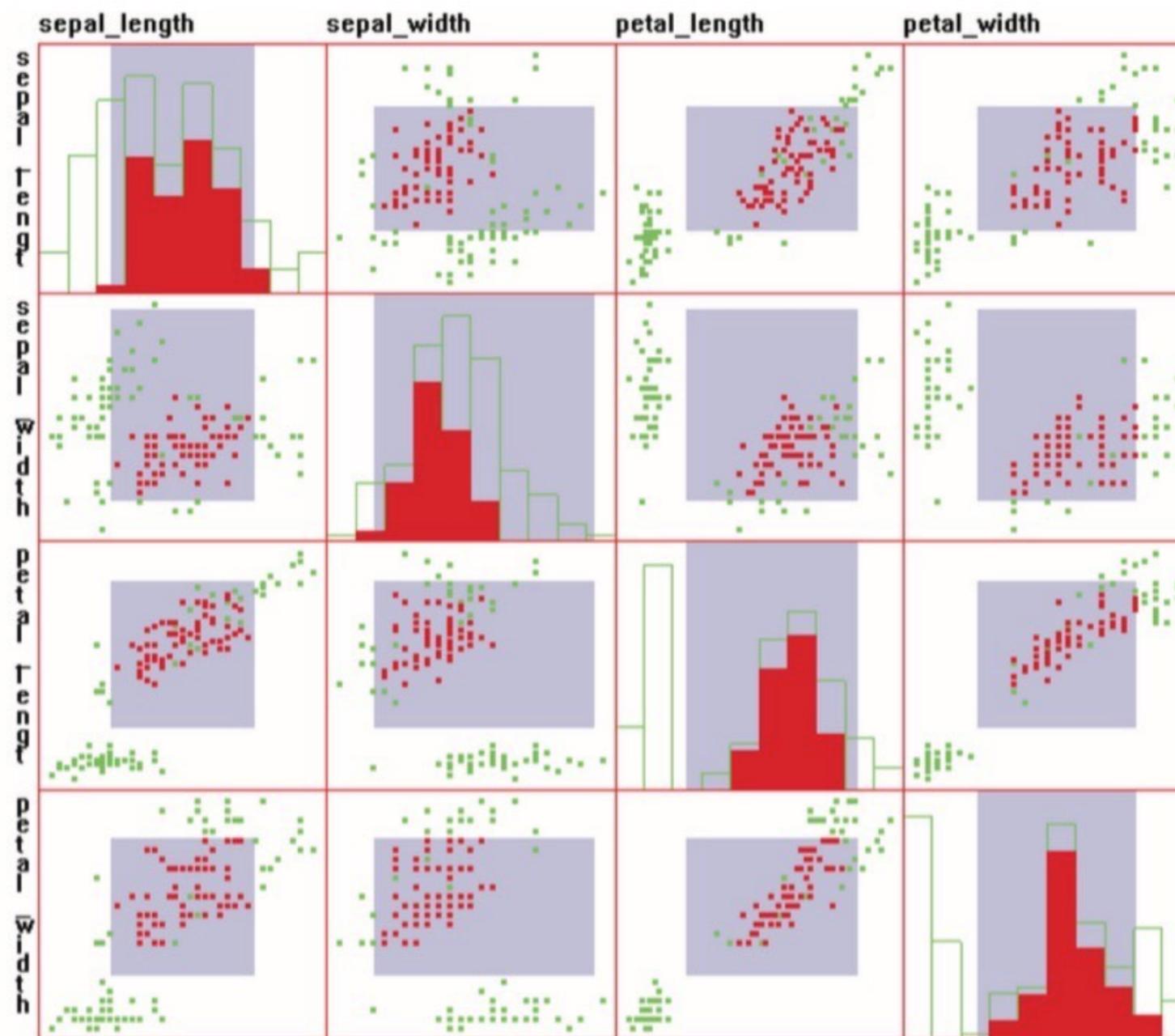
Color of each point: Gibbs energy

Multivariate Data: Point-Based Techniques

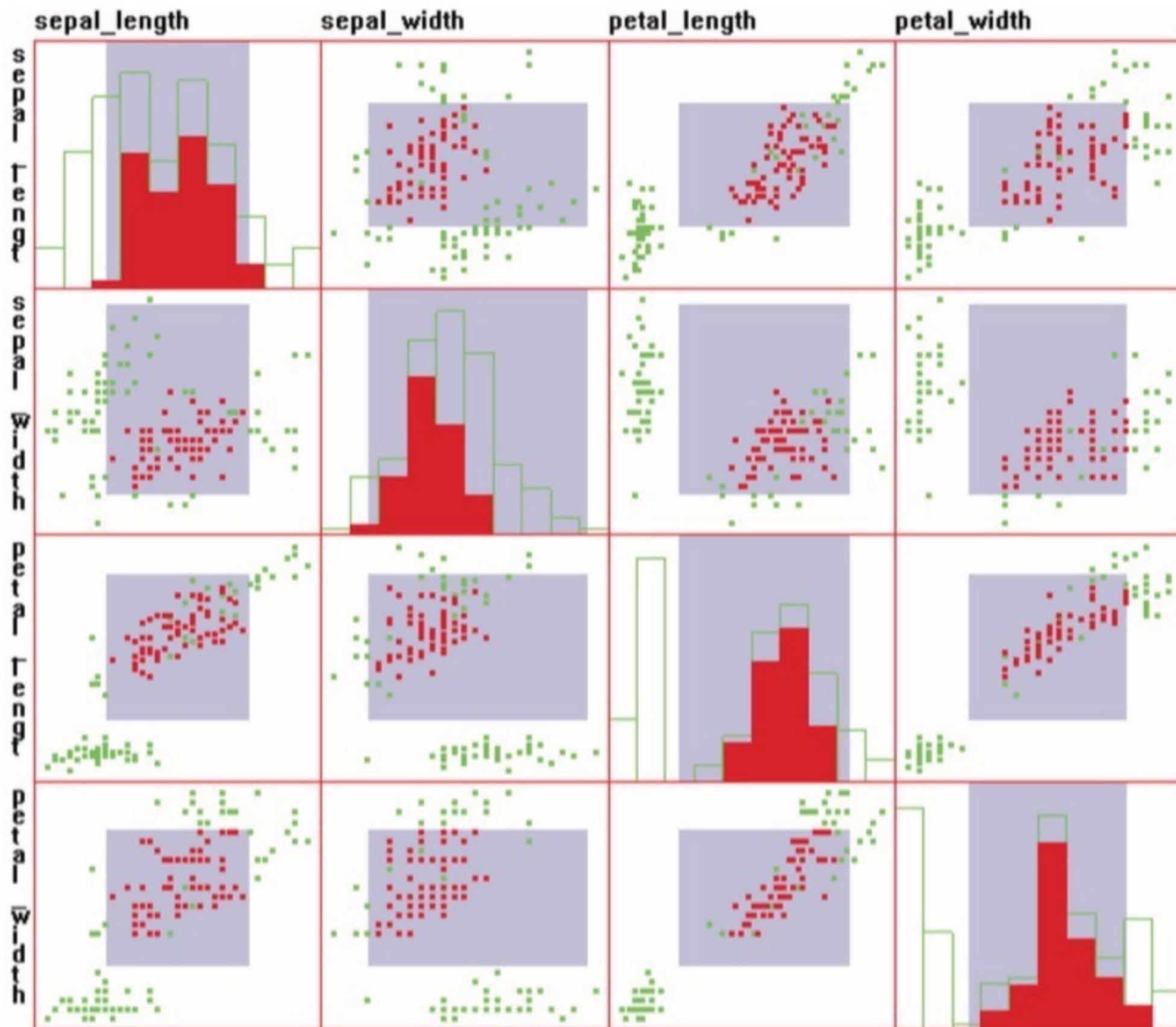
Scatterplots



Multivariate Data: Point-Based Techniques

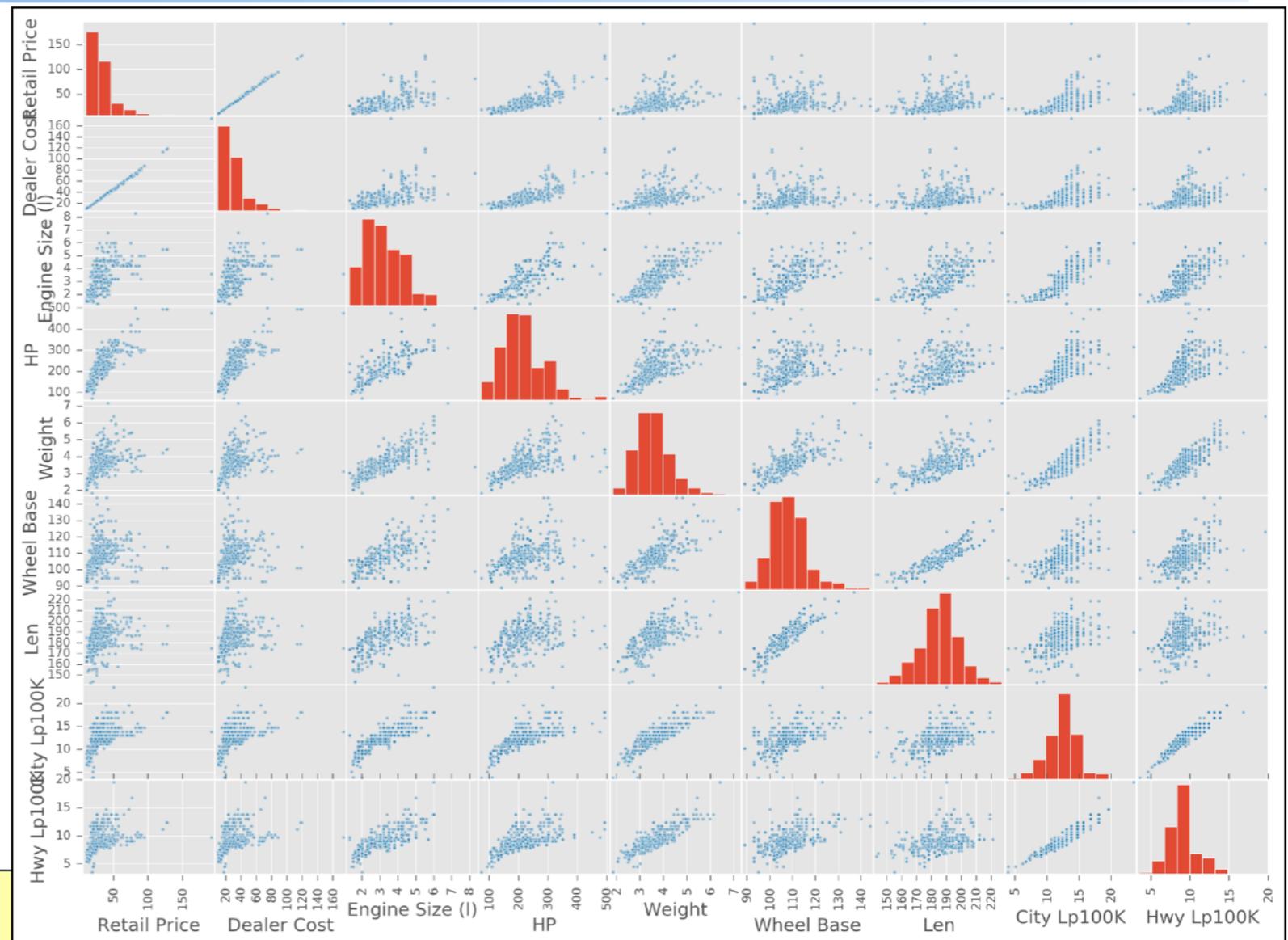


A scatterplot matrix with the diagonal plot showing a histogram of each dimension. Note that the points and histogram regions in red indicate selected data.



A scatterplot matrix with the diagonal plot showing a histogram of each dimension. Note that the points and histogram regions in red indicate selected data.

Scatter Matrix (in Python)

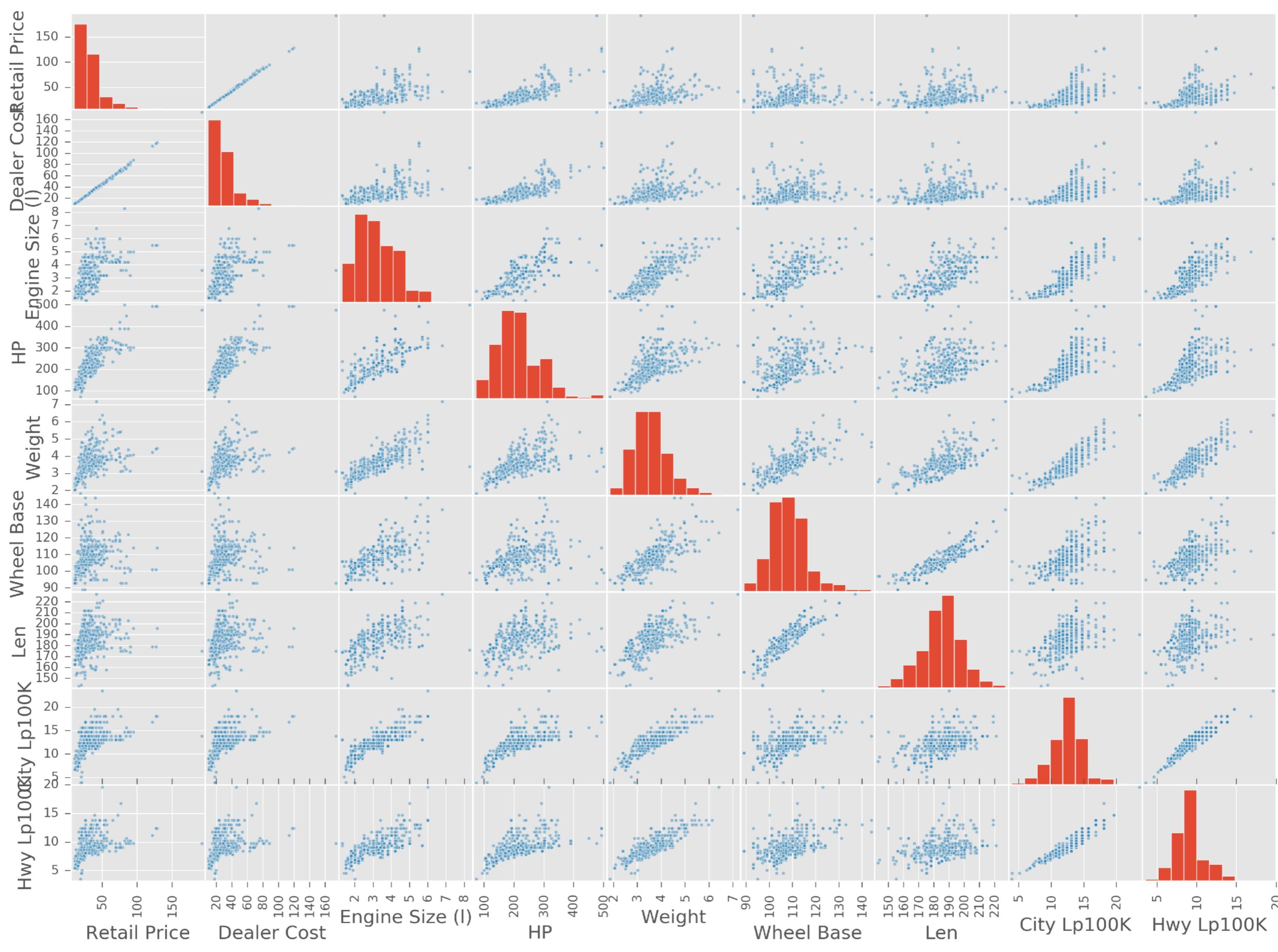


...

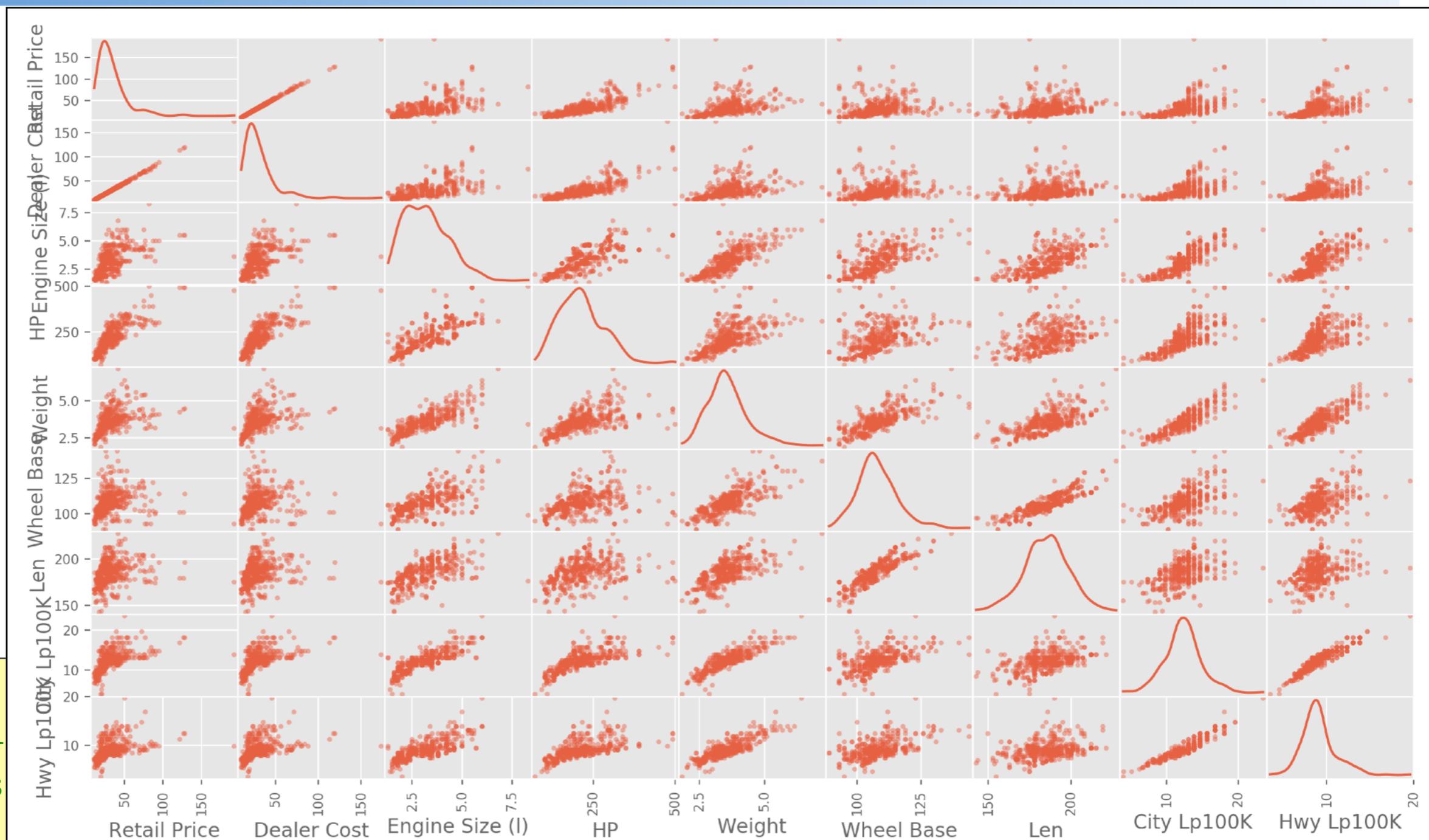
```
# data is the data frame with all variable
```

```
# snc is the subset of numerical variables of interest
```

```
# Let's check how these variables relate to each other  
scatter matrix(data[snc], figsize=(12, 12))
```

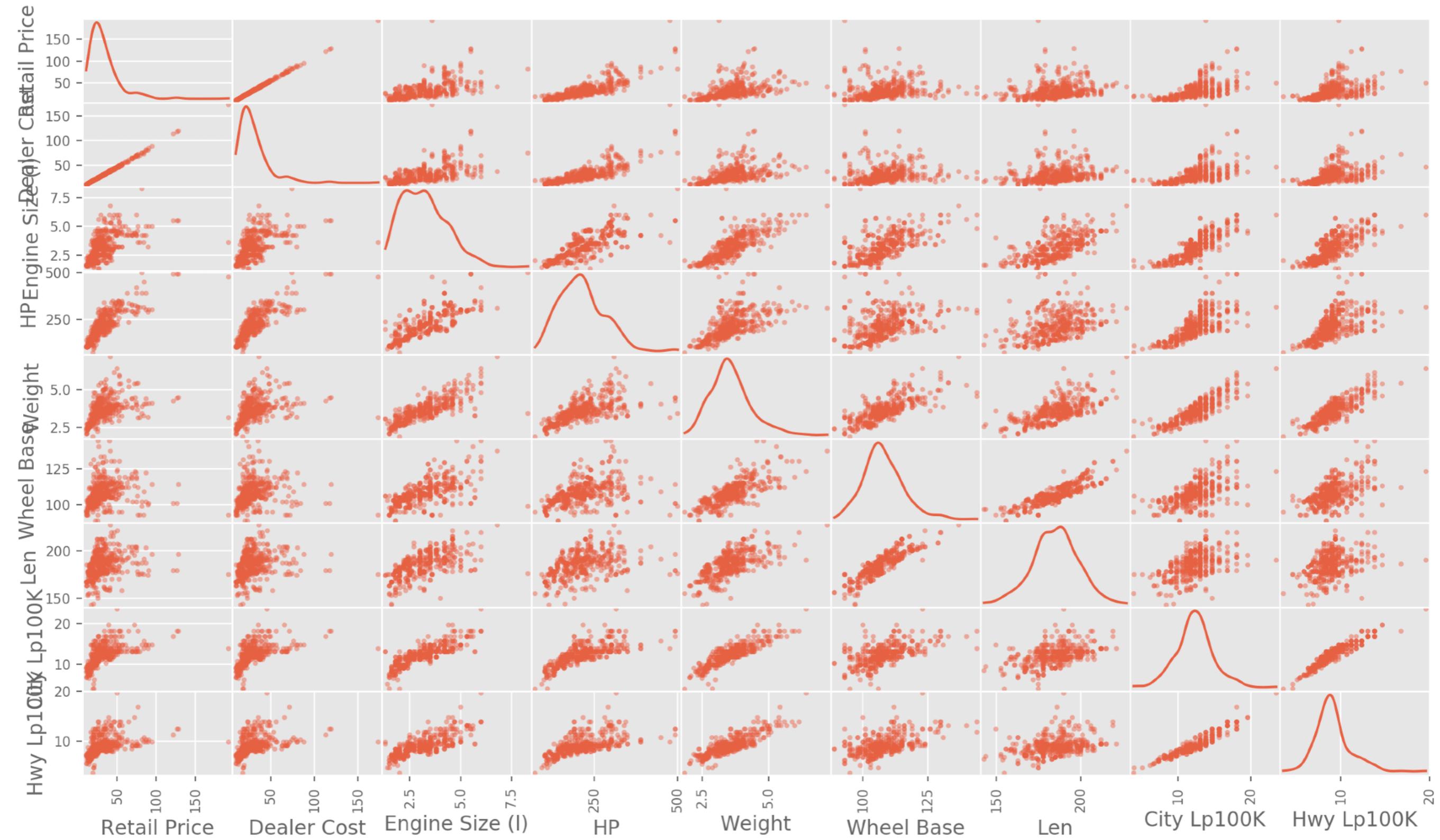


Scatter Matrix (in Python)



```
...  
# data i  
# snc is
```

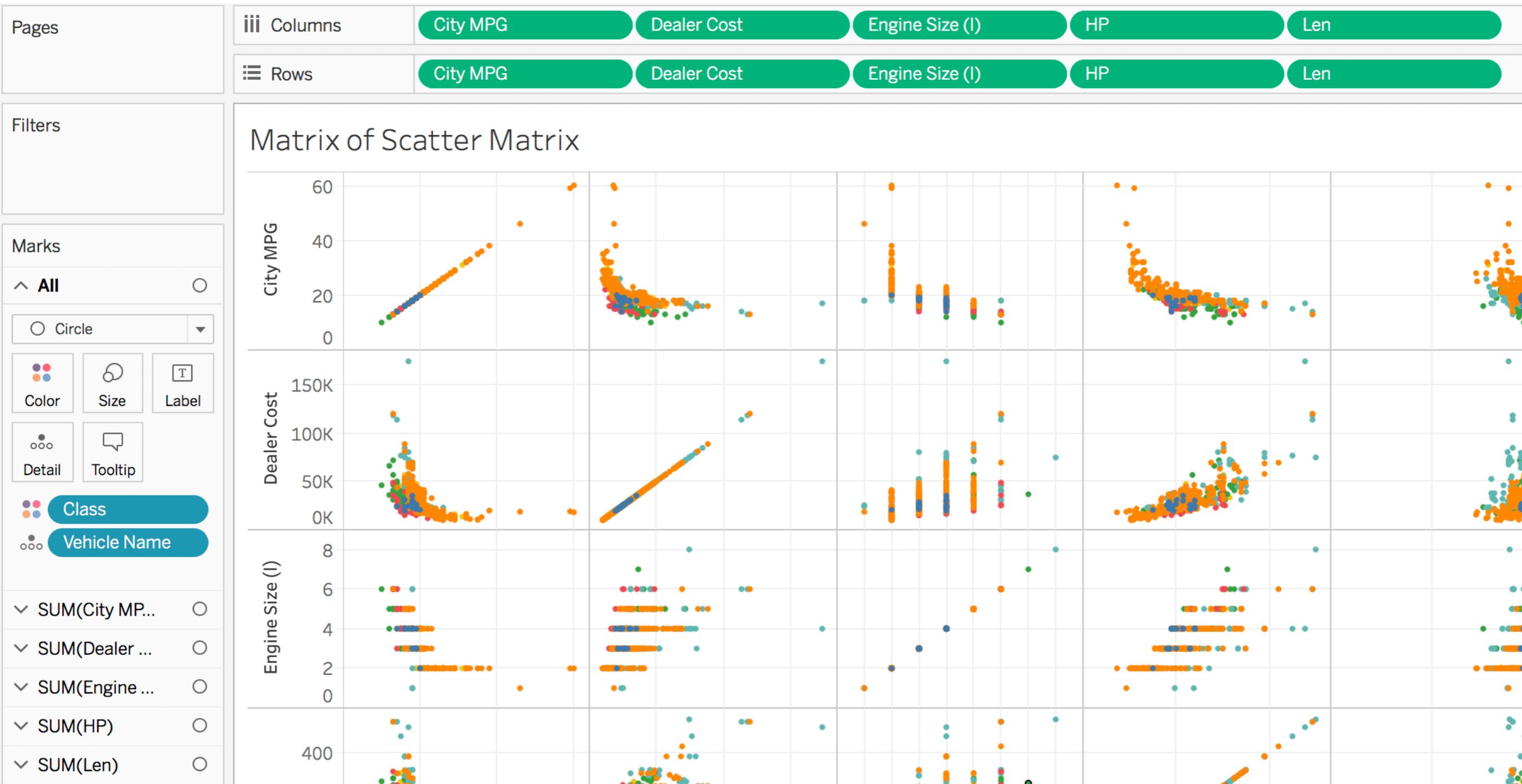
```
# Let's check how these variables relate to each other  
scatter_matrix(data[snc], figsize=(12, 12), diagonal='kde')
```



Scatter Matrix (in Tableau)



Scatter Matrix (in Tableau)



Pages

Columns: City MPG, Dealer Cost, Engine Size (l), HP, Len
Rows: City MPG, Dealer Cost, Engine Size (l), HP, Len

Filters

Marks

^ All

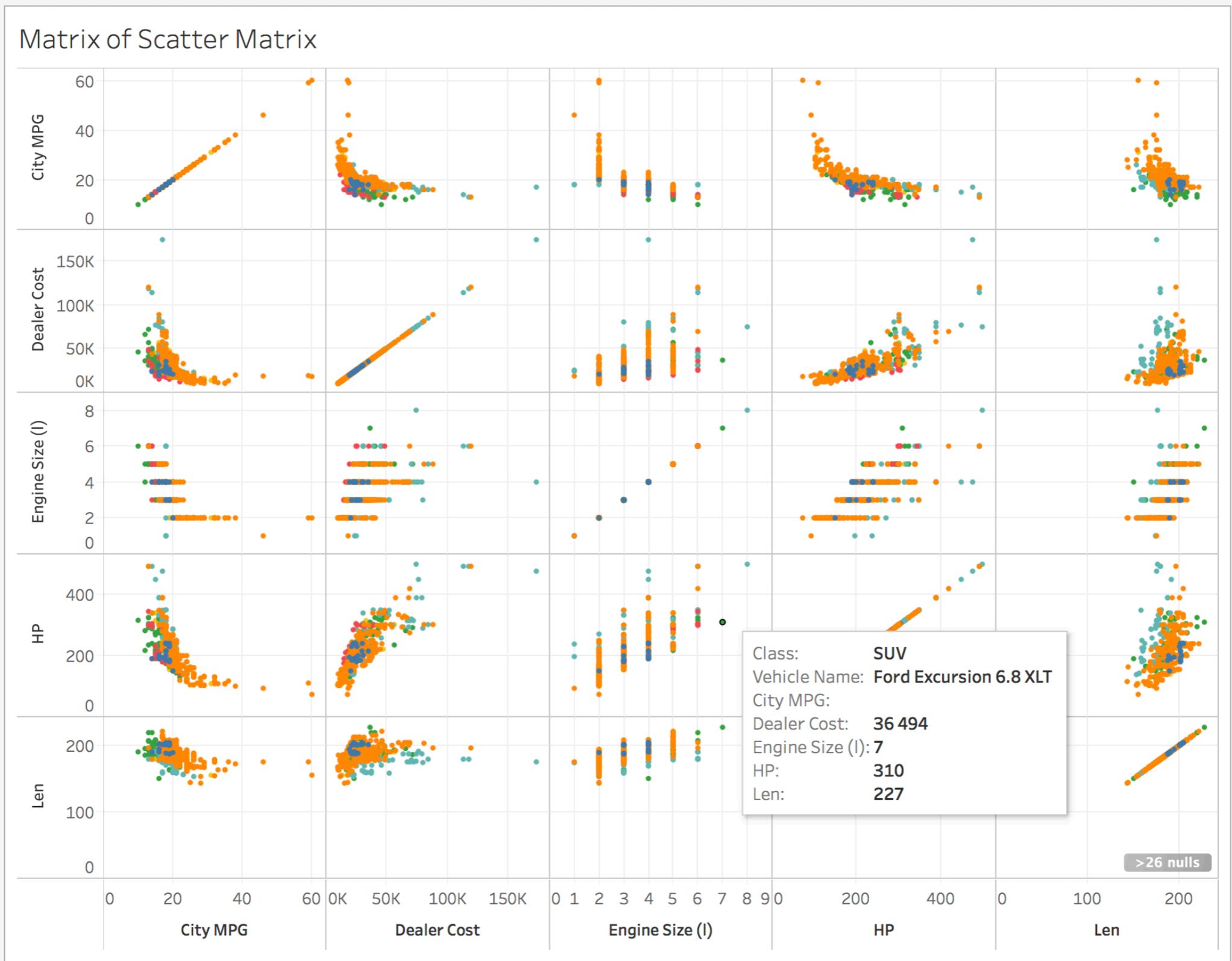
Circle

Color, Size, Label

Detail, Tooltip

Class, Vehicle Name

SUM(City MP...), SUM(Dealer ...), SUM(Engine ...), SUM(HP), SUM(Len)



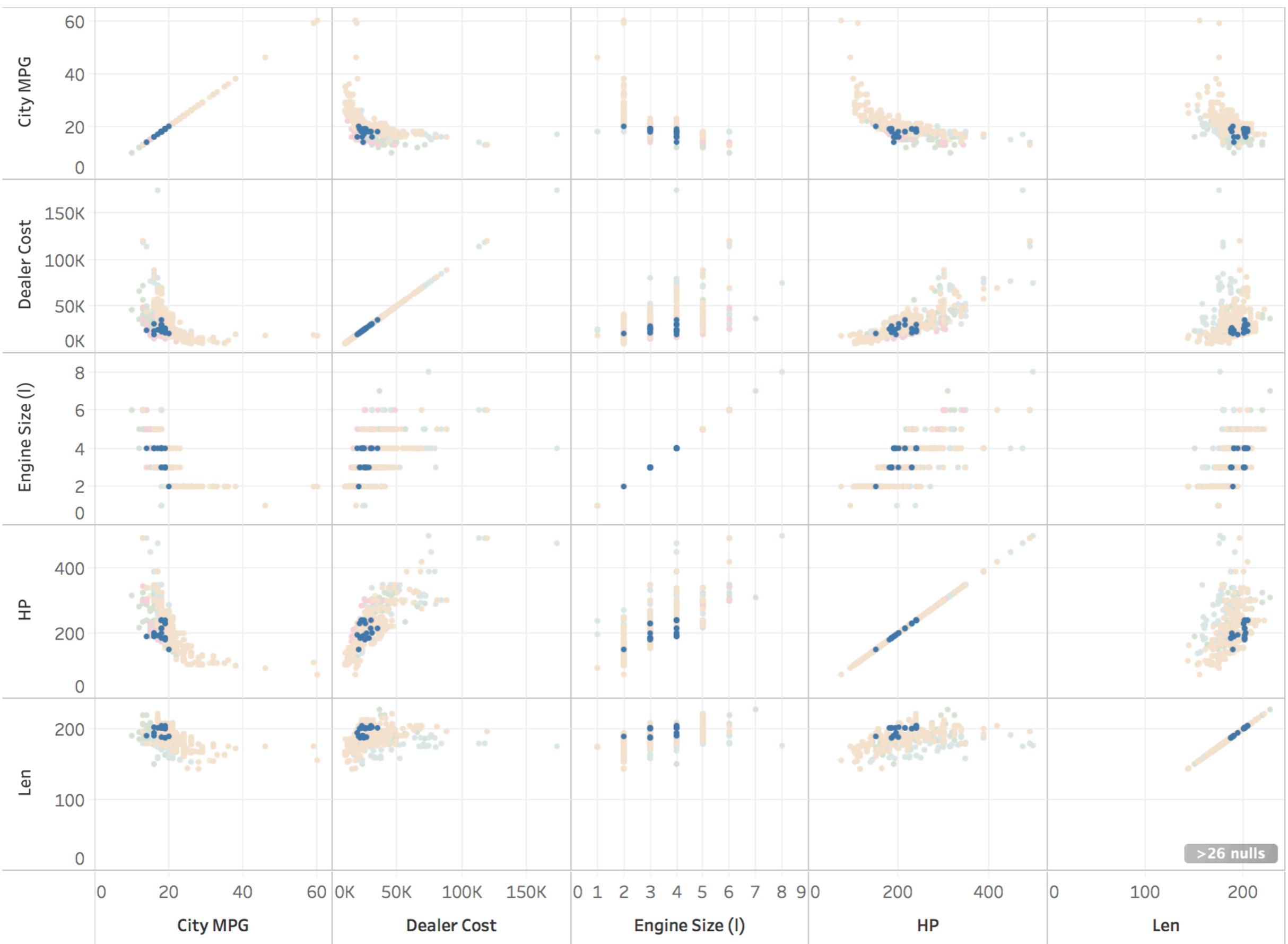
Class

- Minivan
- Normal
- Pickup
- Sports
- SUV
- Wagon

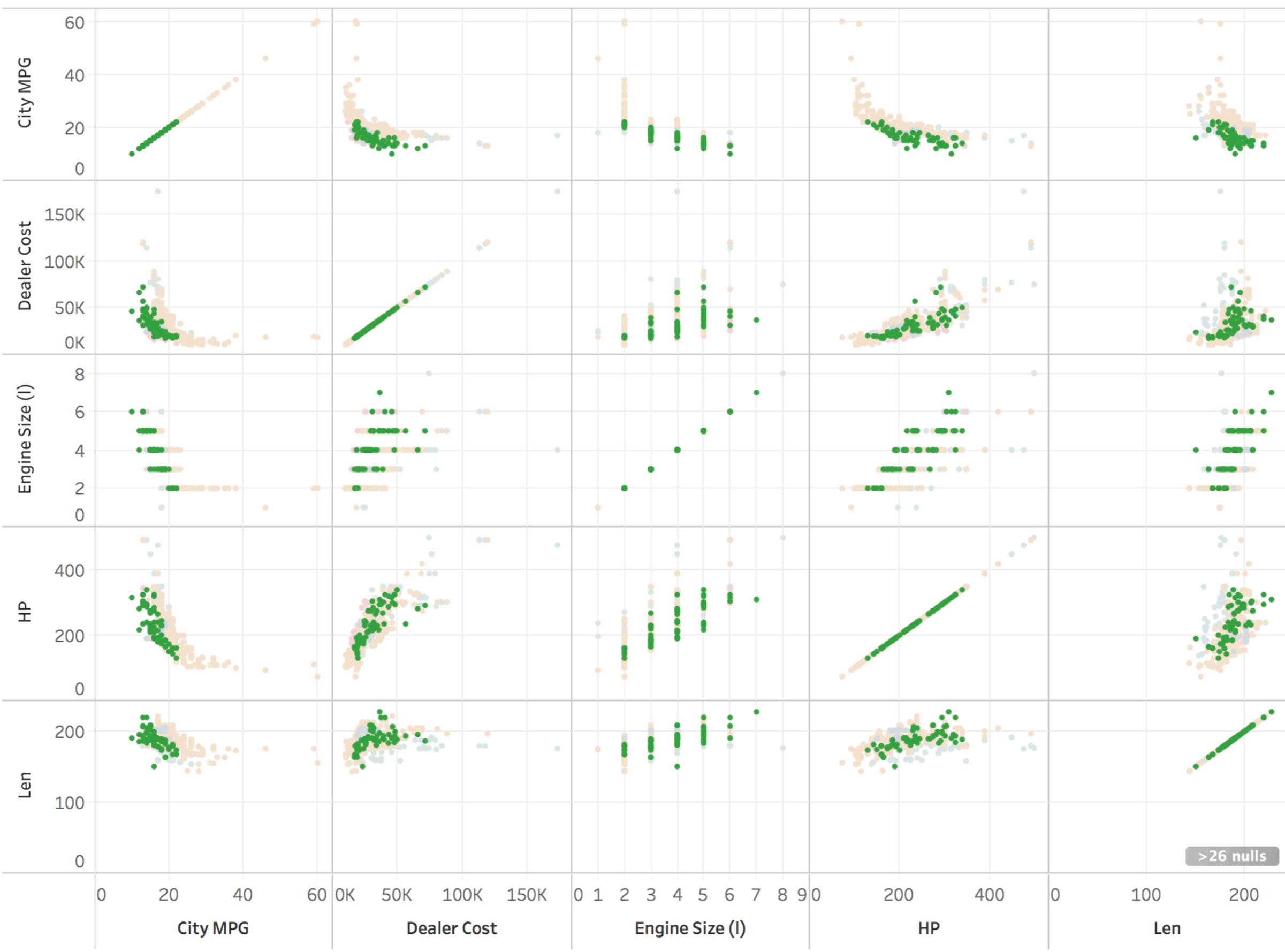
Matrix of Scatter Matrix

Class

- Minivan
- Normal
- Pickup
- Sports
- SUV
- Wagon



Matrix of Scatter Matrix



Class

- Minivan
- Normal
- Pickup
- Sports
- SUV**
- Wagon

>26 nulls

Multivariate Data: Point-Based Techniques

- In situations where the dimensionality of the data exceeds the capabilities of the visualization technique. It is necessary to investigate ways to **reduce the data dimensionality, while at the same time preserving, as much as possible, the information contained within.**
- Principal Component Analysis (PCA) - [read more](#) and see this [implementation](#)
- Multidimensional Scaling (MDS) - [read more](#) and [more](#)
- Non-linear dimension reduction techniques:
 - ◆ Self-organizing Maps (SOMs) - [read more](#)
 - ◆ Local Linear Embeddings (LLE) - [read more](#)

Multidimensional scaling (MDS)

- Projecting **M** points in **N** dimensions into **L** dimensions ($L = 2$ or 3) display space.

Multidimensional scaling (MDS)

- Projecting **M** points in **N** dimensions into **L** dimensions ($L = 2$ or 3) display space.
- The key goal is to **attempt to maintain the N-dimensional features and characteristics** of the data through the projection process, e.g., relationships that exist in the original data must also exist after projection.

Multidimensional scaling (MDS)

- Projecting M points in N dimensions into L dimensions ($L = 2$ or 3) display space.
- The key goal is to **attempt to maintain the N -dimensional features and characteristics** of the data through the projection process, e.g., relationships that exist in the original data must also exist after projection.
 - ◆ The projection may also **unintentionally introduce artifacts** that may appear in the visualization and are not present in the data.

Multidimensional scaling (MDS)

- Projecting M points in N dimensions into L dimensions ($L = 2$ or 3) display space.
- The key goal is to **attempt to maintain the N -dimensional features and characteristics** of the data through the projection process, e.g., relationships that exist in the original data must also exist after projection.
 - ◆ The projection may also **unintentionally introduce artifacts** that may appear in the visualization and are not present in the data.
- ◆ Repeat
 - ◆ Create an Similarity $M \times M$ Matrix (D) (could be distance)
 - ◆ Create a coordinates Matrix $M \times L$ and fill randomly or other method (ex: PCA)
 - ◆ Compute an $M \times M$ matrix (L) based on L coordinates. And compute S the difference between D and L .
 - ◆ Shift the positions of points in L in a direction that will reduce their individual stress levels
- ◆ Until S is small of not changed significantly

Multidimensional scaling (MDS)

- There are many possible variants on this algorithm, including:
 - ◆ **Different similarity and stress measures;**
 - ◆ **Different initial and termination conditions;**
 - ◆ **Different position update strategies.**

Multidimensional scaling (MDS)

- There are many possible variants on this algorithm, including:
 - ◆ **Different similarity and stress measures;**
 - ◆ **Different initial and termination conditions;**
 - ◆ **Different position update strategies.**
- ◆ As in any optimization process, there is the potential to fall into a local minimal configuration that still has a high level of stress.

Multidimensional scaling (MDS)

- There are many possible variants on this algorithm, including:
 - ◆ **Different similarity and stress measures;**
 - ◆ **Different initial and termination conditions;**
 - ◆ **Different position update strategies.**
- ◆ As in any optimization process, there is the potential to fall into a local minimal configuration that still has a high level of stress.
- ◆ Common strategies to alleviate this include occasionally **adding a random jump** in the position of a point to see if it will converge to a different location

Multidimensional scaling (MDS)

- There are many possible variants on this algorithm, including:
 - ◆ **Different similarity and stress measures;**
 - ◆ **Different initial and termination conditions;**
 - ◆ **Different position update strategies.**
- ◆ As in any optimization process, there is the potential to fall into a local minimal configuration that still has a high level of stress.
- ◆ Common strategies to alleviate this include occasionally **adding a random jump** in the position of a point to see if it will converge to a different location
- ◆ Obviously, **the results are not unique**: minor changes in the starting conditions can lead to dramatically different results.

Multivariate Data: Point-Based Techniques

- Iris flower data set



Iris setosa



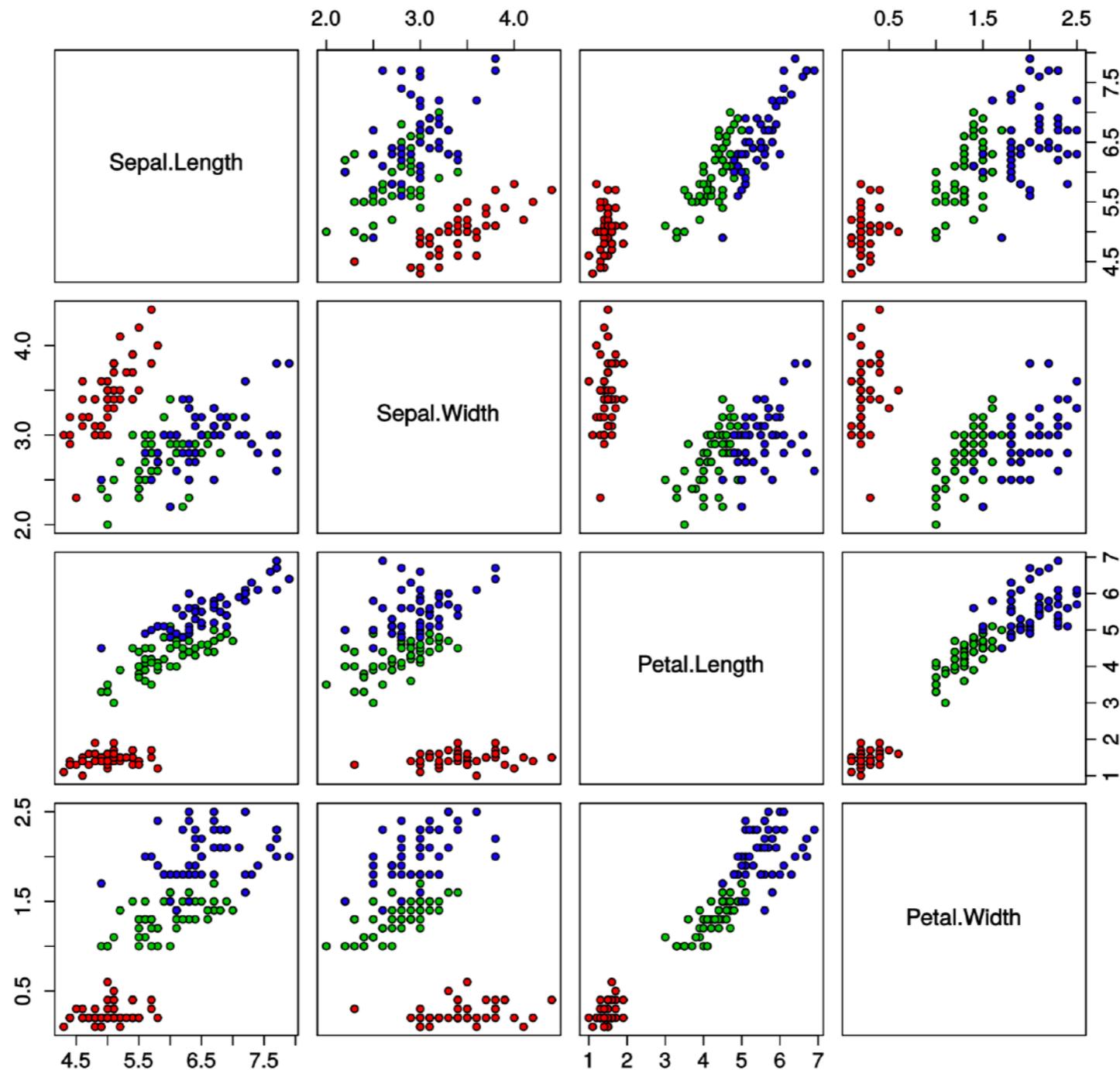
Iris versicolor



Iris virginica

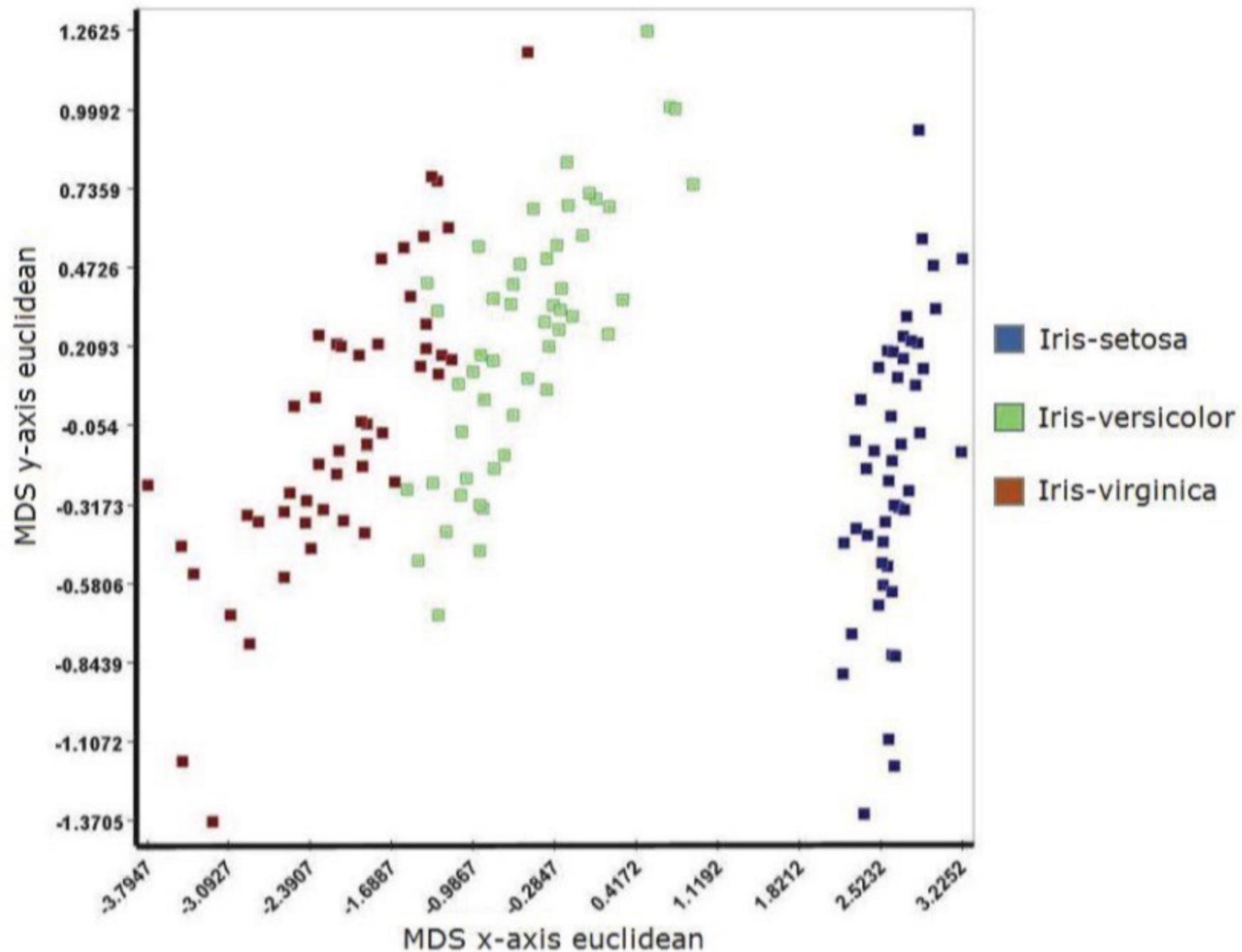
Multivariate Data: Point-Based Techniques

Iris Data (red=setosa,green=versicolor,blue=virginica)



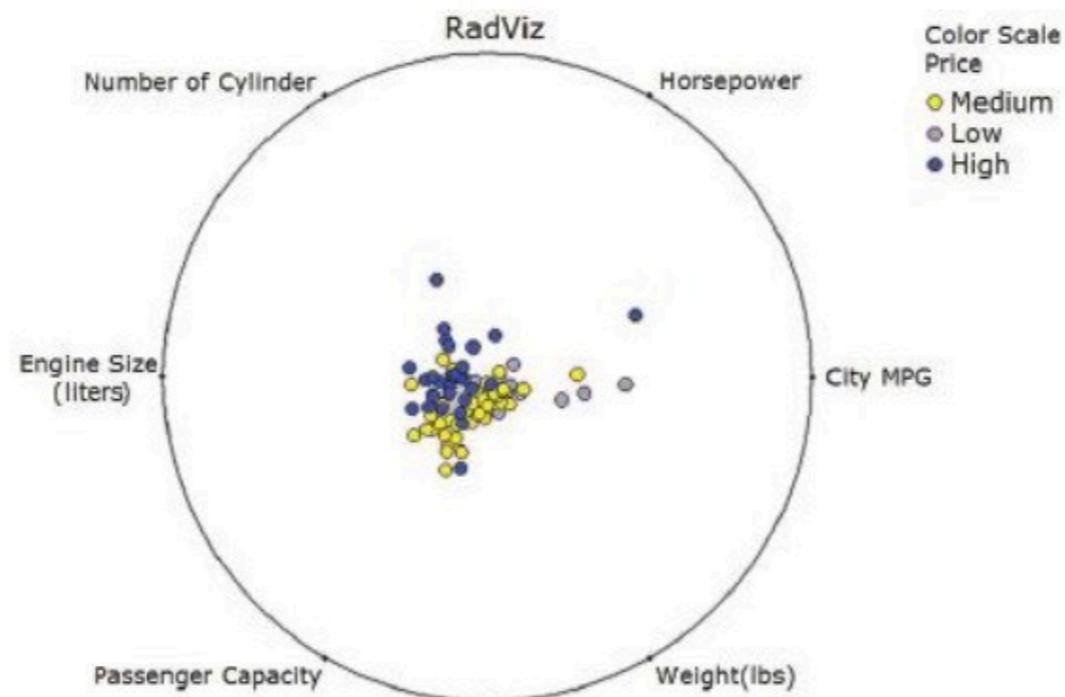
Multivariate Data: Point-Based Techniques

- Iris data set projected using MDS



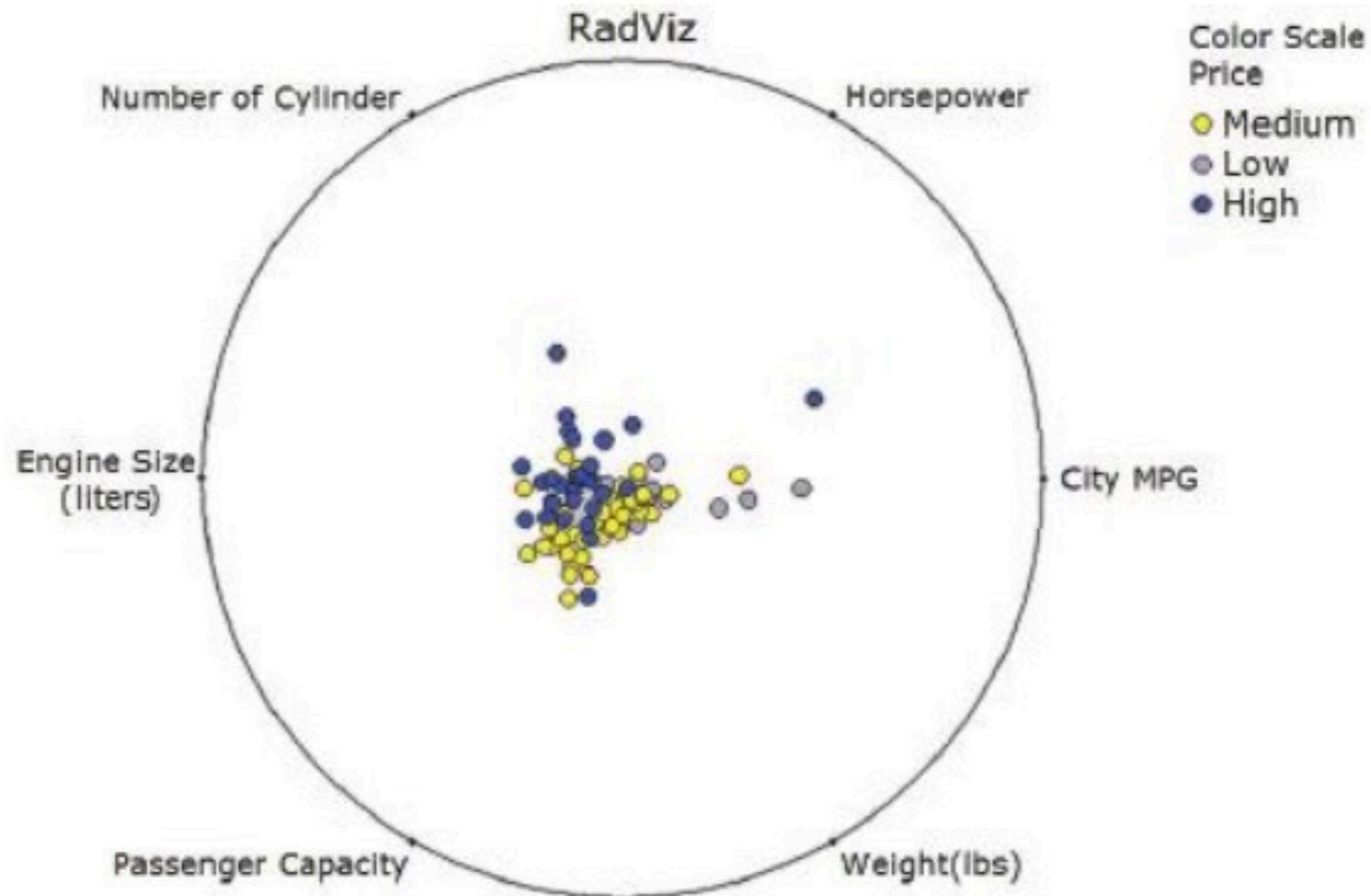
Multivariate Data: Point-Based Techniques

- **RadViz:** is a force-driven point layout technique that is based on Hooke's Law for equilibrium.
- For an N-dimensional data set, **N anchor points** are placed on the circumference of the circle to represent the fixed ends of the **N springs** attached to each data point.
- **Different placement and ordering of the anchors will give different results**, and that points that are quite distinct in N dimensions may map to the same location in 2D.



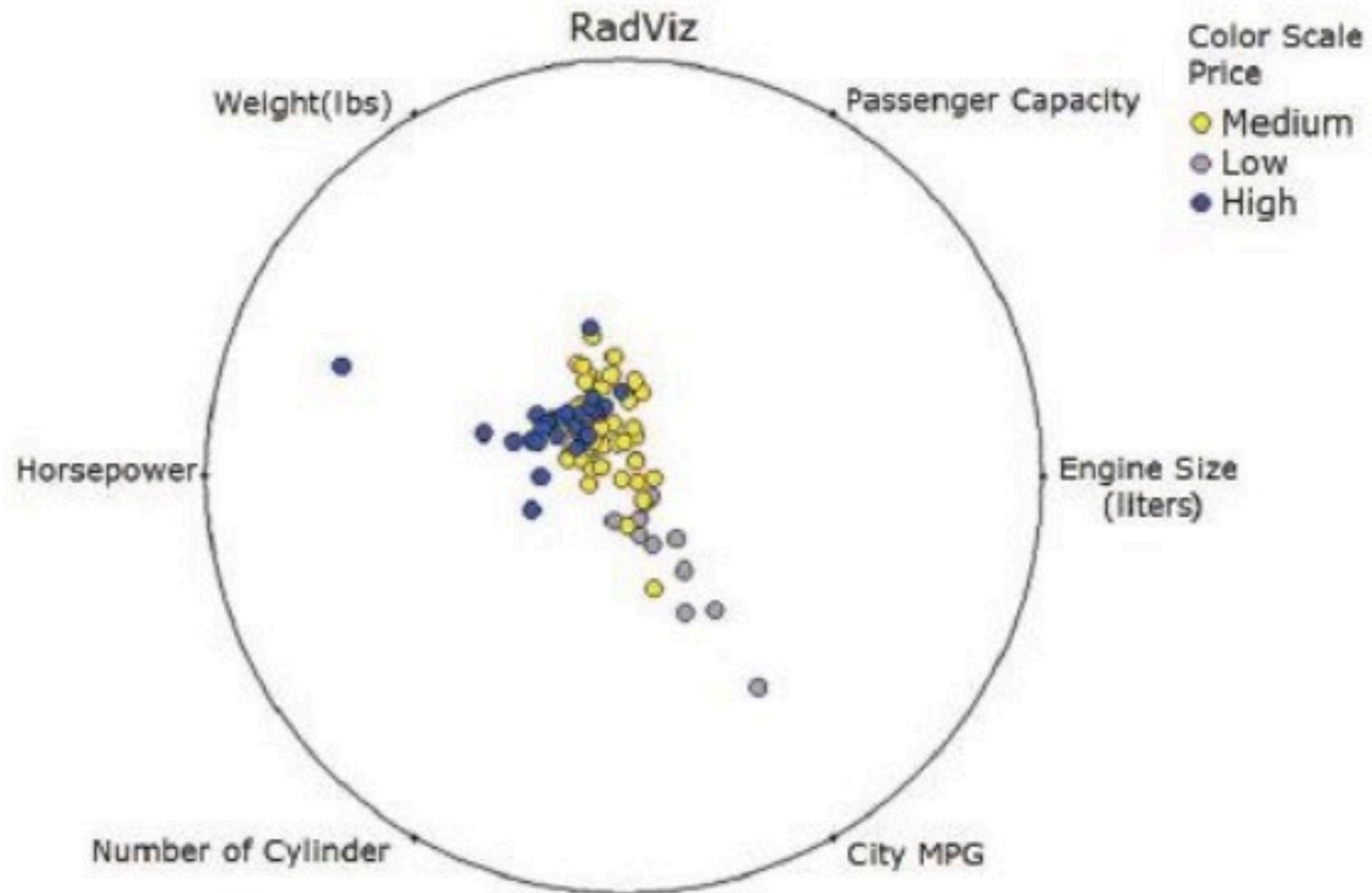
Multivariate Data: Point-Based Techniques

- **RadViz:** different views of the same data set in RadViz, using manual reordering of dimensions.



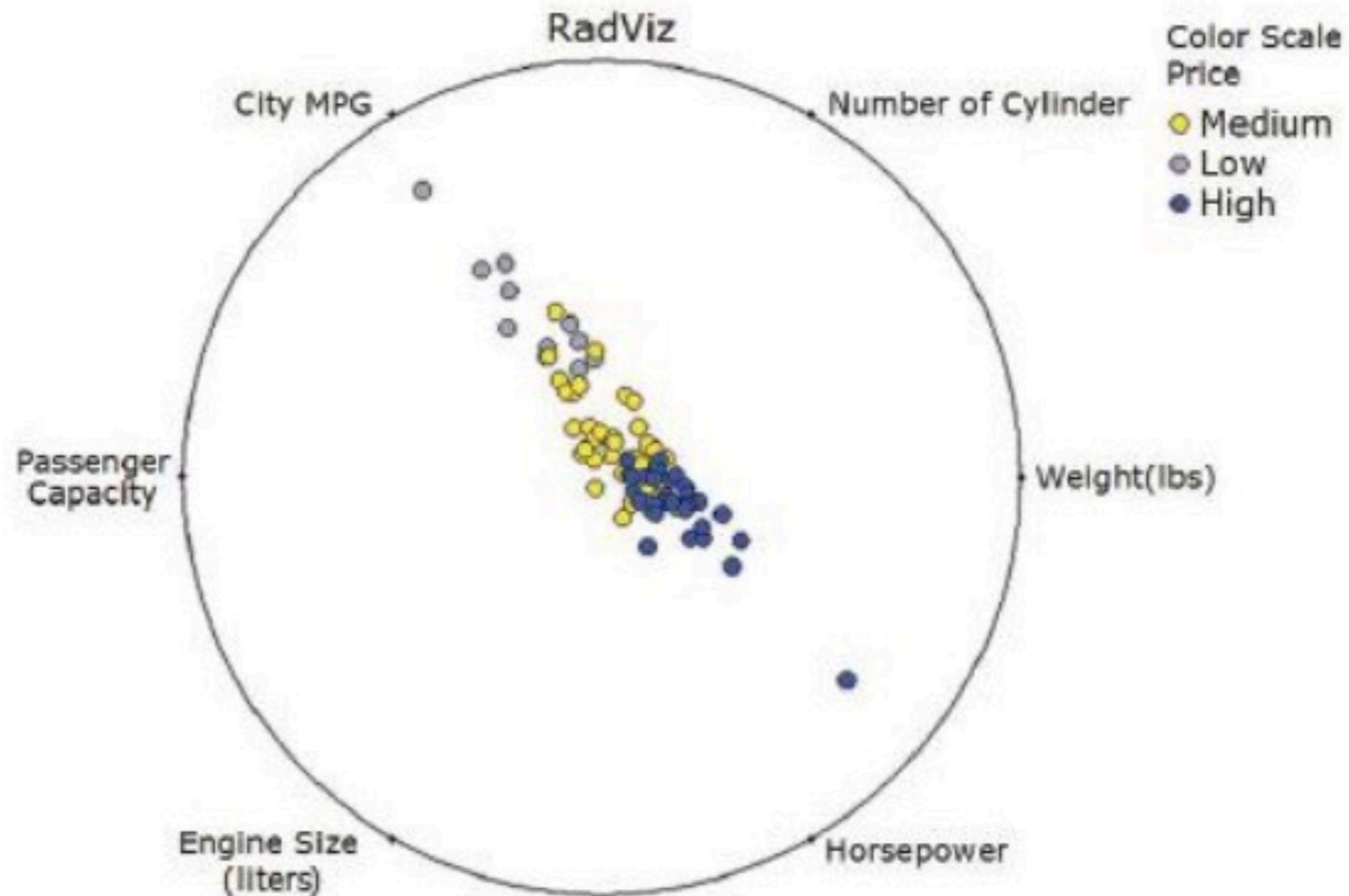
Multivariate Data: Point-Based Techniques

- **RadViz:** different views of the same data set in RadViz, using manual reordering of dimensions.



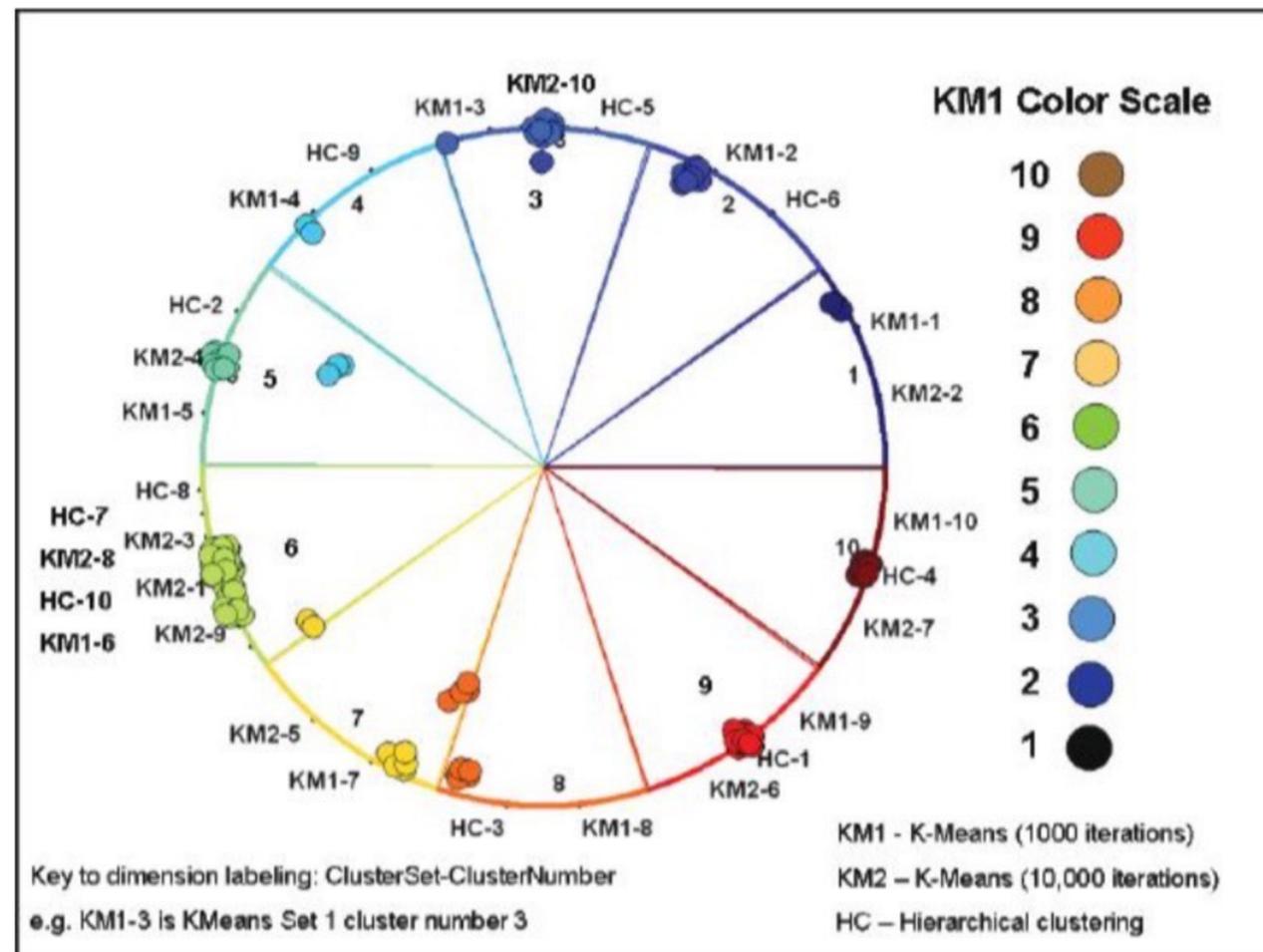
Multivariate Data: Point-Based Techniques

- **RadViz:** different views of the same data set in RadViz, using manual reordering of dimensions.



Multivariate Data: Point-Based Techniques

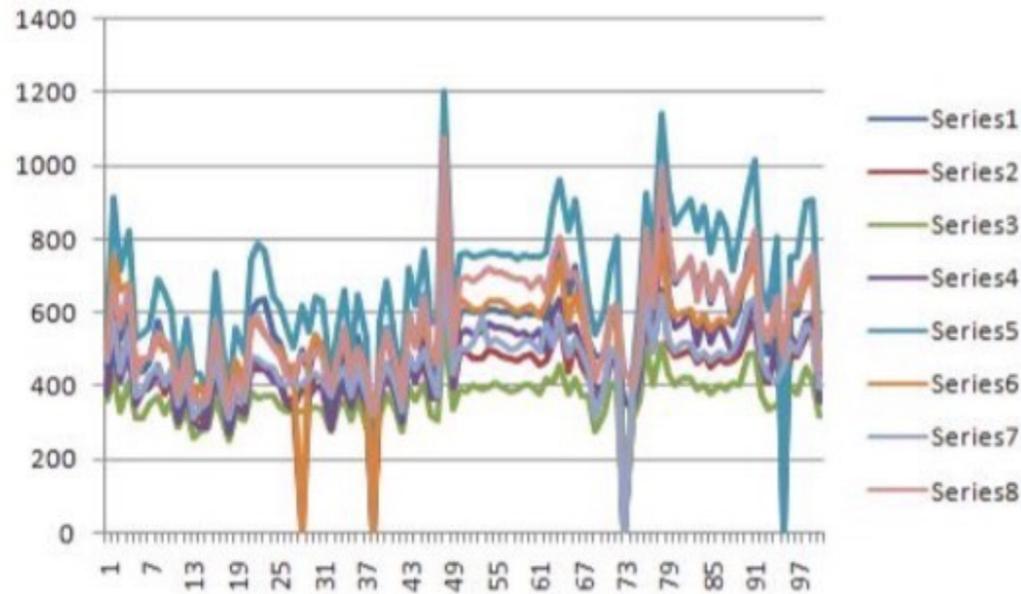
- **Vectorized RadViz, or VRV**, constructs multiple dimensions from individual dimensions by a flattening process, breaking each dimension into many



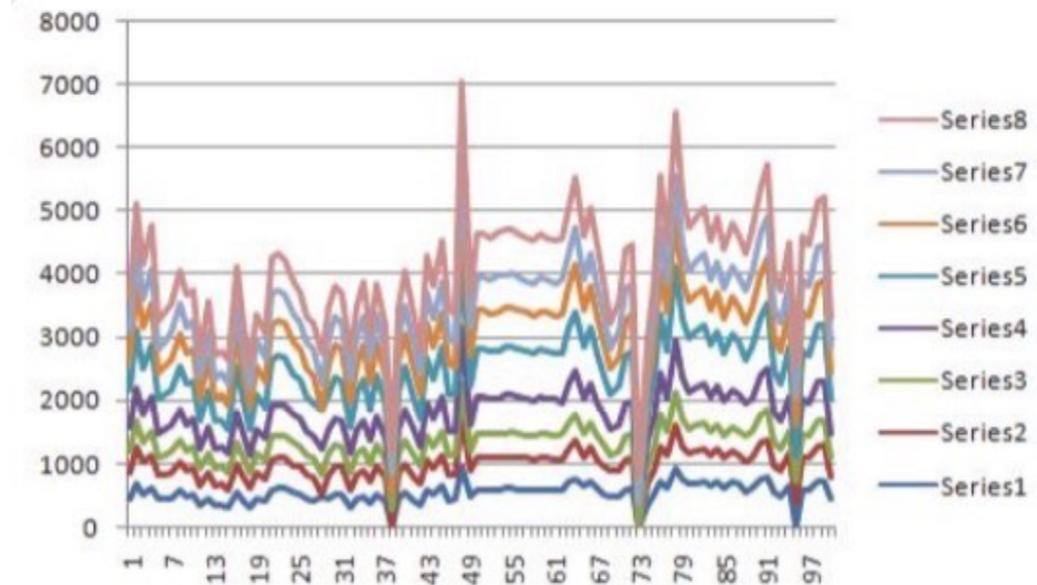
Vectorized RadViz, formed by splitting each dimension into multiple dimensions to create a binary representation for each data record. In this case, each cluster set is separated into multiple dimensions, where each dimension represents a cluster in each cluster set [372].

Line-Based Techniques

Multivariate Data: Line-Based Techniques



(a) superimposed

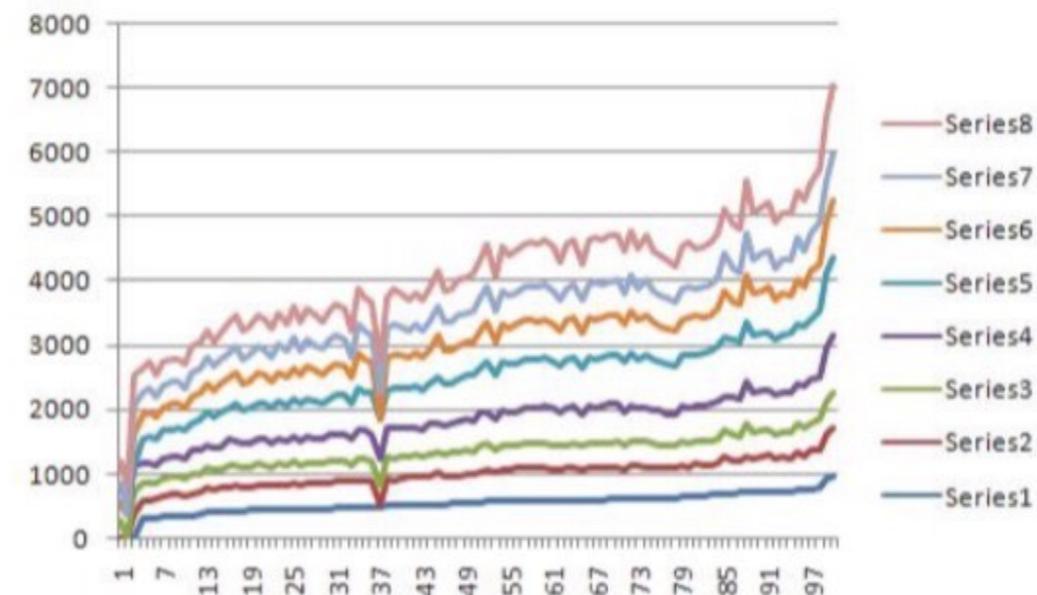


(b) stacked

Line Graphs



(c) ordered superimposed

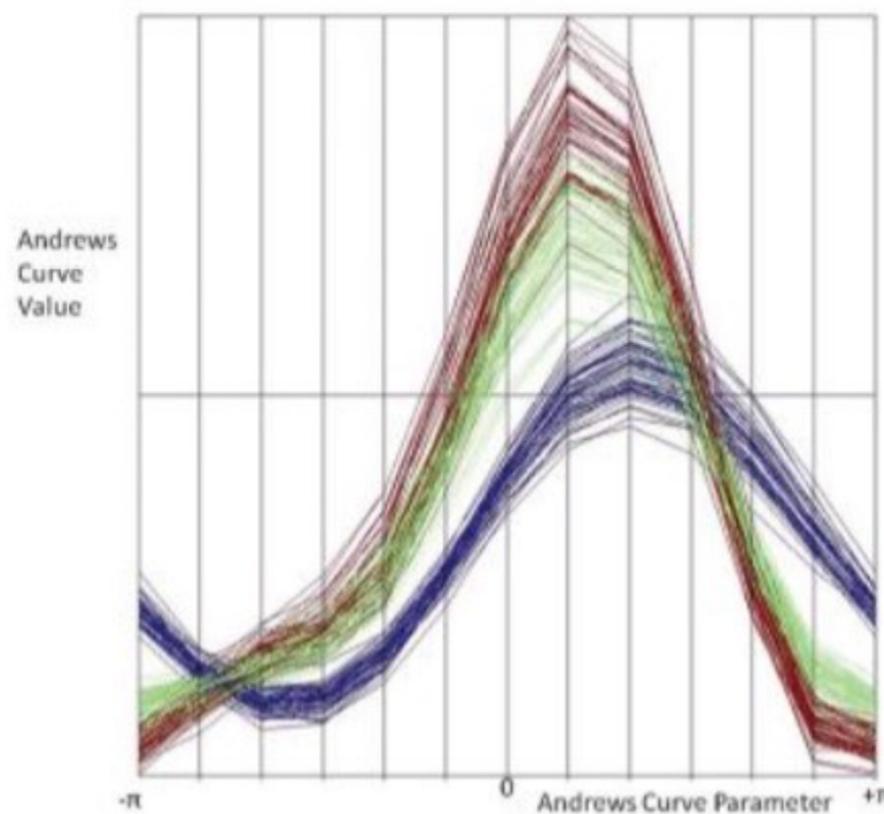


(d) ordered stacked

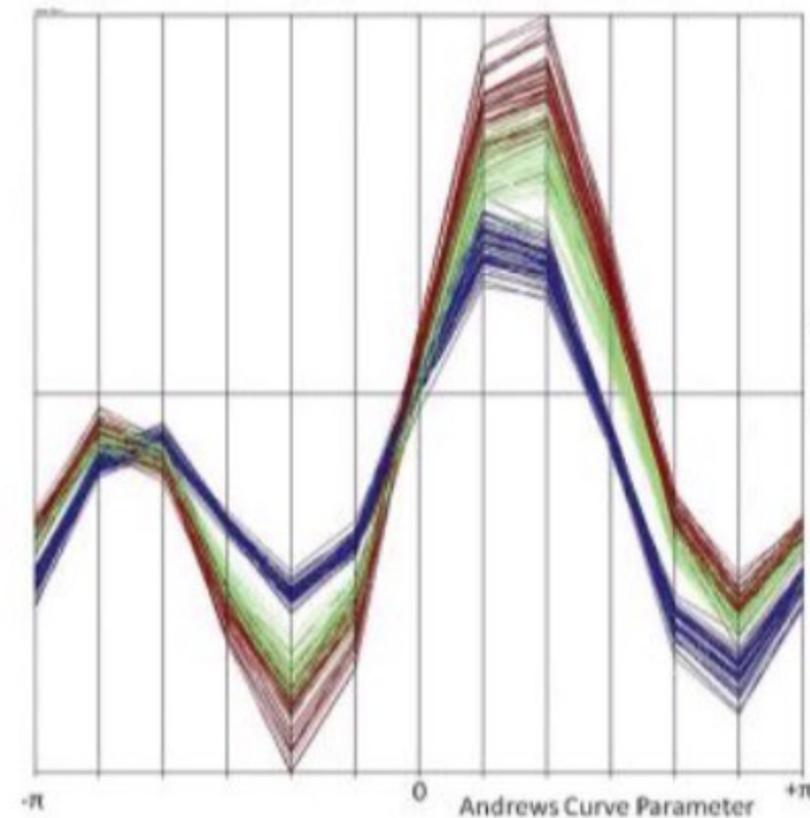
Multivariate Data: Line-Based Techniques

■ Andrews curves

$$f(t) = \frac{d_1}{\sqrt{2}} + d_2 \sin(t) + d_3 \cos(t) + d_4 \sin(2t) + d_5 \cos(2t) + \dots$$



(a)

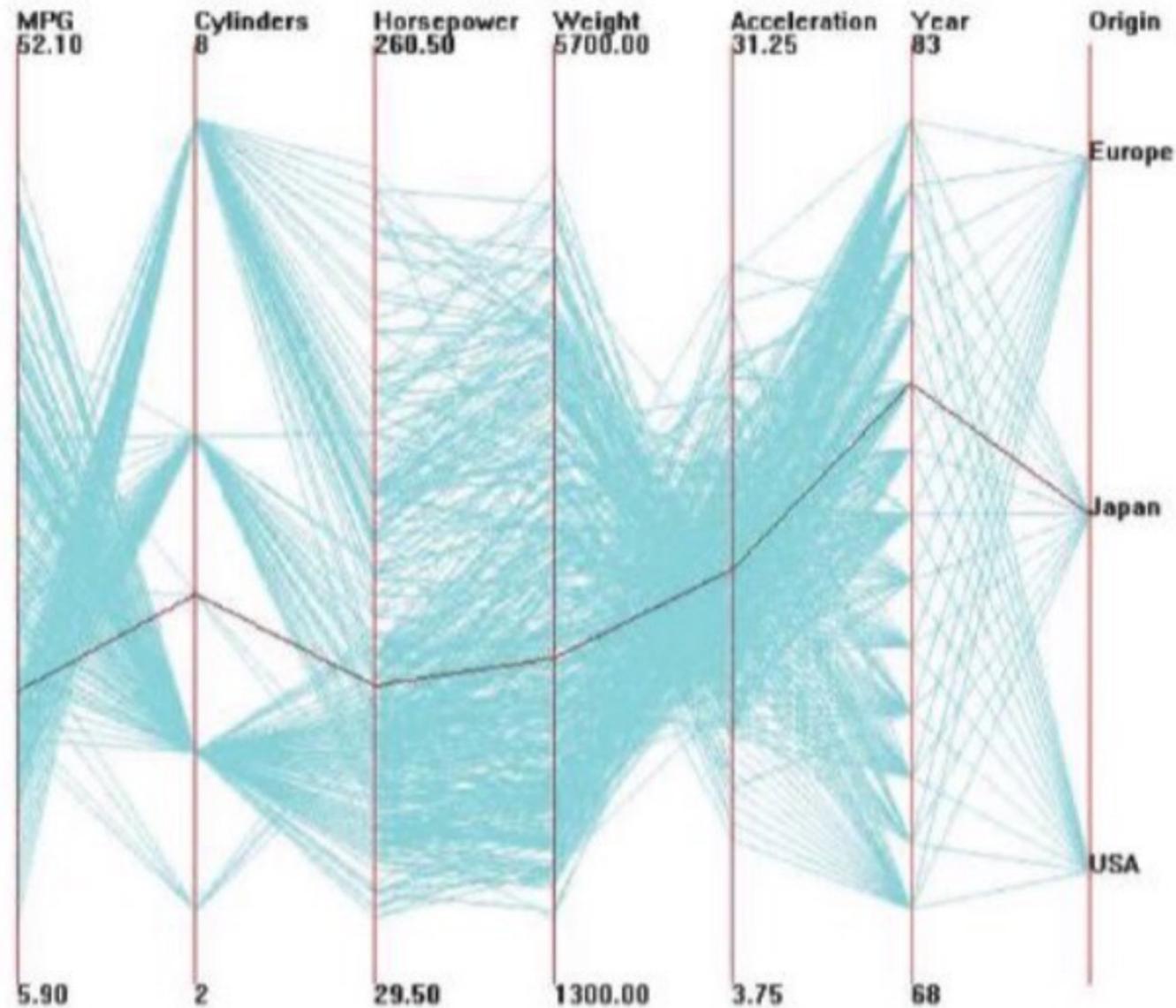


(b)

An example of Andrews curves using two different dimension orders: (a) based on the original order of the dimensions (sepal length, sepal width, petal length, petal width); (b) based on the original order of the dimensions in reverse order.

Multivariate Data: Line-Based Techniques

■ Parallel Coordinates



An example of a 7-dimensional data set visualized with parallel coordinates. A single data point is represented as the darkened polyline.

Parallel Coordinates (\parallel -coords or PCP)

■ Inselberg in 1985

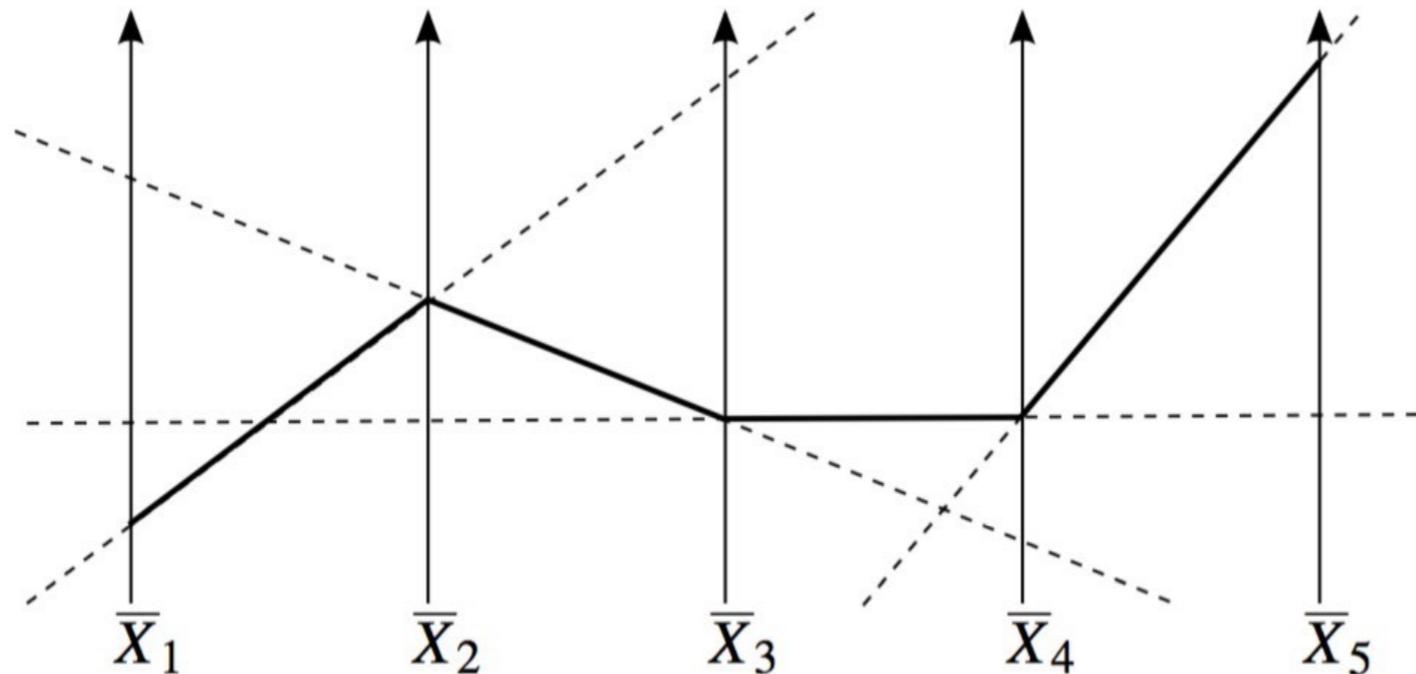


Figure 3: Constructing parallel coordinates with five dimensions represented by $N = 5$ vertical lines. Points in the plane are represented by lines joining the corresponding coordinates at the respective axes. Typically, only the line segments between the axes are drawn (represented by the bold poly-line).

State of the Art of Parallel Coordinates
J. Heinrich and D. Weiskopf

Parallel Coordinates (\parallel -coords or PCP)

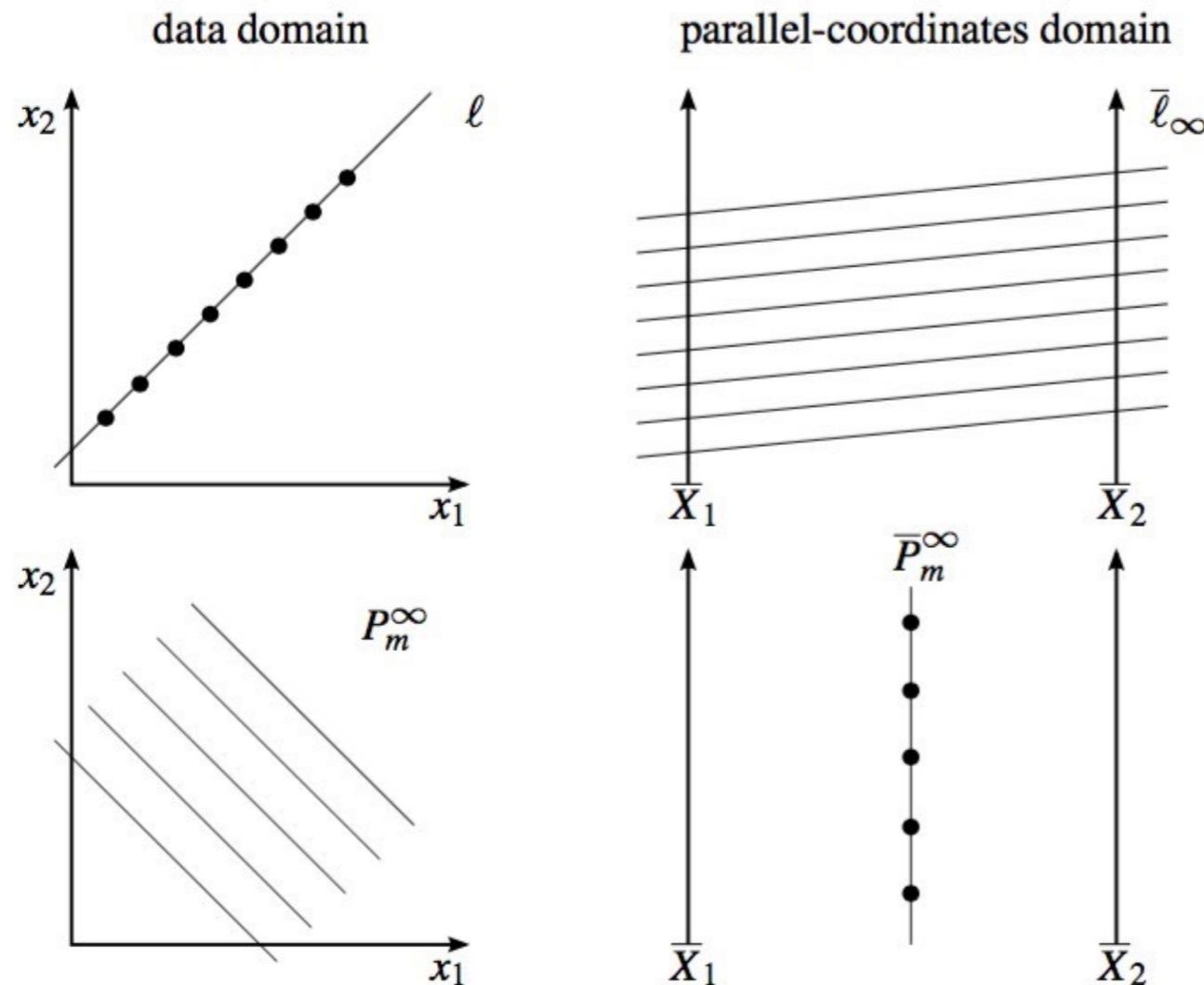


Figure 4: The line with slope $m = 1$ in the data domain is mapped to the ideal point $\bar{\ell}_\infty$ in parallel coordinates (top). The vertical line $\bar{P}_m^\infty : x = \frac{d}{1-m}$ in parallel coordinates is represented by the ideal point P_m^∞ with slope m in the data domain. Both domains are considered projective planes.

State of the Art of Parallel Coordinates
J. Heinrich and D. Weiskopf

Parallel Coordinates (\parallel -coords or PCP)

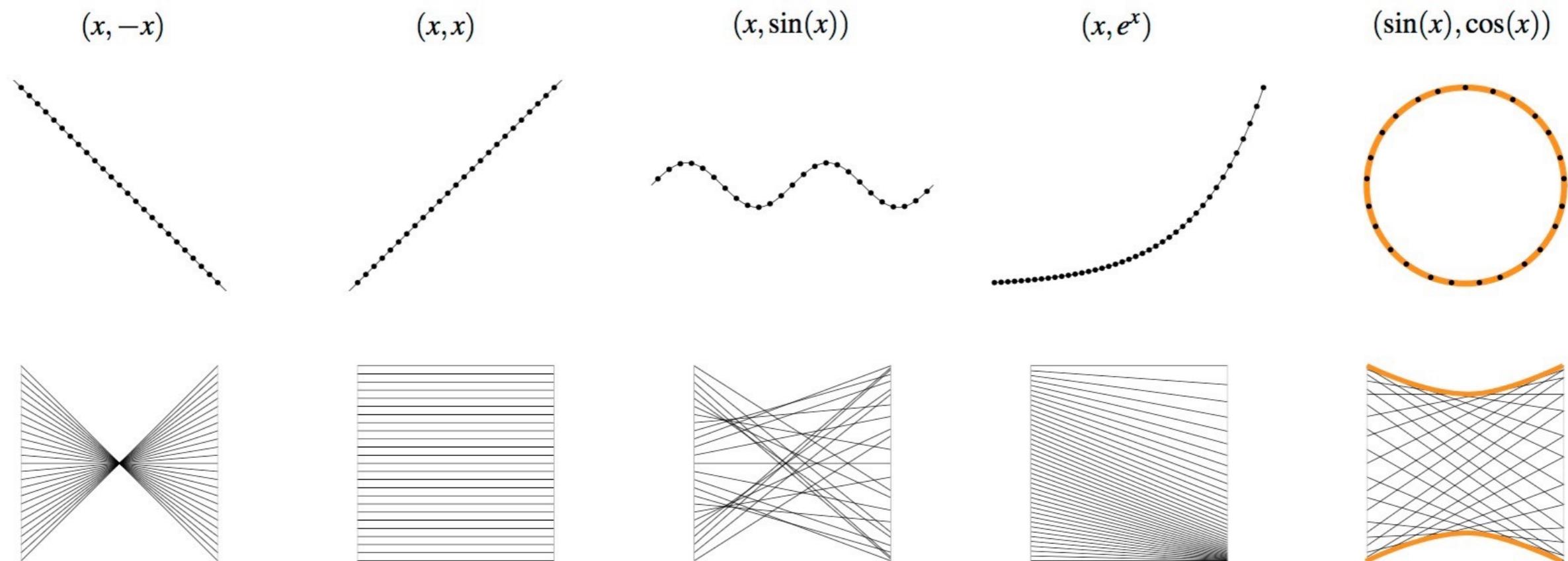


Figure 5: Common patterns in Cartesian coordinates (top) and their dual representation in parallel coordinates (bottom). The envelope of lines is highlighted for the ellipse–hyperbola duality.

State of the Art of Parallel Coordinates
J. Heinrich and D. Weiskopf

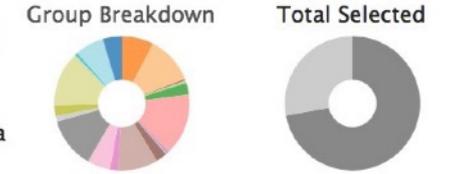
Nutrient Contents – Parallel Coordinates

An interactive visualization of the [USDA Nutrient Database](#). For information on parallel coordinates, read this tutorial.

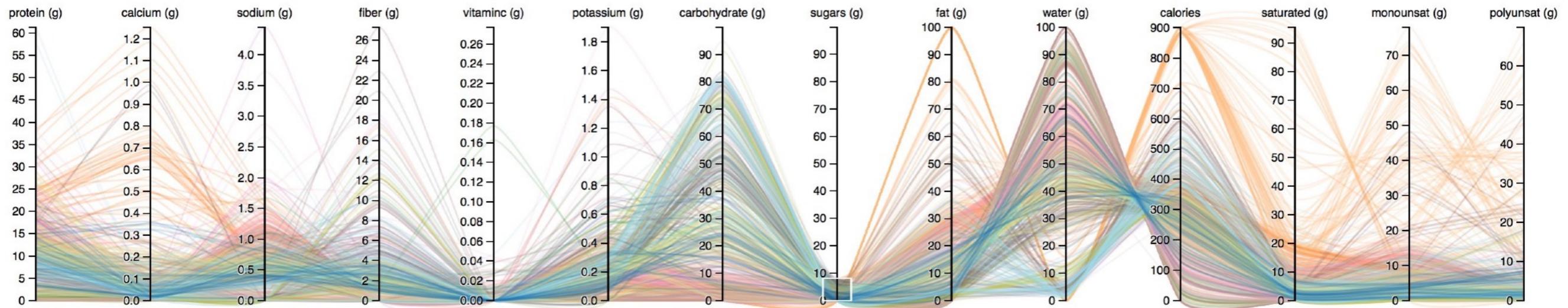
Hide Ticks Dark Shadows Opacity: 17%

Per 100g of Food

Selected 831 rows



- Dairy and Egg Products
- Fats and Oils
- Poultry Products
- Soups, Sauces, and Gravies
- Vegetables and Vegetable Products
- Sausages and Luncheon Meats
- Breakfast Cereals
- Fruits and Fruit Juices
- Nut and Seed Products
- Beverages
- Finfish and Shellfish Products
- Legumes and Legume Products
- Baked Products
- Sweets
- Cereal Grains and Pasta
- Fast Foods
- Meals, Entrees, and Sidedishes
- Snacks
- Restaurant Foods



name	group	protein (g)	calcium ...	sodium ...	fiber (g)	vitaminc...	potassiu...	carbohy...	sugars (g)	fat (g)	water (g)	calories
Butter oil, anhydrous	Dairy and Egg Products	0.28	0.004	0.002	0	0	0.005	0	0	99.48	0.24	876
Butter, salted	Dairy and Egg Products	0.85	0.024	0.714	0	0	0.024	0.06	0.06	81.11	15.87	717
Cheese fondue	Dairy and Egg Products	14.23	0.476	0.132	0	0	0.105	3.77	0	13.47	61.61	229
Cheese food, cold pack, american	Dairy and Egg Products	19.66	0.497	0.966	0	0	0.363	8.32	0	24.46	43.12	331
Cheese food, pasteurized process, swiss	Dairy and Egg Products	21.92	0.723	1.552	0	0	0.284	4.5	0	24.14	43.67	323
Cheese spread, cream cheese base	Dairy and Egg Products	7.1	0.071	0.673	0	0	0.112	3.5	3.5	28.6	58.5	295
Cheese, blue	Dairy and Egg Products	21.4	0.528	1.395	0	0	0.256	2.34	0.5	28.74	42.41	353
Cheese, brick	Dairy and Egg Products	23.24	0.674	0.56	0	0	0.136	2.79	0.51	29.68	41.11	371
Cheese, brie	Dairy and Egg Products	20.75	0.184	0.629	0	0	0.152	0.45	0.45	27.68	48.42	334

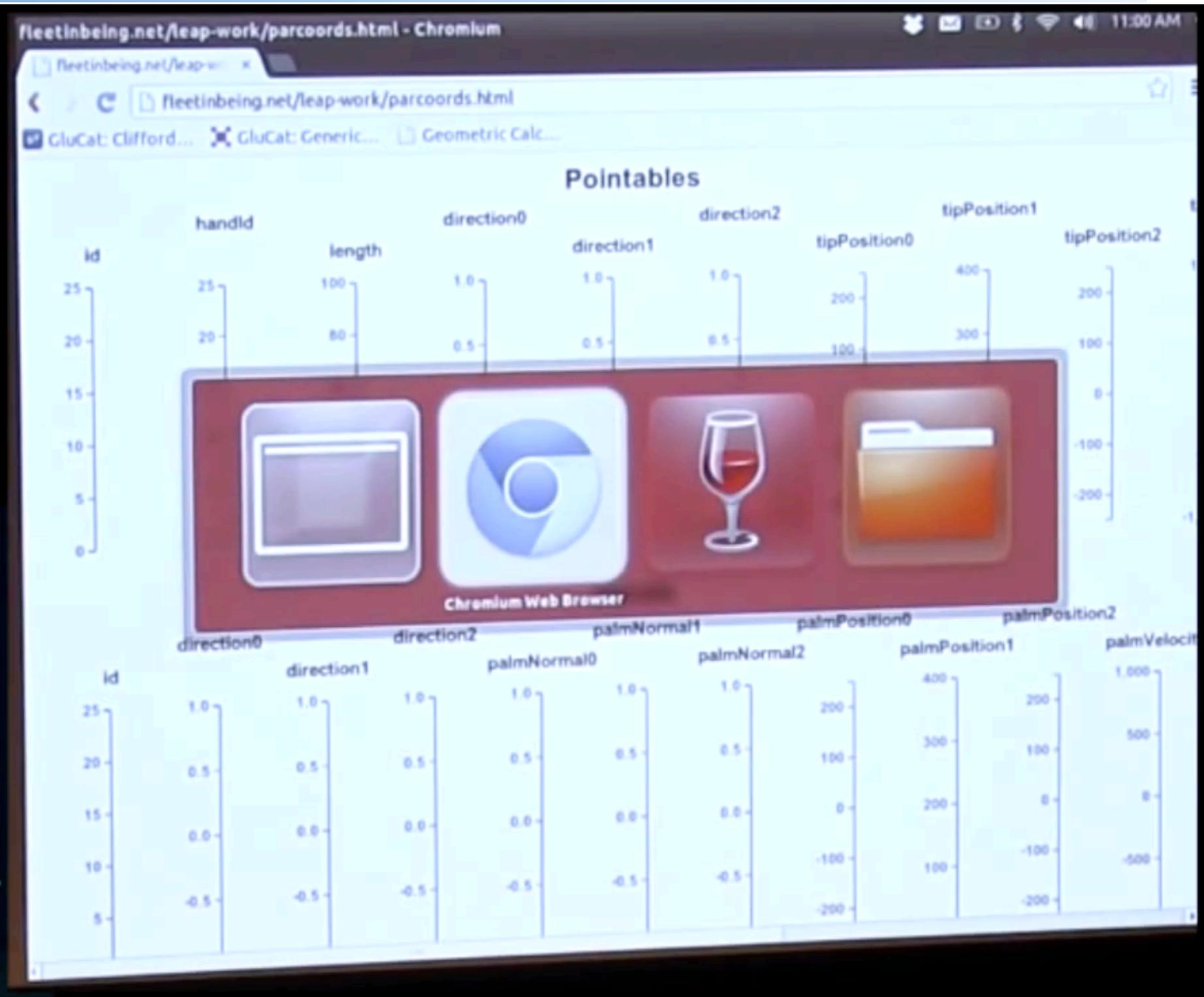
Kai Chang

Visually Exploring Multidimensional Data

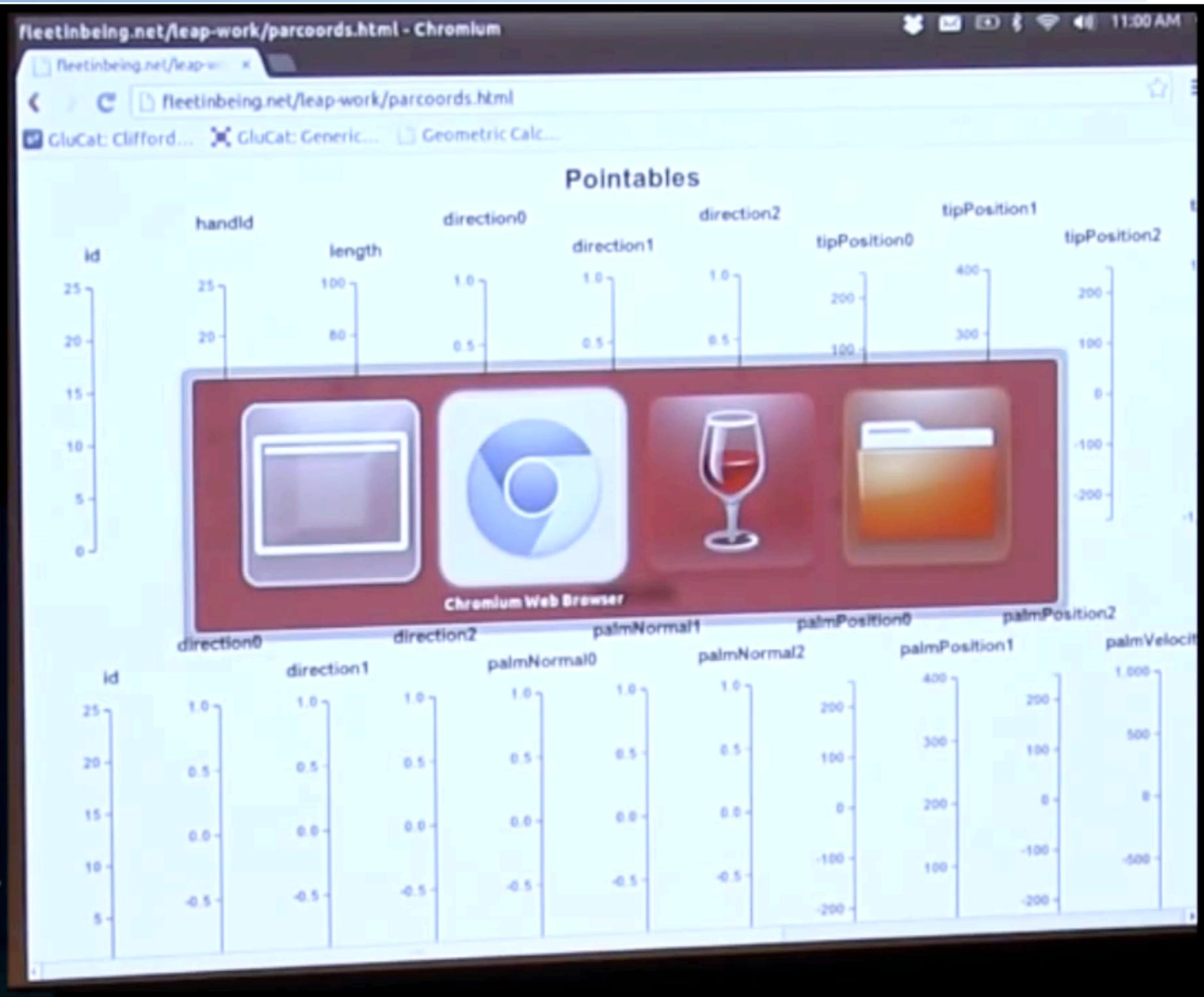
Kai Chang

Visually Exploring Multidimensional Data

Parallel Coordinates (||-coords or PCP)



Parallel Coordinates (||-coords or PCP)



Parallel Coordinates (||-coords or PCP)

having
fun



Parallel Coordinates (||-coords or PCP)

having
fun



Parallel Coordinates (\parallel -coords or PCP)



Parallel Coordinates (||-coords or PCP)



Parallel Coordinates (||-coords or PCP)

- Check <https://eagereyes.org/techniques/parallel-coordinates>
- **Check** <https://syntagmatic.github.io/parallel-coordinates/>
- See the video: <https://youtu.be/ypc7UI9LkxA>

- <http://www.xdat.org/>

- **Check** <http://www.parallelcoordinates.de/paco/#>

Parallel Coordinates (||-coords or PCP)

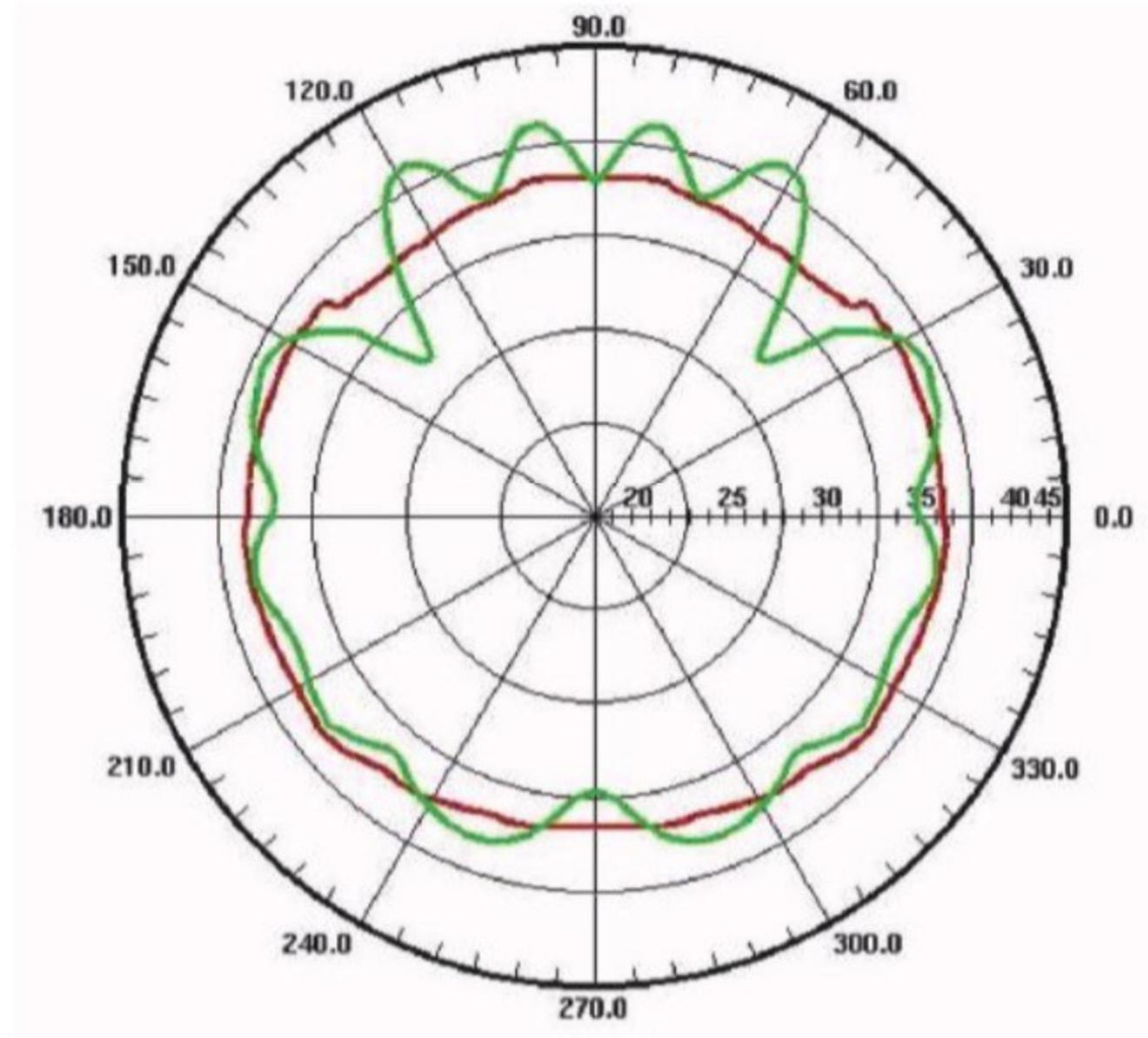
- **Very special videos !**
- **Tutorial by Alfred Inselberg at iV 2016 (at Lisbon) (FB and Twitter)**
 - **Part1**
 - **Part2**
 - **Part3**

State of the Art of Parallel Coordinates
J. Heinrich and D. Weiskopf

Multivariate Data: Line-Based Techniques

- **Radial Axis Techniques**
 - **circular line graph**;
 - **polar graphs**: point plots using polar coordinates;
 - **circular bar charts**: like circular line graphs, but plotting bars on the base line;
 - **circular area graphs**: like a line graph, but with the area under line filled in with a color or texture;
 - **circular bar graphs**: with bars that are circular arcs with a common center point and base line.

Multivariate Data: Line-Based Techniques

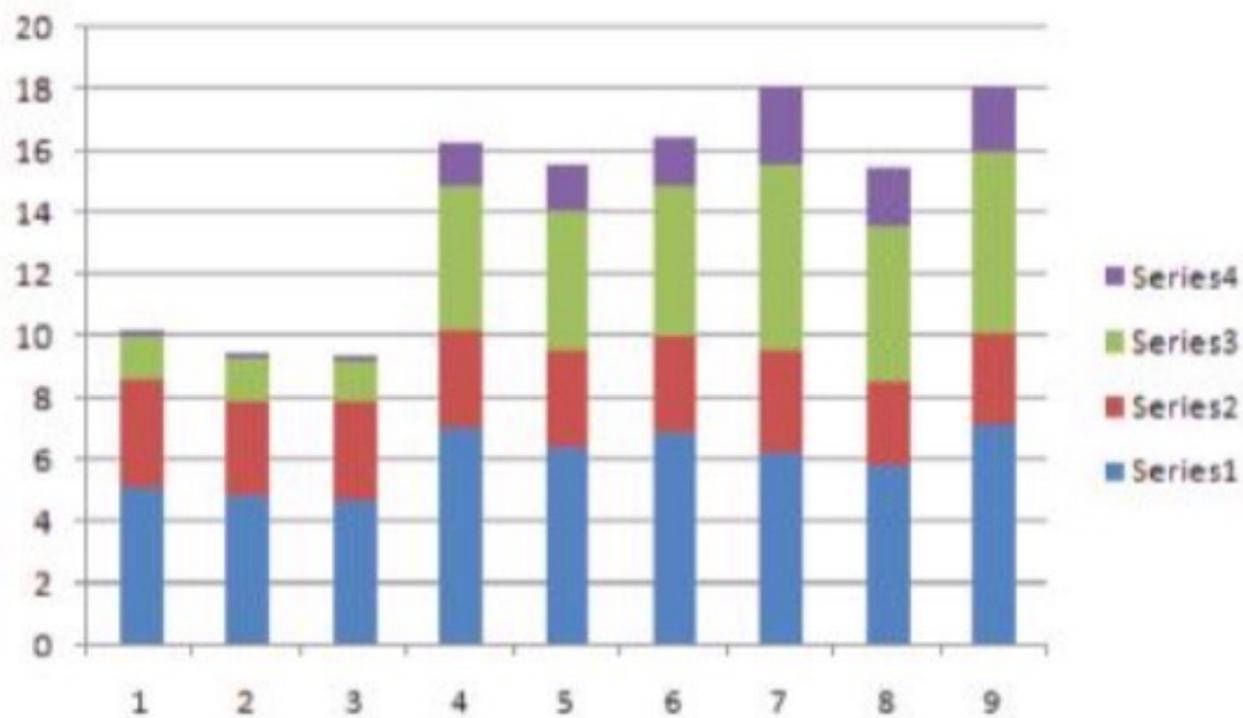


An example of a circular line graph. (Image courtesy <http://www.cemframework.com/img/PolarPlot1.png>.)

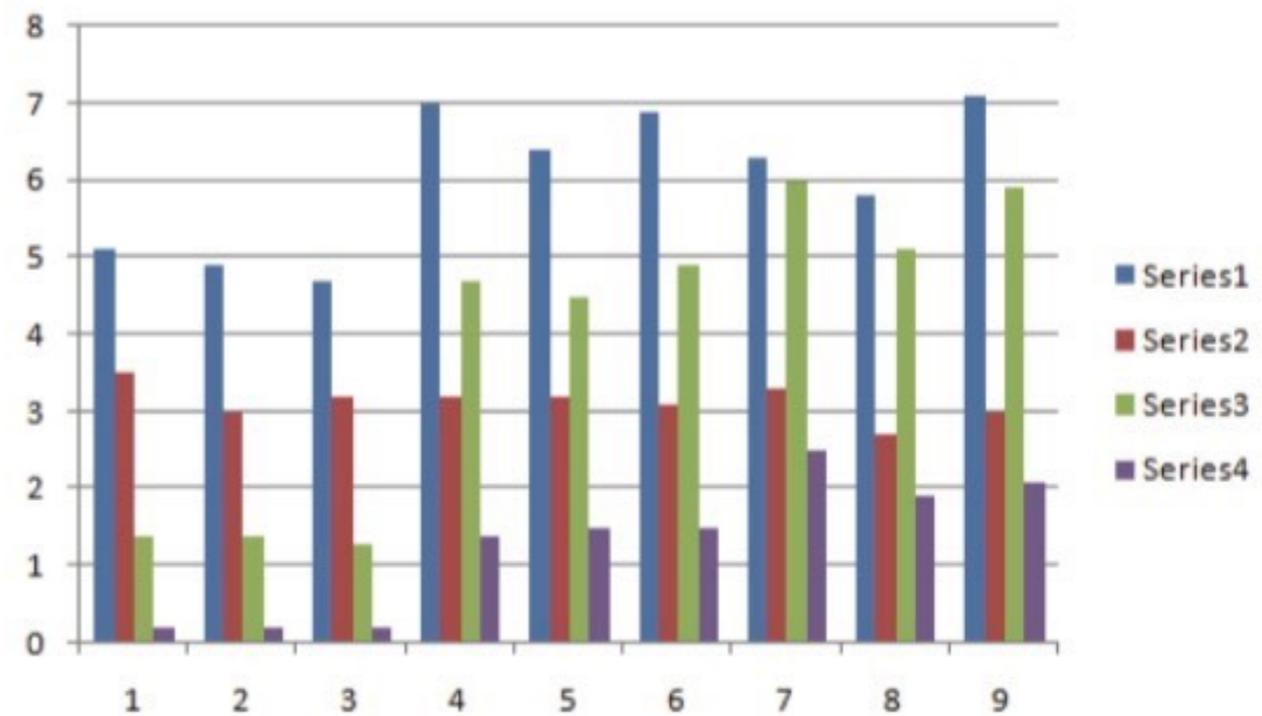
Region-Based Techniques

Multivariate Data: Region-Based Techniques

■ Bar Charts/Histograms



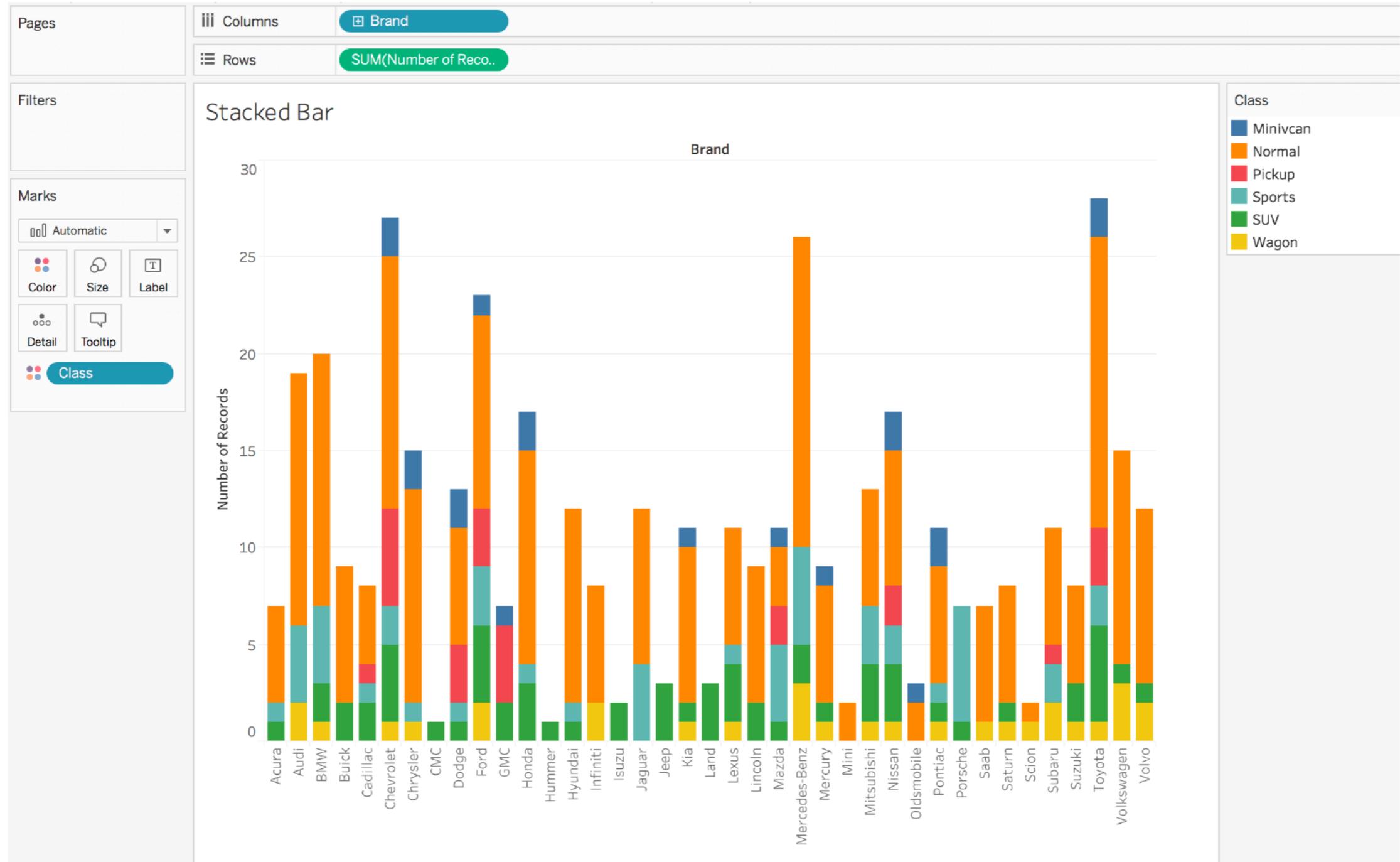
(a) Stacked bar chart.



(b) Clustered bar chart.

Multivariate Data: Region-Based Techniques

■ Bar Charts



Columns

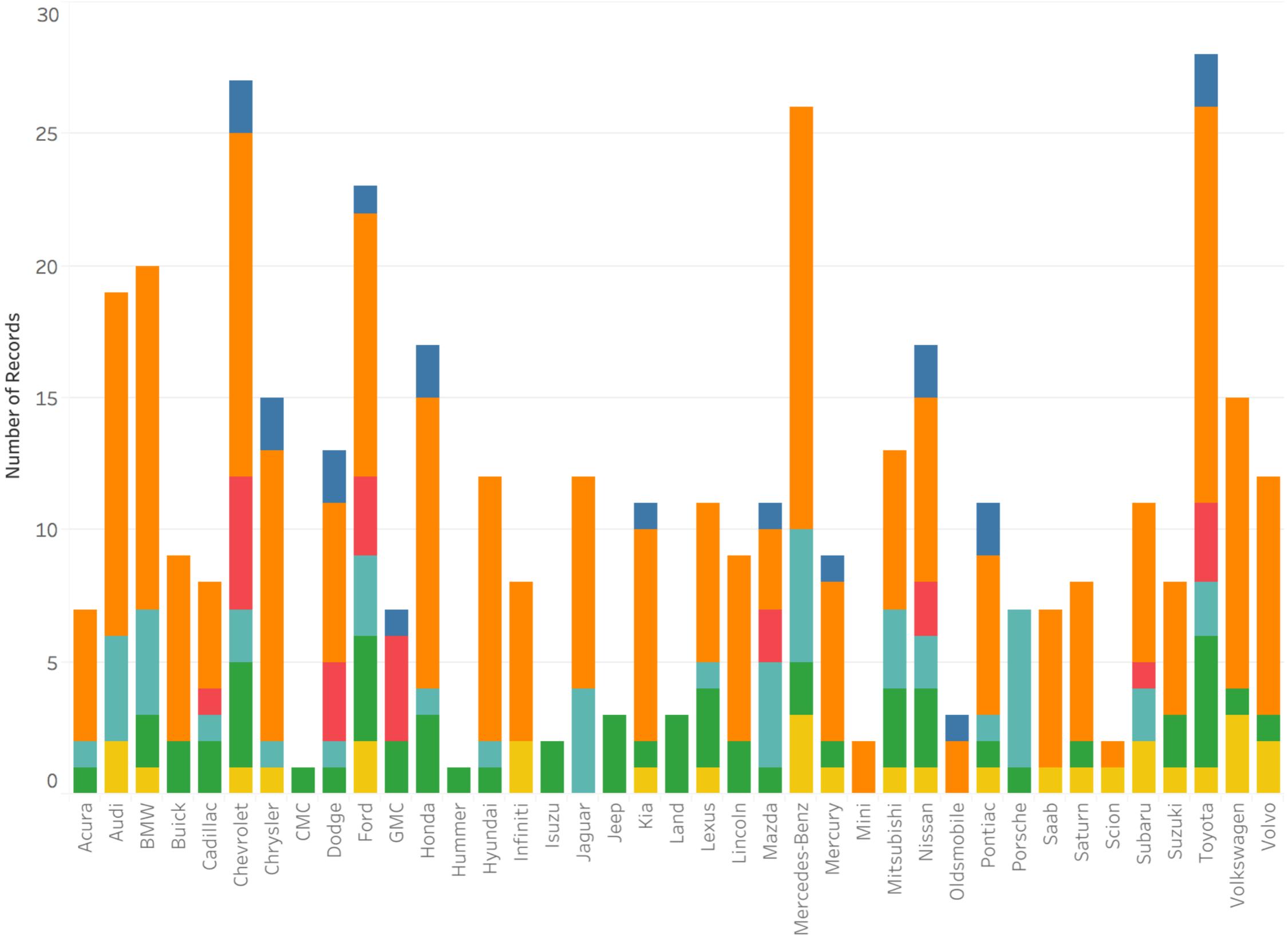
Brand

Rows

SUM(Number of Reco..

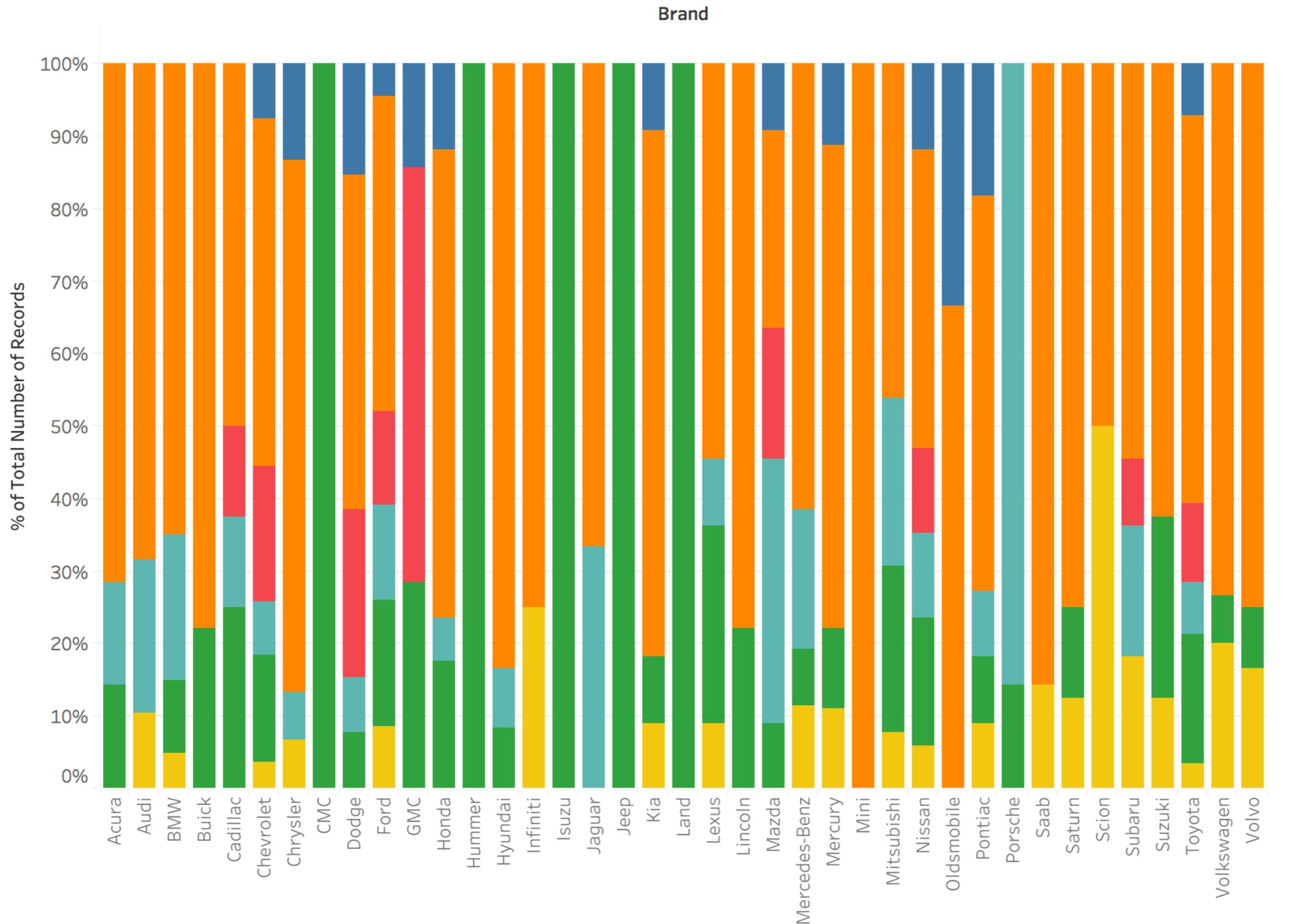
Stacked Bar

Brand



- Class
- Minivan
 - Normal
 - Pickup
 - Sports
 - SUV
 - Wagon

Stacked Bar 100%

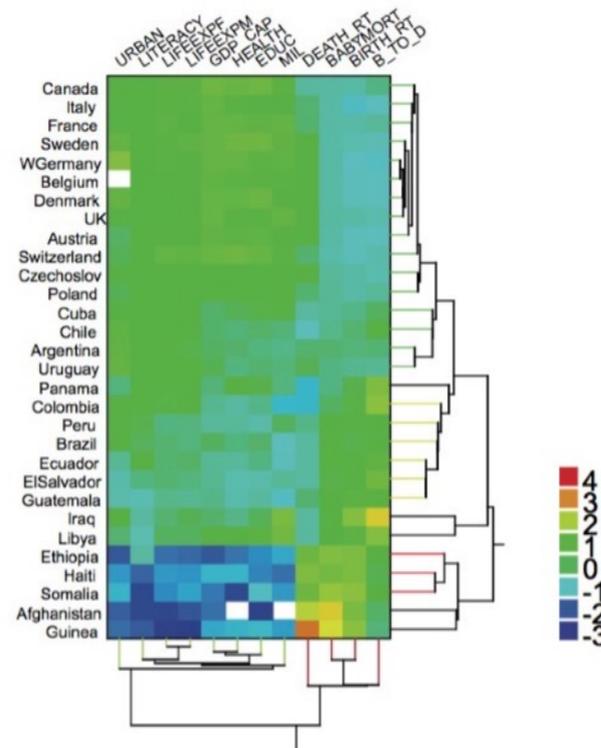


- Class**
- Minivan
 - Normal
 - Pickup
 - Sports
 - SUV
 - Wagon

Multivariate Data: Region-Based Techniques

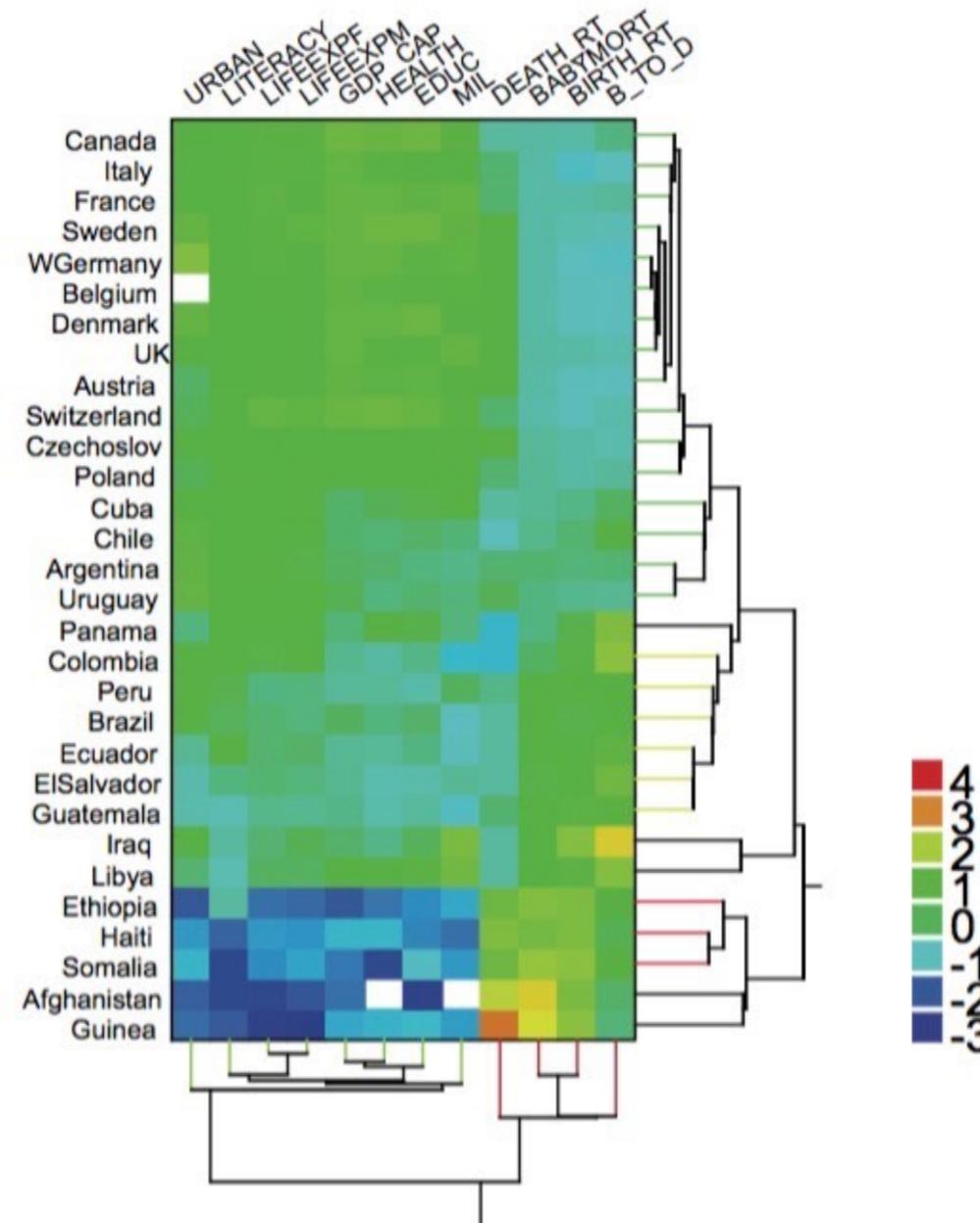
■ Tabular Displays

- ◆ **Heatmaps** are created by displaying the table of record values **using color rather than text**. All **data values are mapped to the same normalized color space**, and each is rendered as a colored square or rectangle.



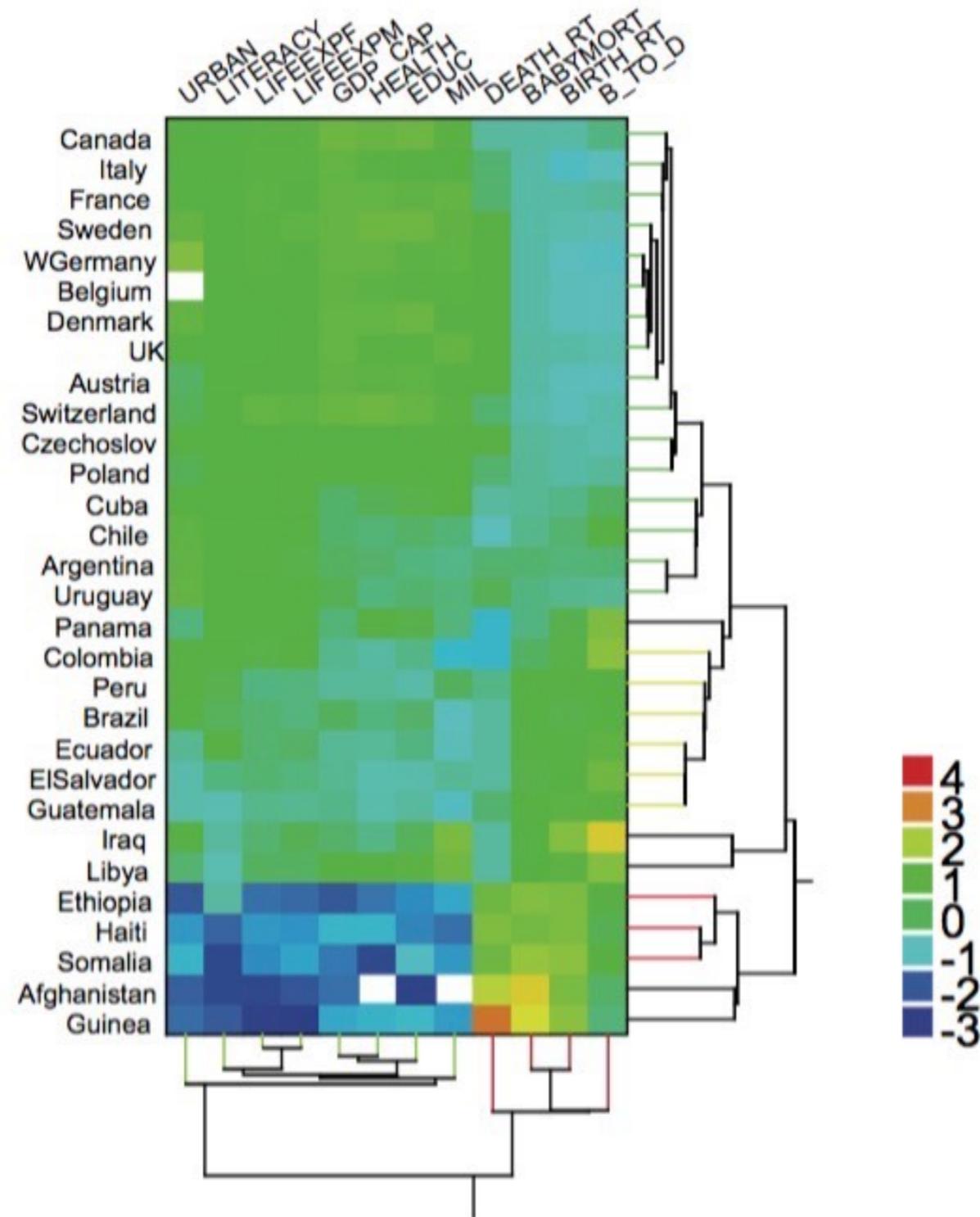
A heatmap showing social statistics for several countries from a U.N. survey. Rows and columns have been reordered via clustering. (Image courtesy Leland Wilkinson [459].)

Multivariate Data: Region-Based Techniques



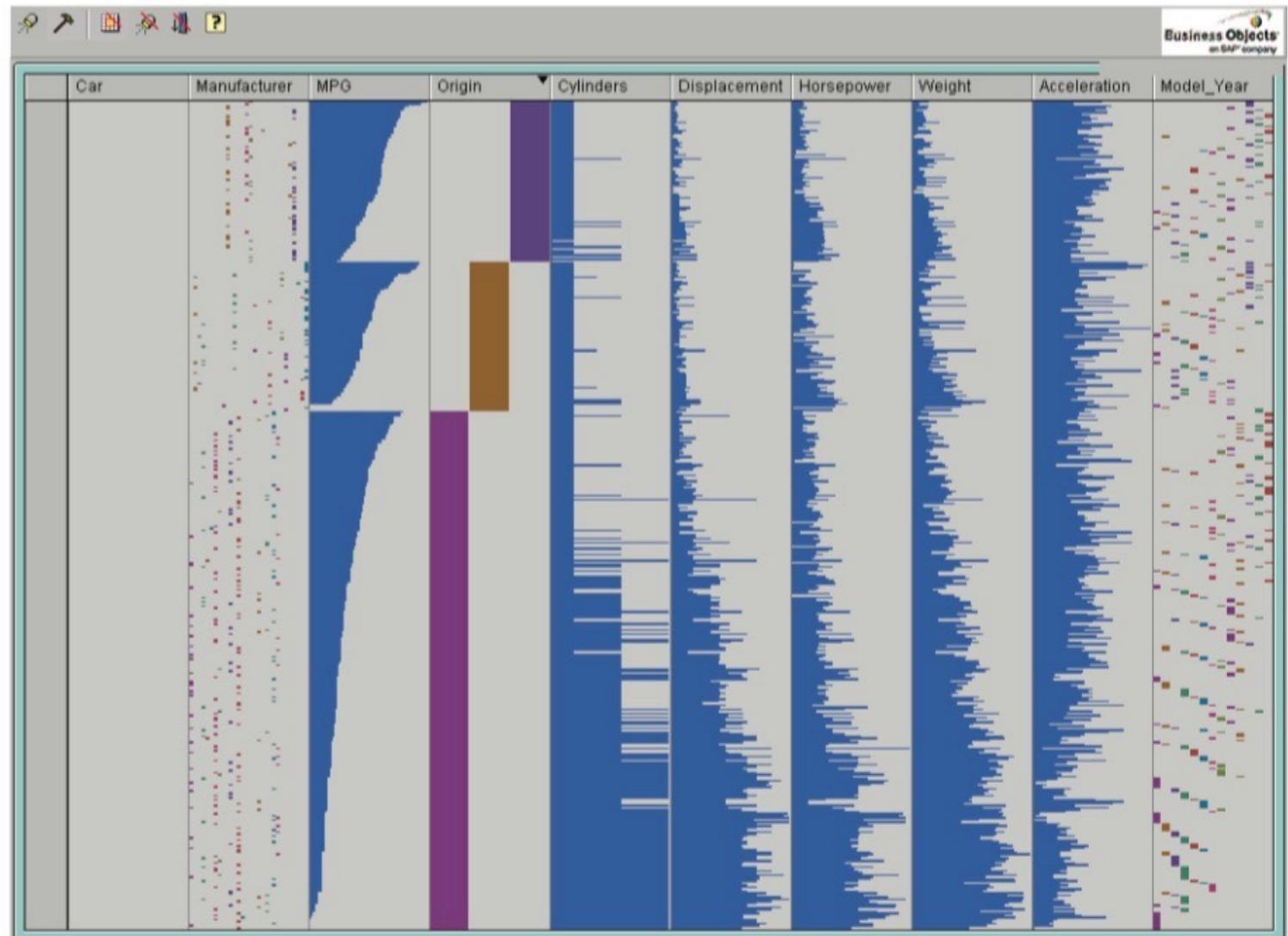
A heatmap showing social statistics for several countries from a U.N. survey. Rows and columns have been reordered via clustering. (Image courtesy Leland Wilkinson [459].)

Multivariate Data: Region-Based Techniques



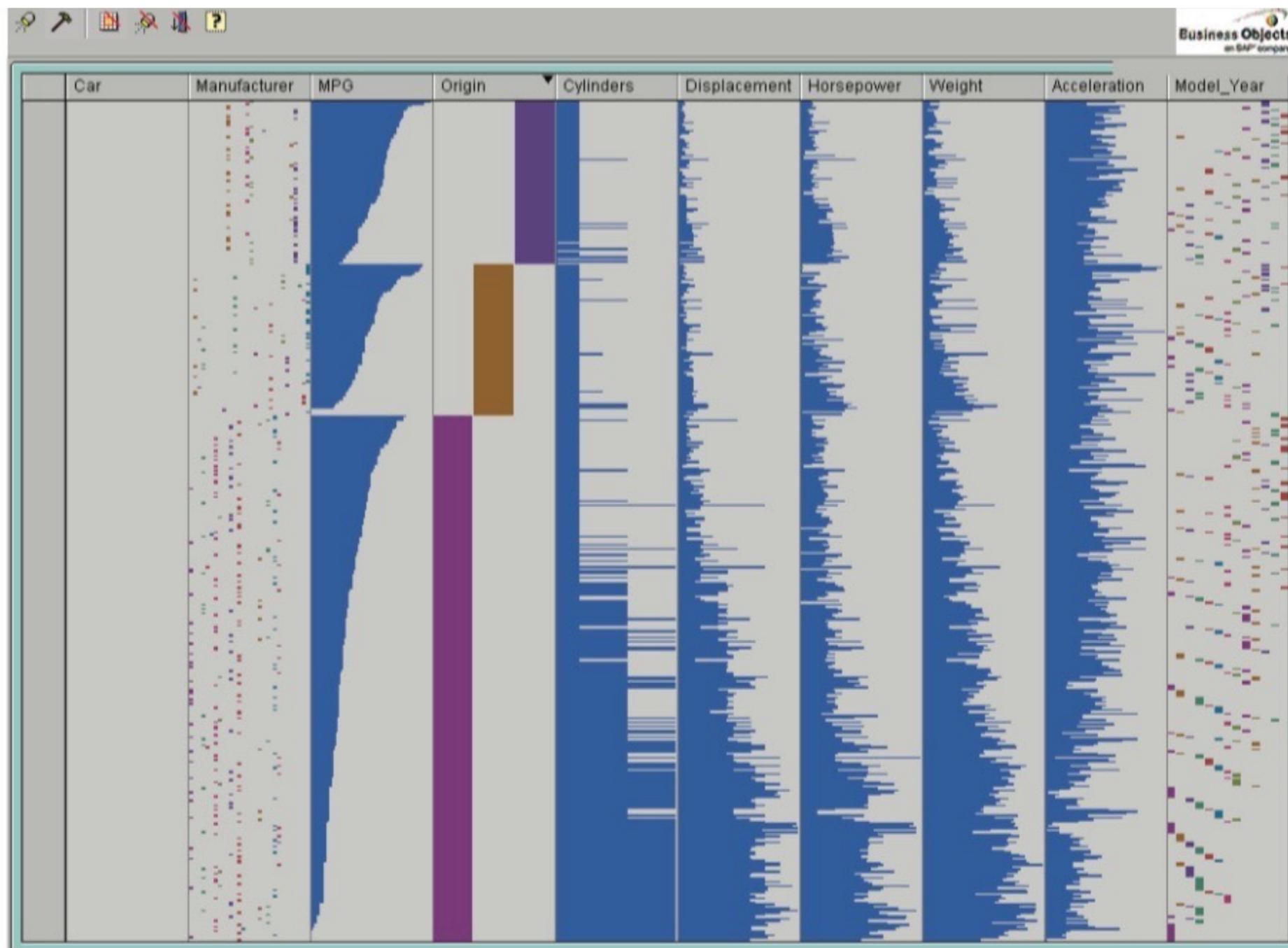
Multivariate Data: Region-Based Techniques

- **table lens** combines all these ideas and includes a **level-of-detail mechanism** for providing panning and zooming capabilities to display whole table views, while still providing some detail through local table lenses



An example of Inxight Table Lens showing the cars data set sorted first by car origin and then by MPG.

Multivariate Data: Region-Based Techniques



An example of Inxight Table Lens showing the cars data set sorted first by car origin and then by MPG.

Multivariate Data: Region-Based Techniques

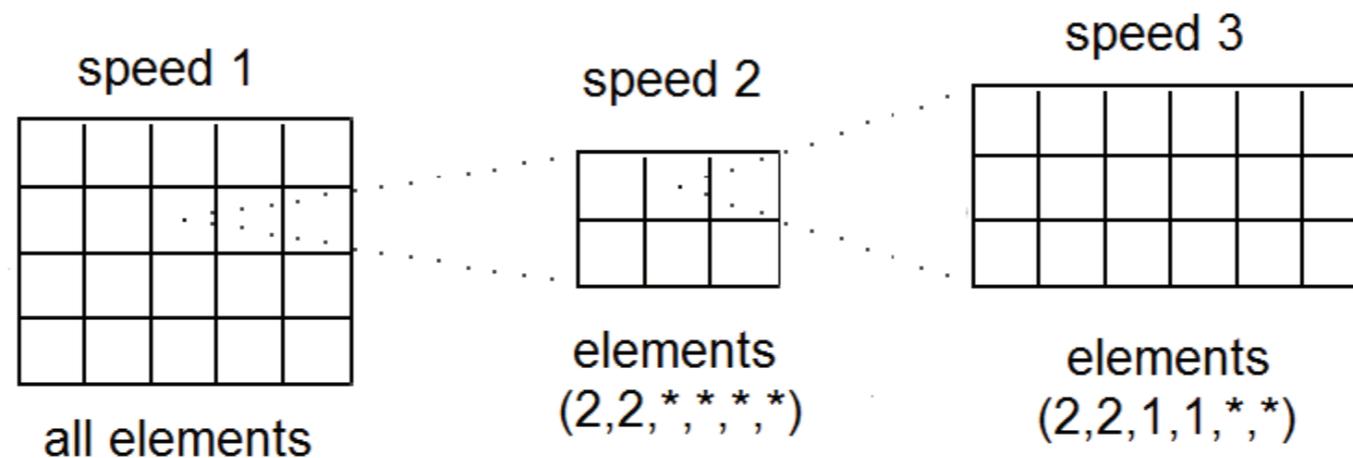
■ Dimensional Stacking

- ◆ Begin with data of dimension $2N + 1$ (for an even number of dimensions there would be an additional implicit dimension of cardinality one).
- ◆ Select a **finite cardinality/discretization** for each dimension.
- ◆ Choose **one** of the dimensions **to be the dependent variable**. The rest will be considered independent
- ◆ Create ordered pairs of the independent dimensions (**N pairs**) and assign to each pair a unique value (speed) from 1 to N.
- ◆ The pair corresponding to speed 1 will create a virtual image whose size coincides with the cardinality of the dimensions (the first dimension in the pair is oriented horizontally, the second vertically).

Multivariate Data: Region-Based Techniques

■ Dimensional Stacking

- ◆ Create ordered pairs of the independent dimensions (**N pairs**) and assign to each pair a unique value (speed) from 1 to N.
- ◆ The pair corresponding to speed 1 will create a virtual image whose size coincides with the cardinality of the dimensions (the first dimension in the pair is oriented horizontally, the second vertically).

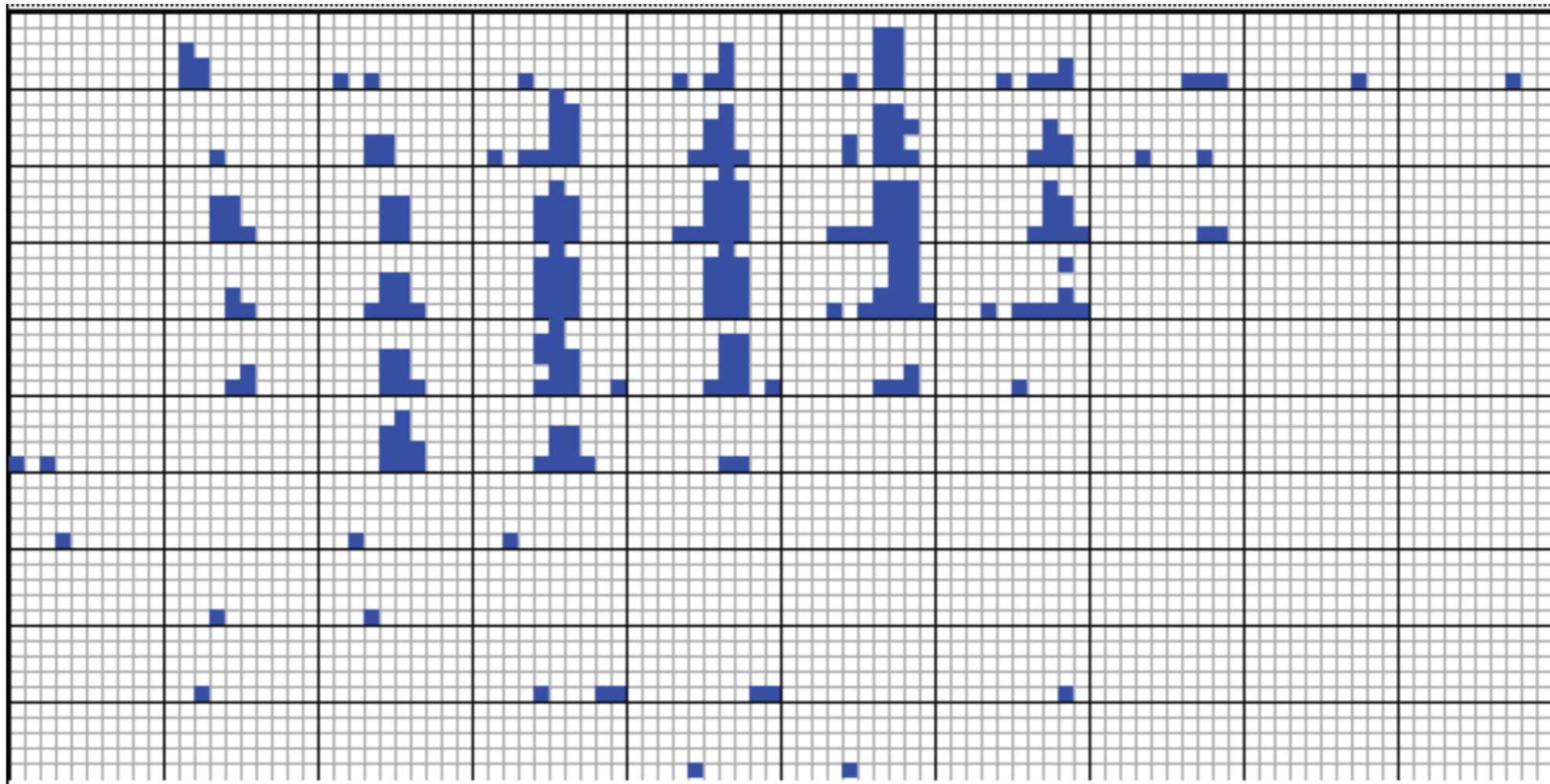


Conceptualization of dimensional stacking; collapsing six dimensions into two dimensions.

d1, . . . , d6 have cardinalities 4, 5, 2, 3, 3, and 6, respectively

Multivariate Data: Region-Based Techniques

■ Dimensional Stacking



An example of 4D data visualized using dimensional stacking. The data consists of drill-hole data, with three spatial dimensions, and the ore grade as the fourth dimension.

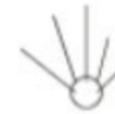
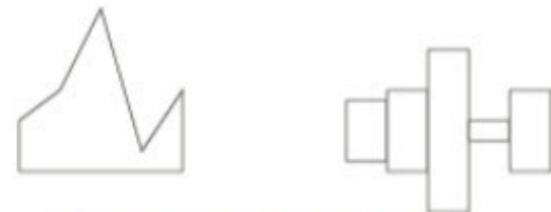
Combinations of Techniques

Multivariate Data: Combinations of Techniques

- **Glyphs and Icons**
- **Dense Pixel Displays**
- **Many others**

Multivariate Data: Combinations of Techniques

■ Glyphs and Icons



PROFILE GLYPHS

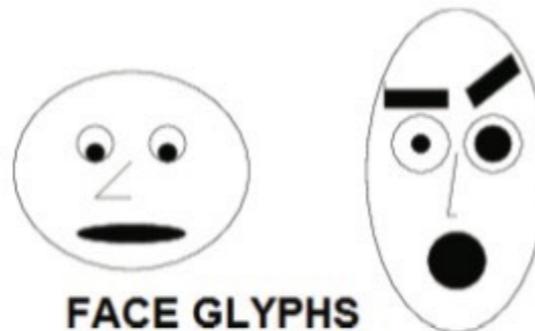
STARS AND METROGLYPHS

STICKS AND TREES

(a)

(b)

(c)



AUTOGLYPH/BOX GLYPH

FACE GLYPHS

ARROWS/WEATHERVANES

(d)

(e)

(f)

Figure 8.20. Examples of multivariate glyphs (from [445]).

Further Reading and Summary

Further Reading

- **Recommend Readings**

- ◆ Interactive Data Visualization: Foundations, Techniques, and Applications, Matthew O. Ward et al, 2015, pages 285-314.

- **Supplemental readings:**

- ◆ Visualization Analysis & Design , Tamara Munzner, Chapter 7

What you should know

■ Point based techniques

- ◆ Classical point base techniques have a limited dimensionality - Scatter based
- ◆ Dimension reduction or selection for data viz

■ Line based

- ◆ Classical line based
- ◆ Radial Axis Techniques
- ◆ Parallel coordinates techniques and related stuff

■ Region based

- ◆ Reordering the data in graphical tables

■ Combination Techniques

- ◆ Dense

- Glyphs