

CSE 564

VISUALIZATION & VISUAL ANALYTICS

VISUALIZING HIGH-DIMENSIONAL DATA:  
LINEAR METHODS

**KLAUS MUELLER**

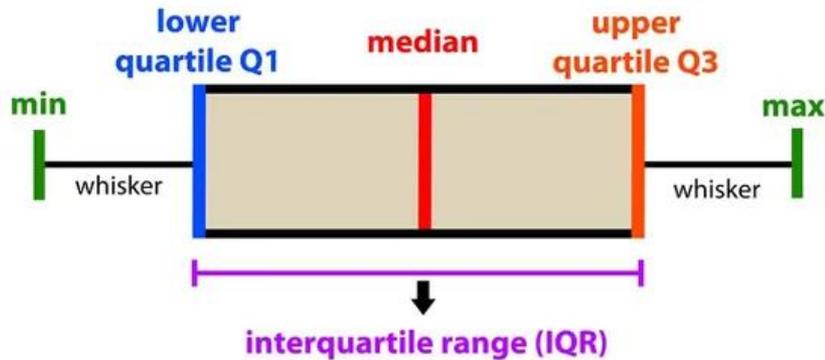
COMPUTER SCIENCE DEPARTMENT  
STONY BROOK UNIVERSITY

Lecture	Topic	Projects
1	Intro and logistics	
2	Basic visualizations and tasks, data types, examples, ethical considerations	
3	Data preparation (cleaning, imputation, data set integration)	
4	AI-assisted coding for VIS applications (design, debugging, refactoring)	Project #1 out
5	Big data and data reduction (distance/sim metrics, intro to clustering)	
6	High-D data: concept, subspaces, dimension reduction, PCA	
7	Cluster analysis: hierarchical, density, model, embedding, temporal	
8	Perception and cognition (human visual system, color, contrast)	Project #2(a) out
9	Visual design and aesthetics	
10	Visualization of multivariate and high-D data: linear methods, projections	
11	Vis. of multivariate and high-D data: non-linear methods, embeddings	
12	Visualization and AI: mutual support and capabilities (VIS4AI, AI4VIS)	Project #2(b) out
13	Principles of interaction: drive what is visualized, analyzed & how (HCI4VIS)	
14	Visual analytics (VA), human-centered AI, mixed-initiative system	
15	Midterm #1 (tentative date)	
16	VA system design and evaluation, collaborative VA, uncertainty, provenance	
17	Midterm #1 discussion (tentative date)	Final proj. proposal call out
18	Visualization of hierarchical data	
19	Visualization of maps and data with geo-reference	
20	Visualization of graphs, networks (incl. derivation of causal networks)	Final project proposal due
21	Vis. of time-varying, time-series, streaming data, progressive visualization	
22	Visualization of text, LLMs, and semantic data	
23	Ed Tufte revisited: principles, critiques and limits, responsible visualization	
24	Design of effective infographics	Final proj. prelim report due
25	Foundations scientific and medical visualization, intro to volume rendering	
26	Scientific visualization	Bonus project out (Vol Ren)
27	Story telling with data, data journalism	
28	Midterm #2 (tentative date)	
Final	Final project demo on zoom (public)	All final proj. materials due

# VISUALIZING DISTRIBUTIONS

# BOX PLOTS

You may have heard about box plots

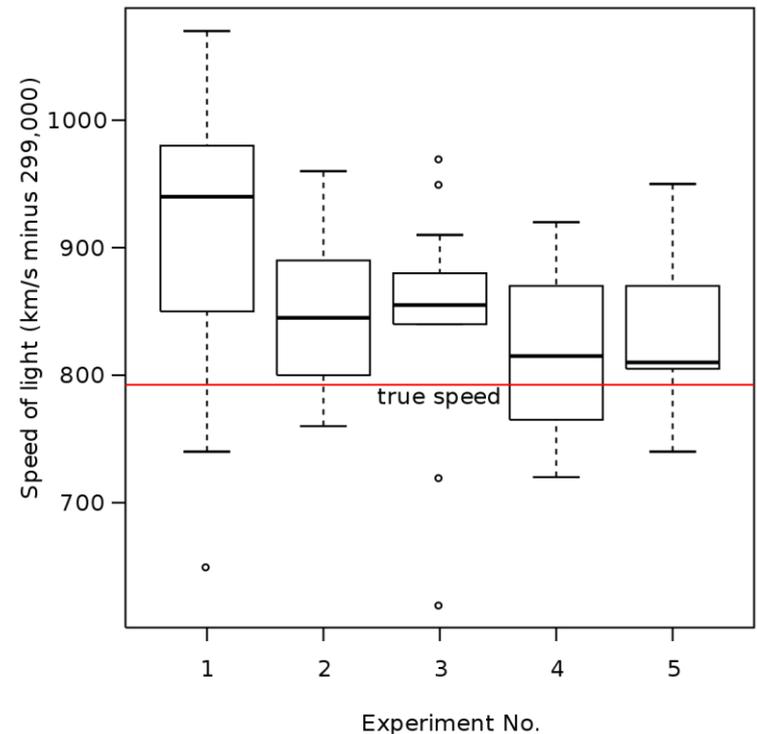


Tend to be bewildering to many

- hard to interpret

They can also give the wrong representation of data

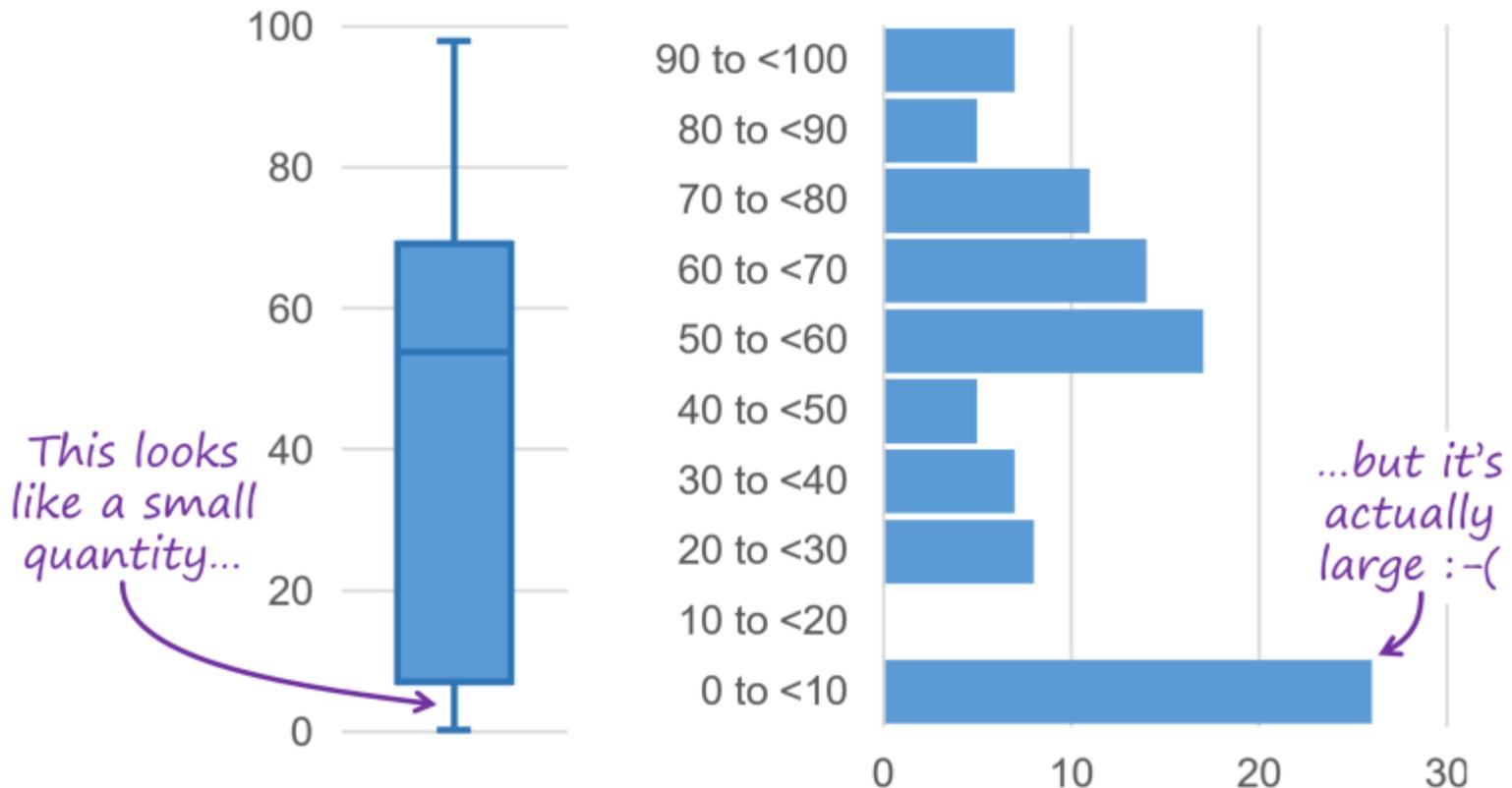
- assume normal distributed data



# BOX PLOTS

Non-normal distributed data give “wrong” box plots

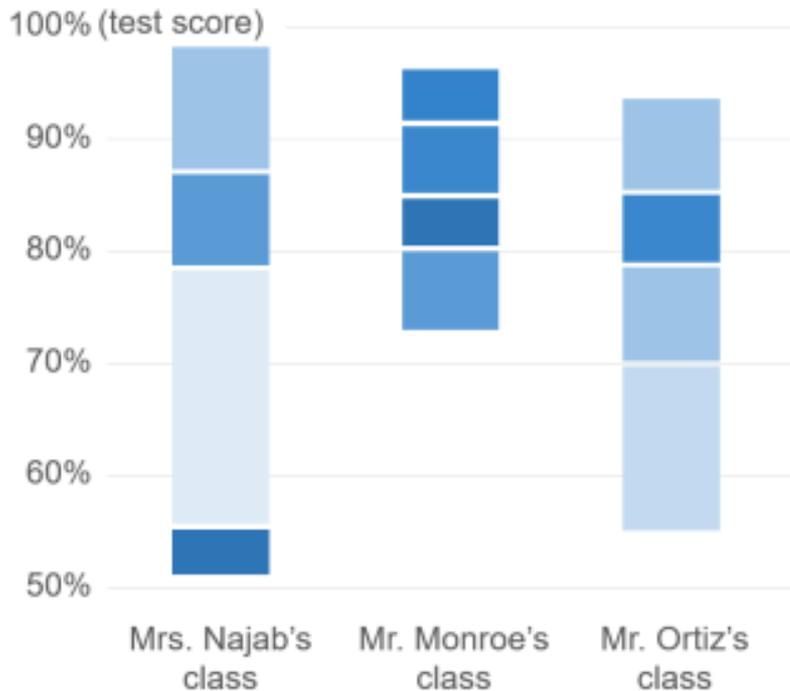
- shown here: data on student test scores



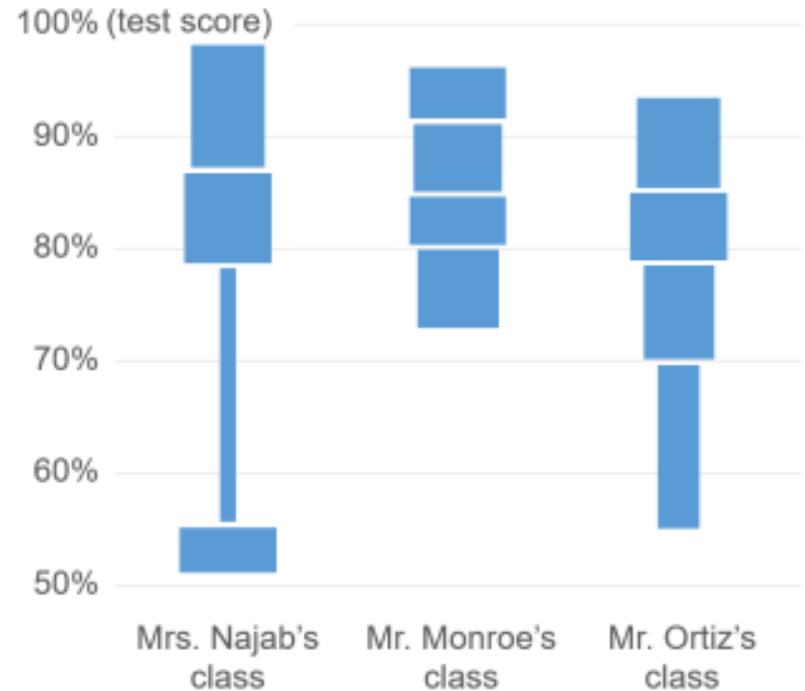
# DENSITY PLOTS

Same data than last side, multiple classes

Student Test Scores by Class

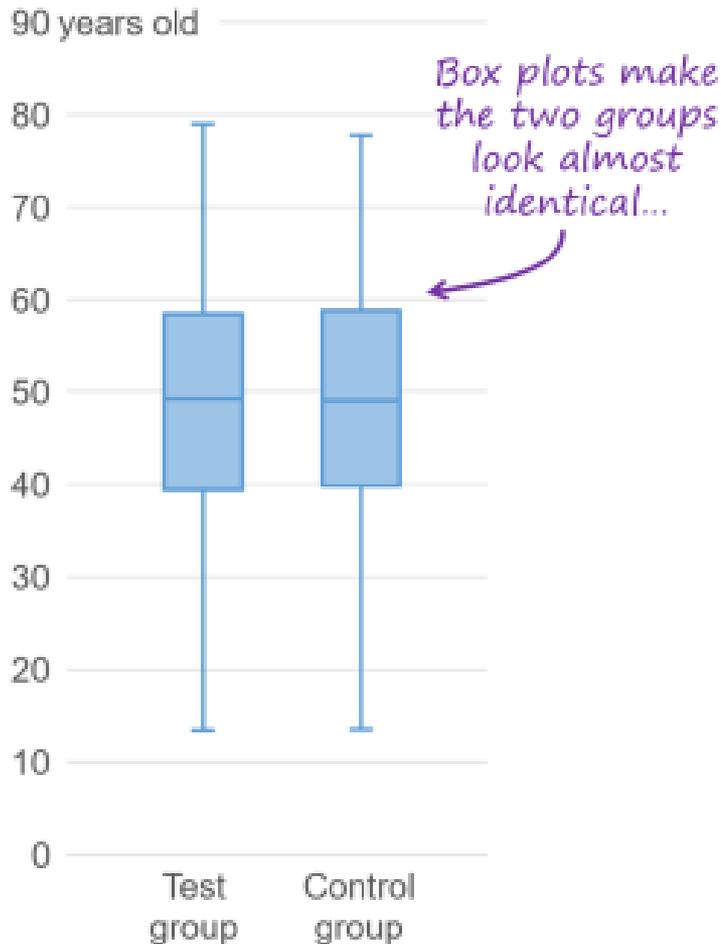


Student Test Scores by Class

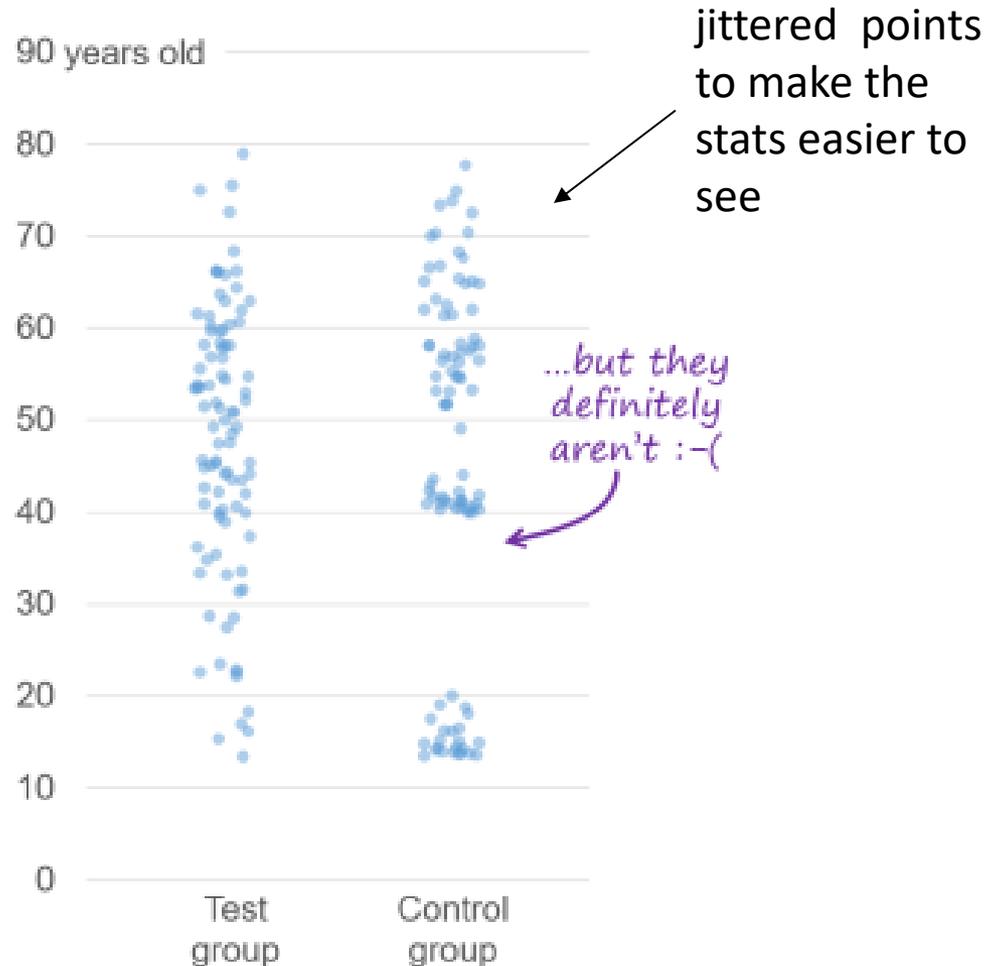


# STRIP PLOTS

Study Participants by Age

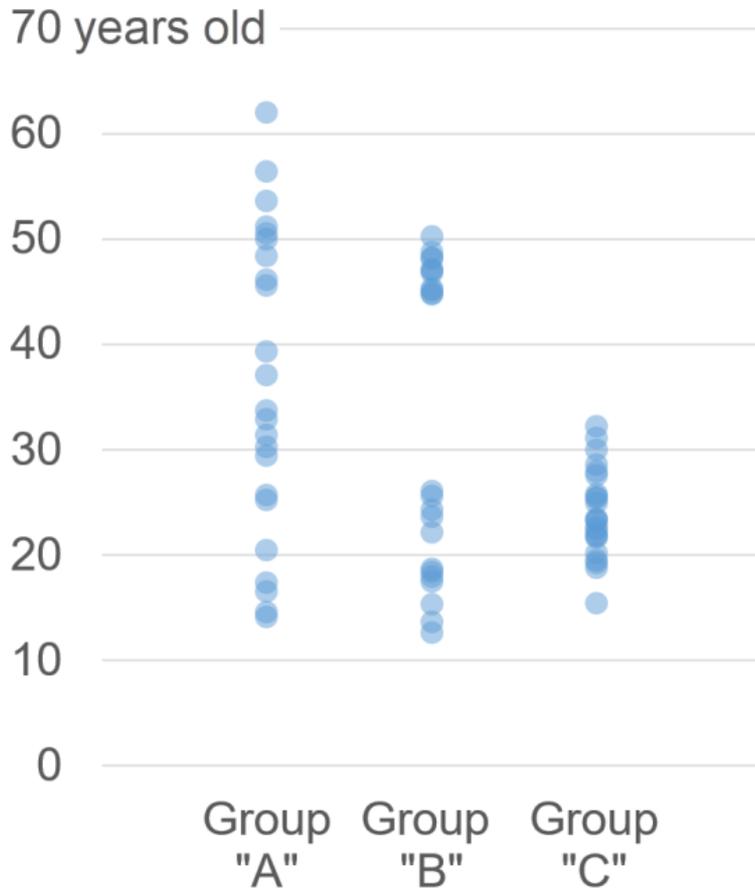


Study Participants by Age

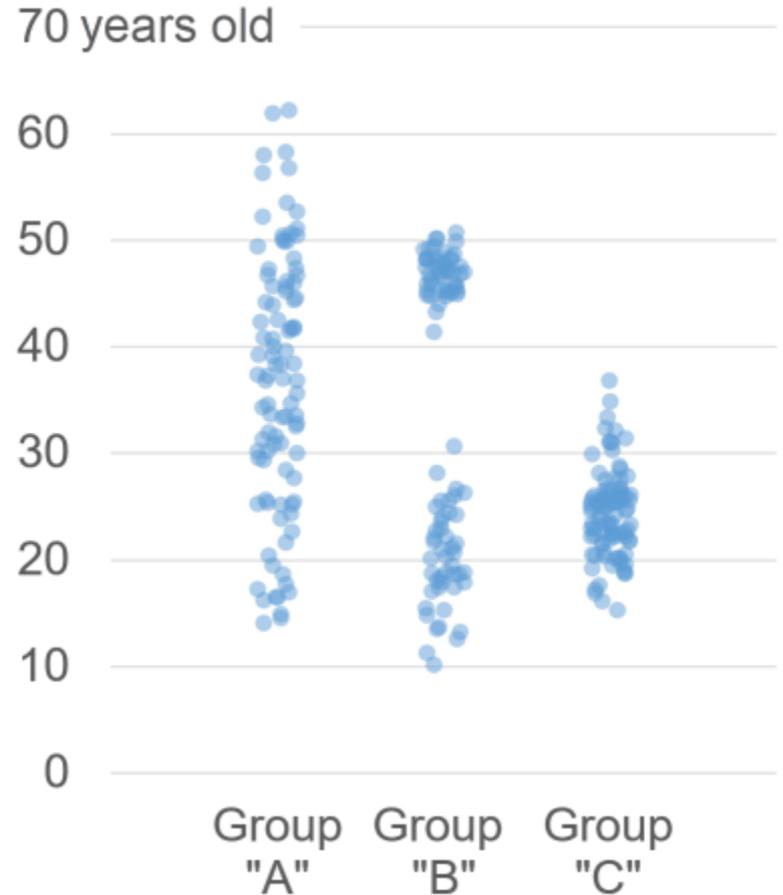


# SEMITRANSSPARENT VS. JITTERING

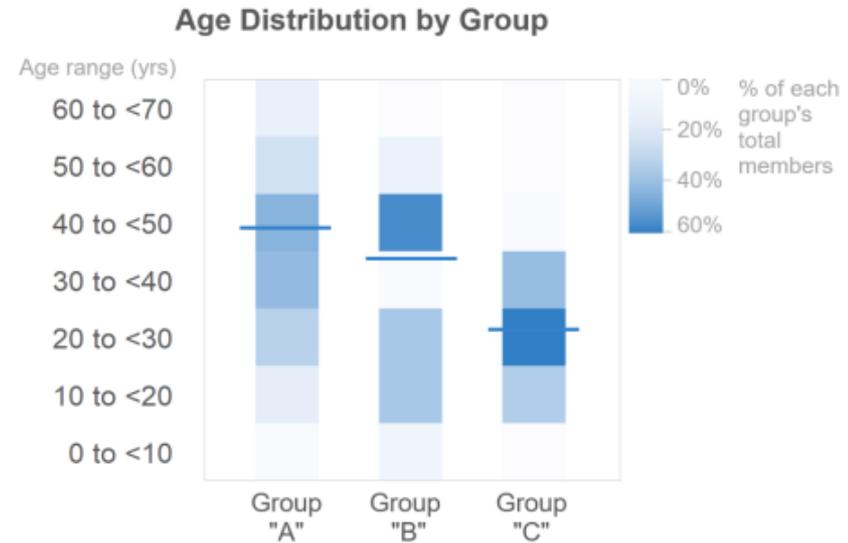
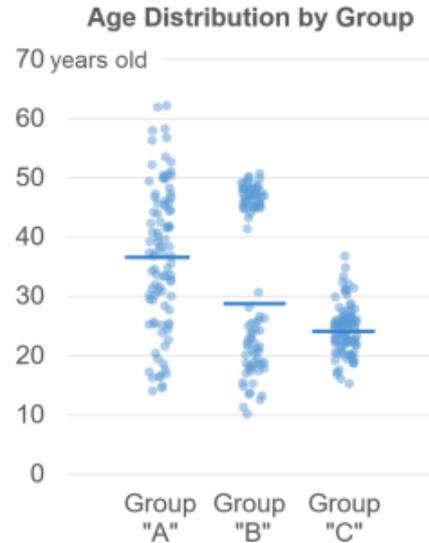
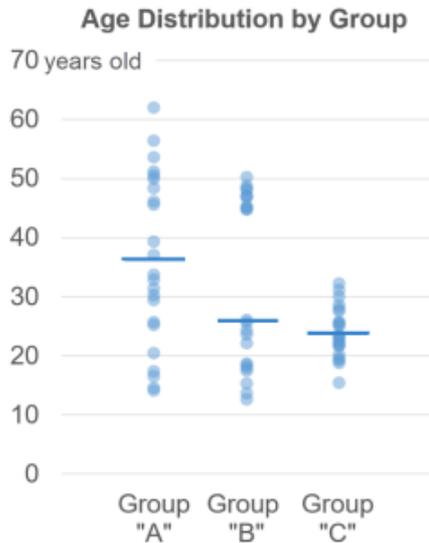
## Age Distribution by Group



## Age Distribution by Group



# COMPARISON

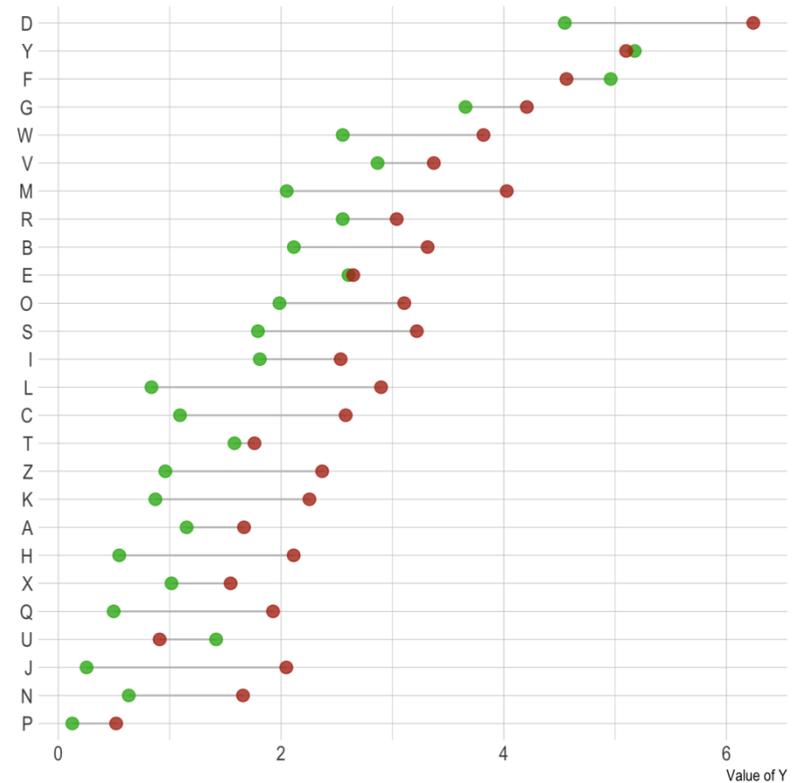
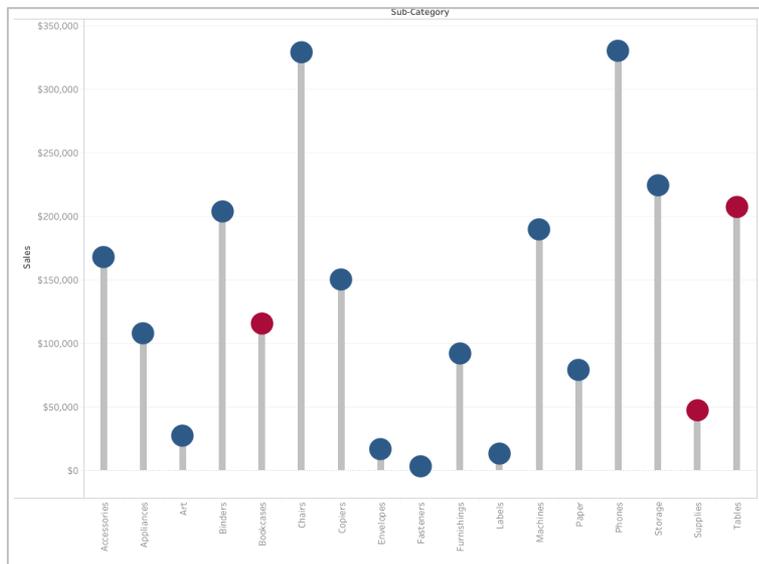


With median lines

Read more here:

<https://nightingaledvs.com/ive-stopped-using-box-plots-should-you/>

# LOLLIPOP CHARTS

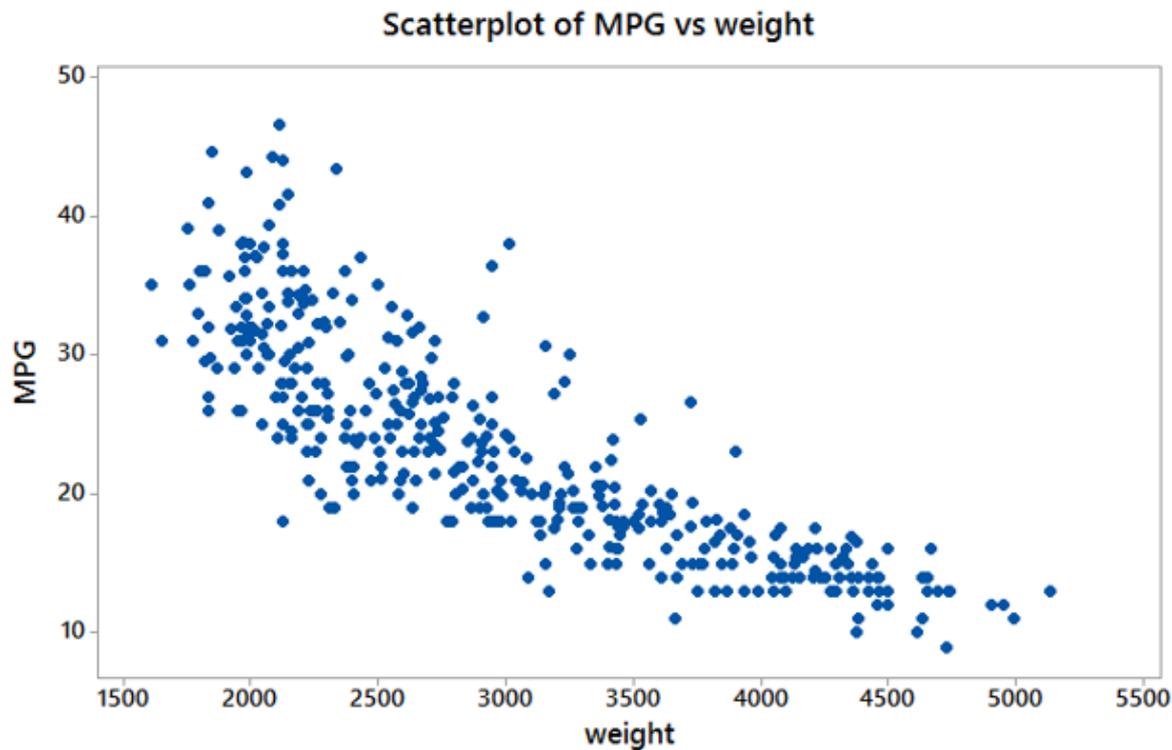


makes it easier to see and compare positions than scatter plots

# SCATTERPLOTS

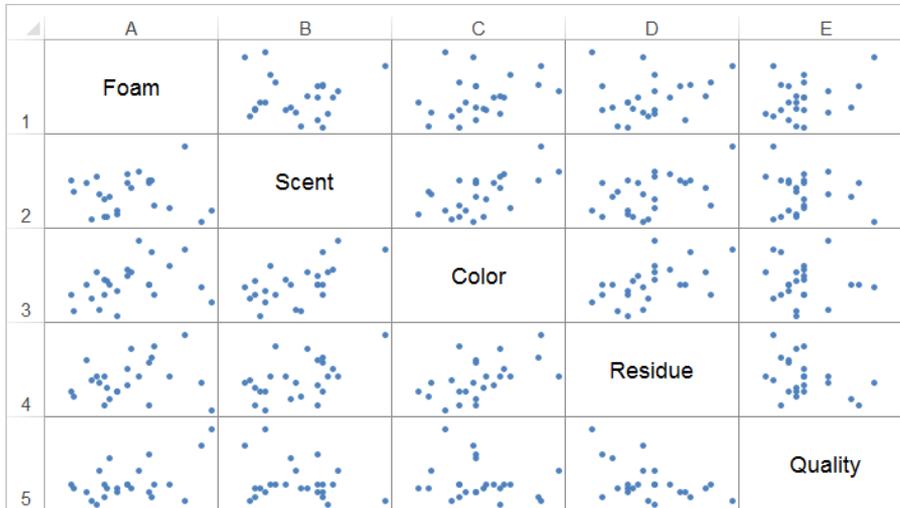
# SCATTERPLOTS

Projection of the data items into a bivariate basis of axes

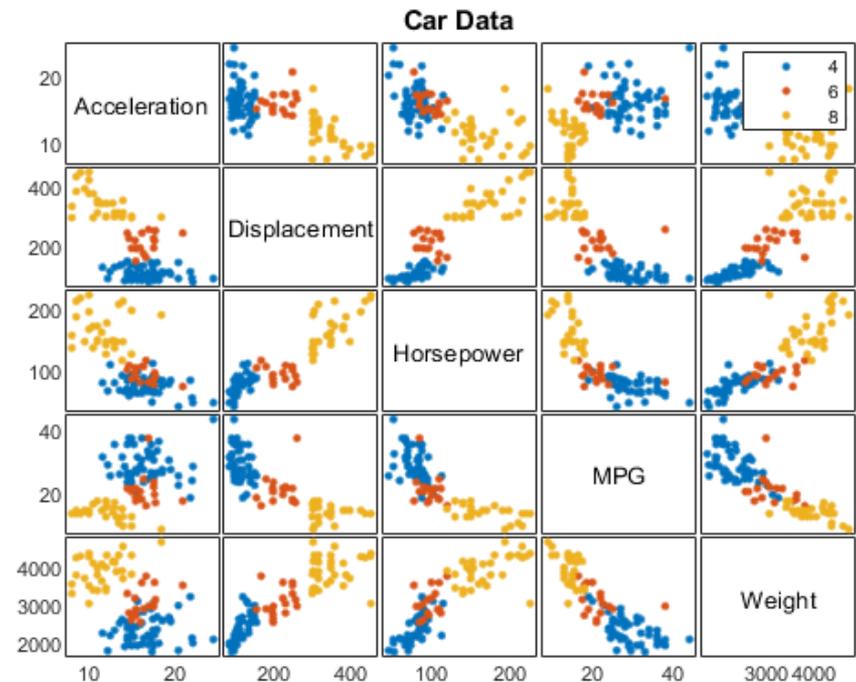


But what if you have more than two variables?

# SCATTERPLOT MATRIX



raw data



colored by cluster or class

## Problem:

- multivariate relationships are scattered across the tiles
- difficult to see multivariate relationships
- biplots are one way to visualize these – there are others

# BIVARIATE TILE SELECTION

# SCATTERPLOT MATRIX: WHICH BIVARIATE TILES TO SHOW?

How many tiles are there?

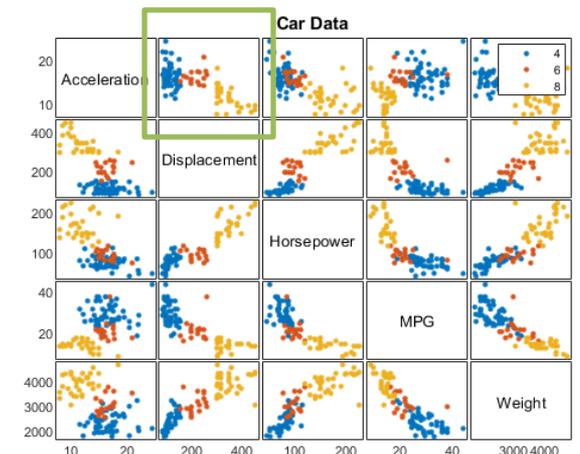
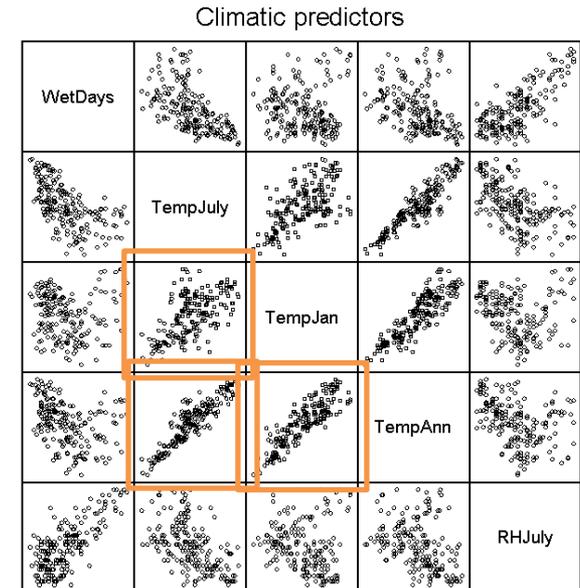
- distributes  $n(n-1)$  bivariate relationships over a set of tiles
- for  $n=4$  get 16 tiles
- can use  $n(n-1)/2$  tiles

For even moderately large  $n$ :

- there will be too many tiles

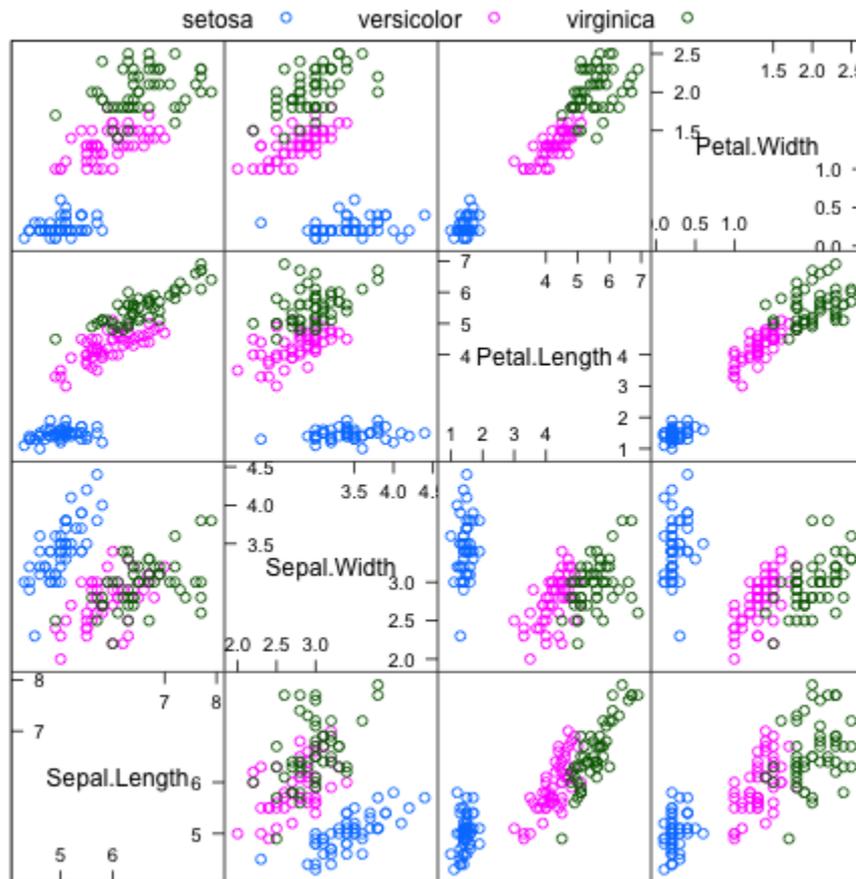
Which plots to select?

- plots that show **correlations** well
- plots that **separate clusters** well



# TILE SELECTION

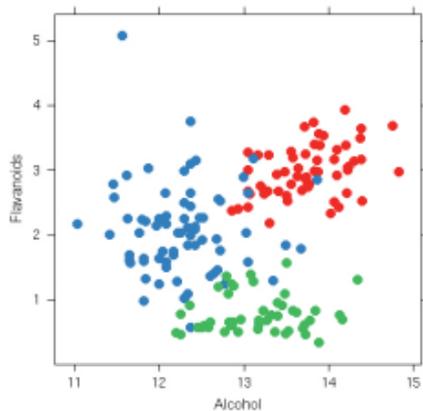
Select the most interesting tiles and show them to the user



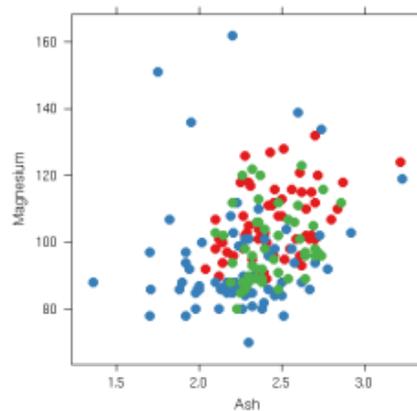
Scatter Plot Matrix

# AUTOMATED TILE SELECTION

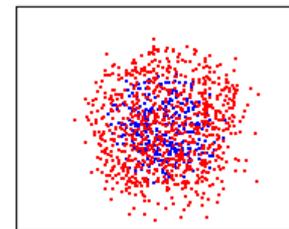
Several metrics, a good one is Distance Consistency (DSC)



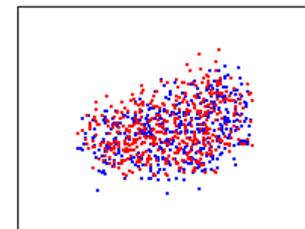
(a) DSC=90



(b) DSC=49

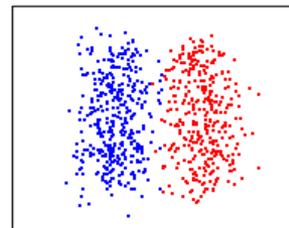


(d) 29

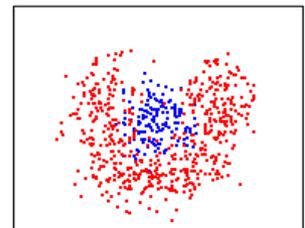


(e) 15

bad



(a) 99



(b) 74

OK

$$\text{DSC} = \frac{|\{x' \in v(X) : \mathbf{CD}(x', \text{centr}'(c_{\text{label}(x)})) = \text{true}\}|}{k}$$

- measures how "pure" a cluster is
- rank and pick the views with highest normalized DSC

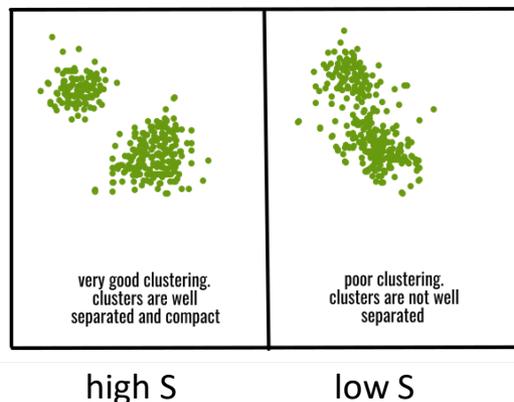
# ANOTHER METRIC: SILHOUETTE SCORE

## Comparison

- DSC → % of correctly assigned points under nearest-centroid rule
- Silhouette score → looks at good margin separability

## Compute for each point $i$

- $a(i)$ : average distance of  $i$  to all points in its own cluster
- $b(i)$ : lowest average distance of  $i$  to points in any other cluster
- Overall score  $S$  is the average of all  $s(i)$



$$s(i) = \frac{b(i) - a(i)}{\max(a(i), b(i))}$$

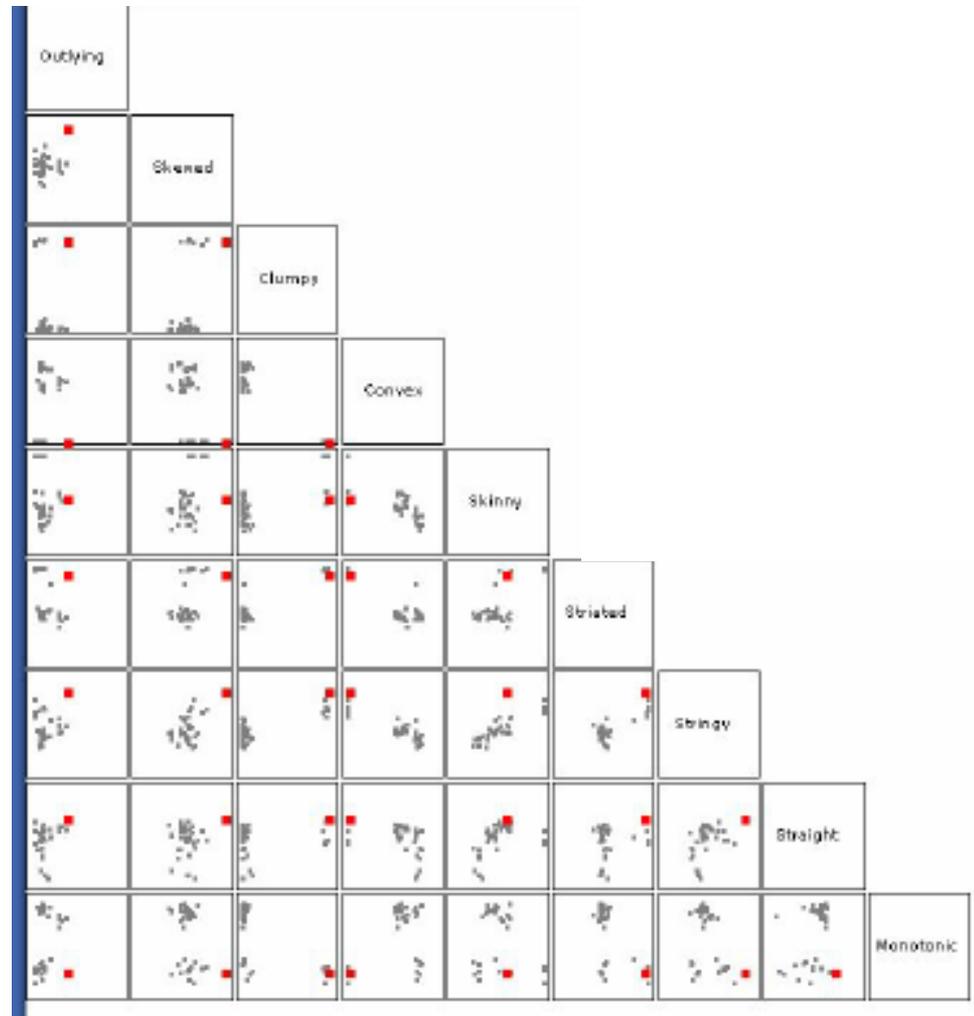
$$S = \frac{1}{N} \sum_{i=1}^N s(i)$$



# SCATTERPLOT OF SCATTERPLOTS

Use scagnostics to quickly survey 1,000s of scatterplots

- compute scagnostics measures
- create scatterplot matrix of these measures
- each scatterplot is a point



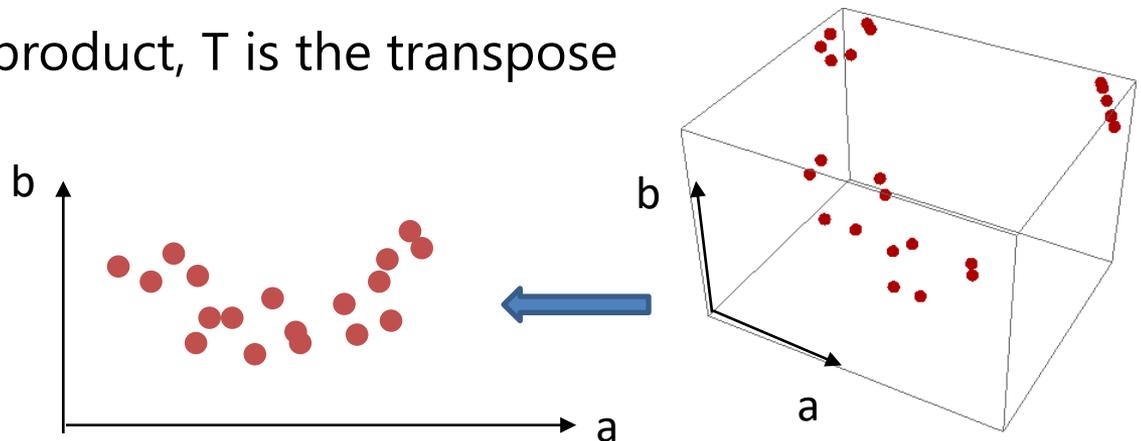
# BIPLOTS

# PROJECTION OPERATIONS

How does 2D projection work in practice?

- N-dimensional point  $x = \{x_1, x_2, x_3, \dots, x_N\}$
- a basis of two orthogonal axis vectors defined in N-D space
$$a = \{a_1, a_2, a_3, \dots, a_N\}$$
$$b = \{b_1, b_2, b_3, \dots, b_N\}$$
- a projection  $\{x_a, x_b\}$  of  $x$  into the 2D basis spanned by  $\{a, b\}$  is:
$$x_a = a \cdot x^T$$
$$x_b = b \cdot x^T$$

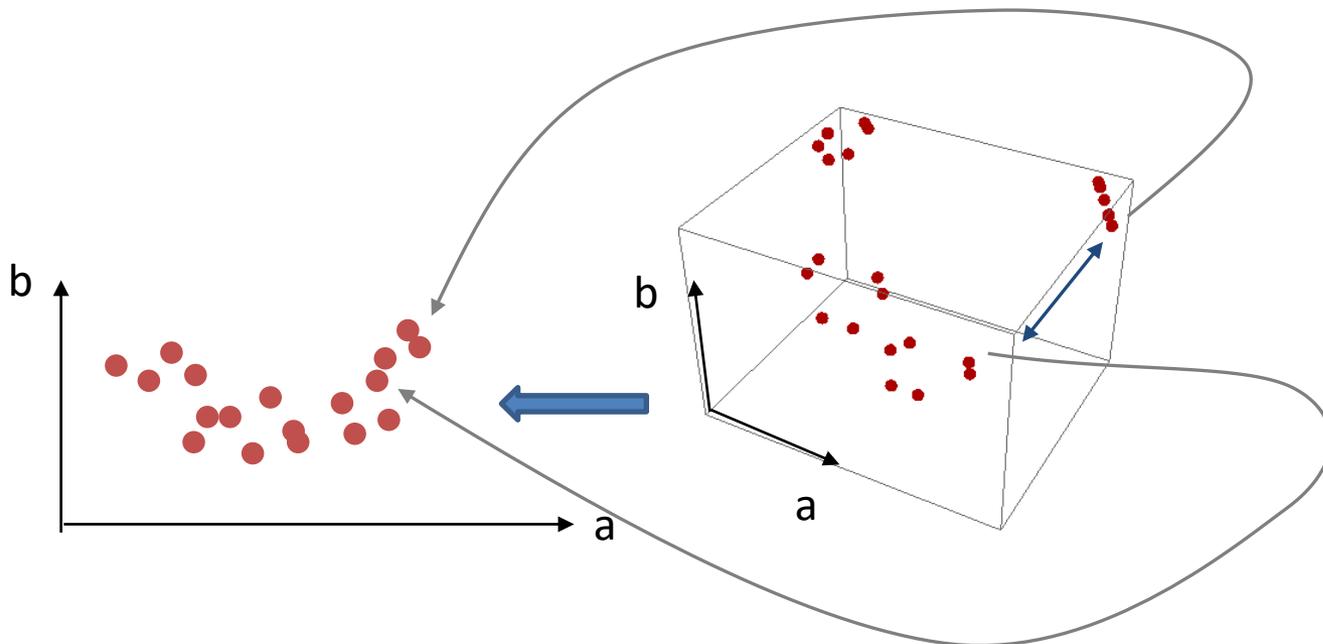
where  $\cdot$  is the dot product, T is the transpose



# PROJECTION AMBIGUITY

Projection causes inaccuracies

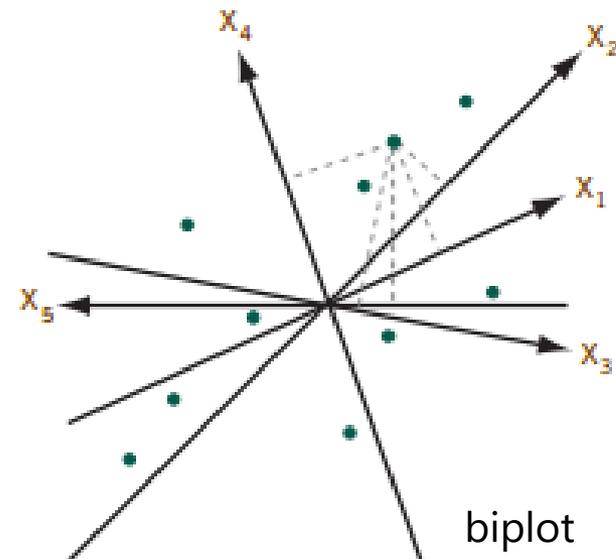
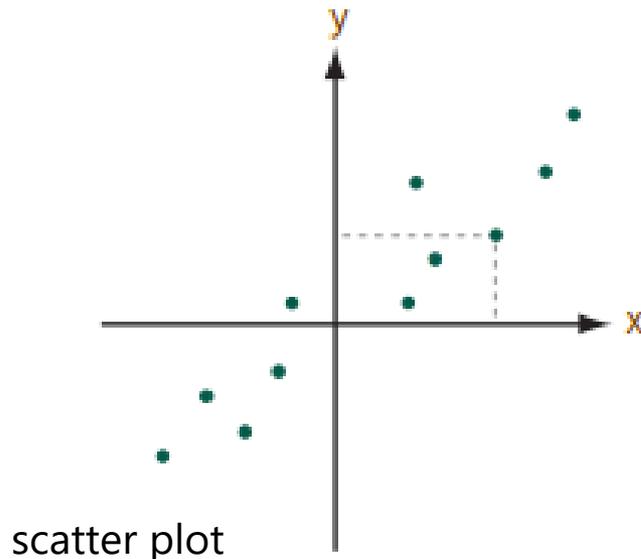
- close neighbors in the projections may not be close neighbors in the original higher-dimensional space
- this is called *projection ambiguity*



# BIPLOTS

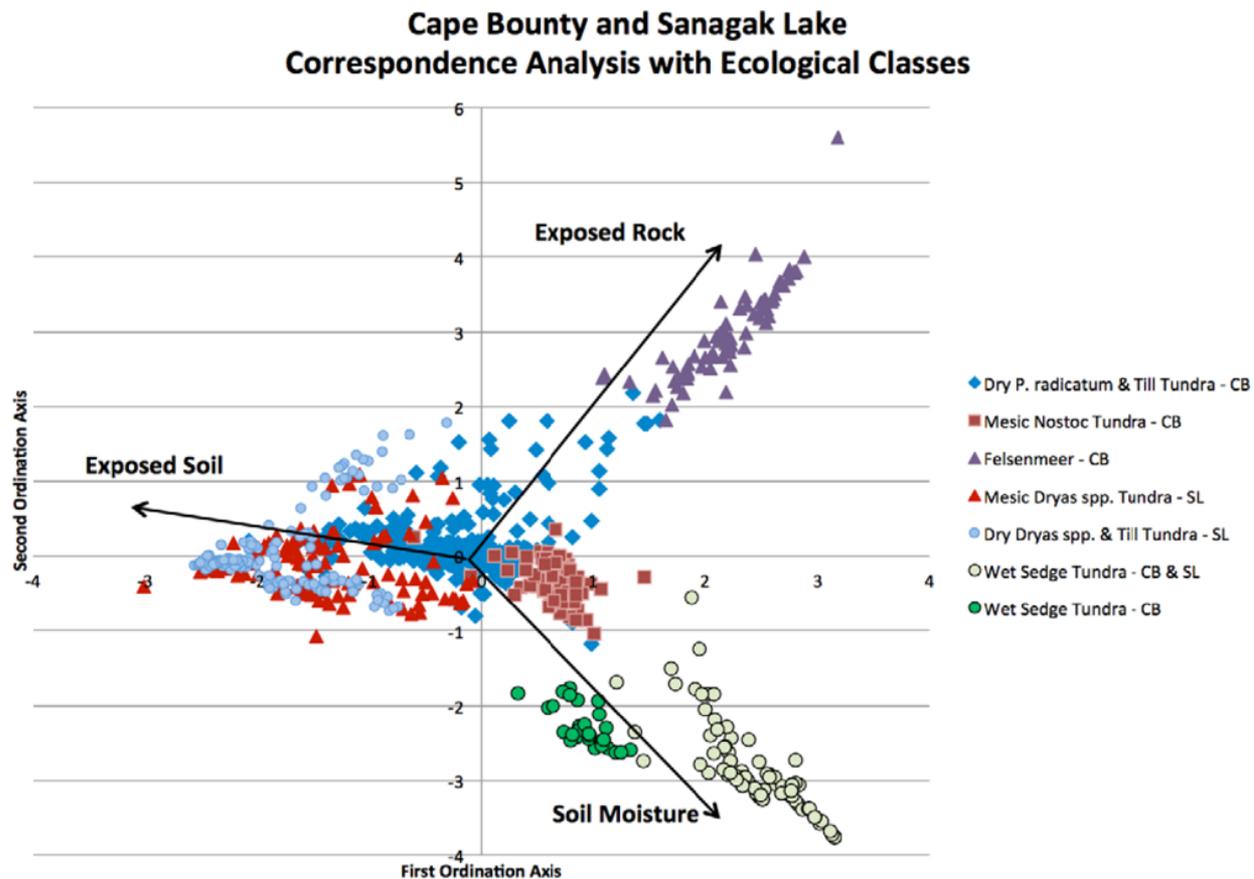
Plots data points and dimension axes into a single visualization

- uses **first two PCA** vectors as the basis to project into
- find plot coordinates [x] [y]  
for data points:  $[PCA_1 \cdot \text{data vector}] [PCA_2 \cdot \text{data vector}]$   
for dimension axes:  $[PCA_1[\text{dimension}]] [PCA_2[\text{dimension}]]$



# BIPLOTS CAN HAVE PROJECTION AMBIGUITIES

Are just a linear projection into the 2D basis generated by PCA



# BIPLOTS – A WORD OF CAUTION

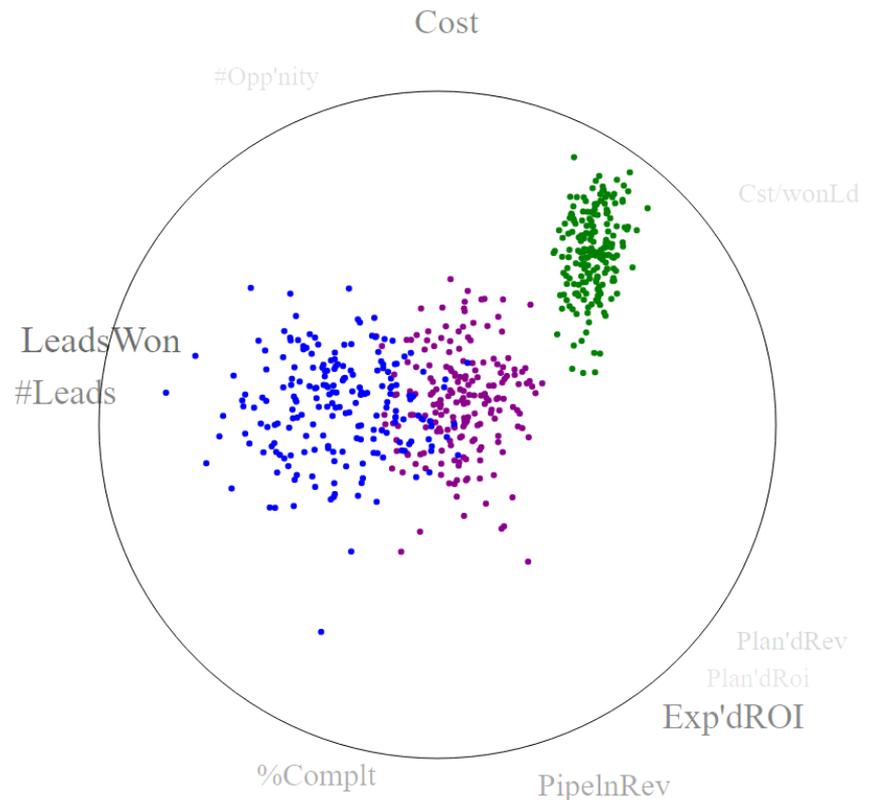
Do be aware that the projections may not be fully accurate

- you are projecting N-D into 2D by a linear transformation
- if there are more than 2 significant PCA vectors then some variability will be lost and won't be visualized
- remote data points might project into nearby plot locations suggesting false relationships → projection ambiguity
- always check out the PCA scree plot to gauge accuracy

# INTERACTIVE BIPLLOTS

Also called multivariate scatterplot

- biplot-axes length vis replaced by graphical design
- less cluttered view
- but there's more to this .....



# MEET THE *SUBSPACE VOYAGER*

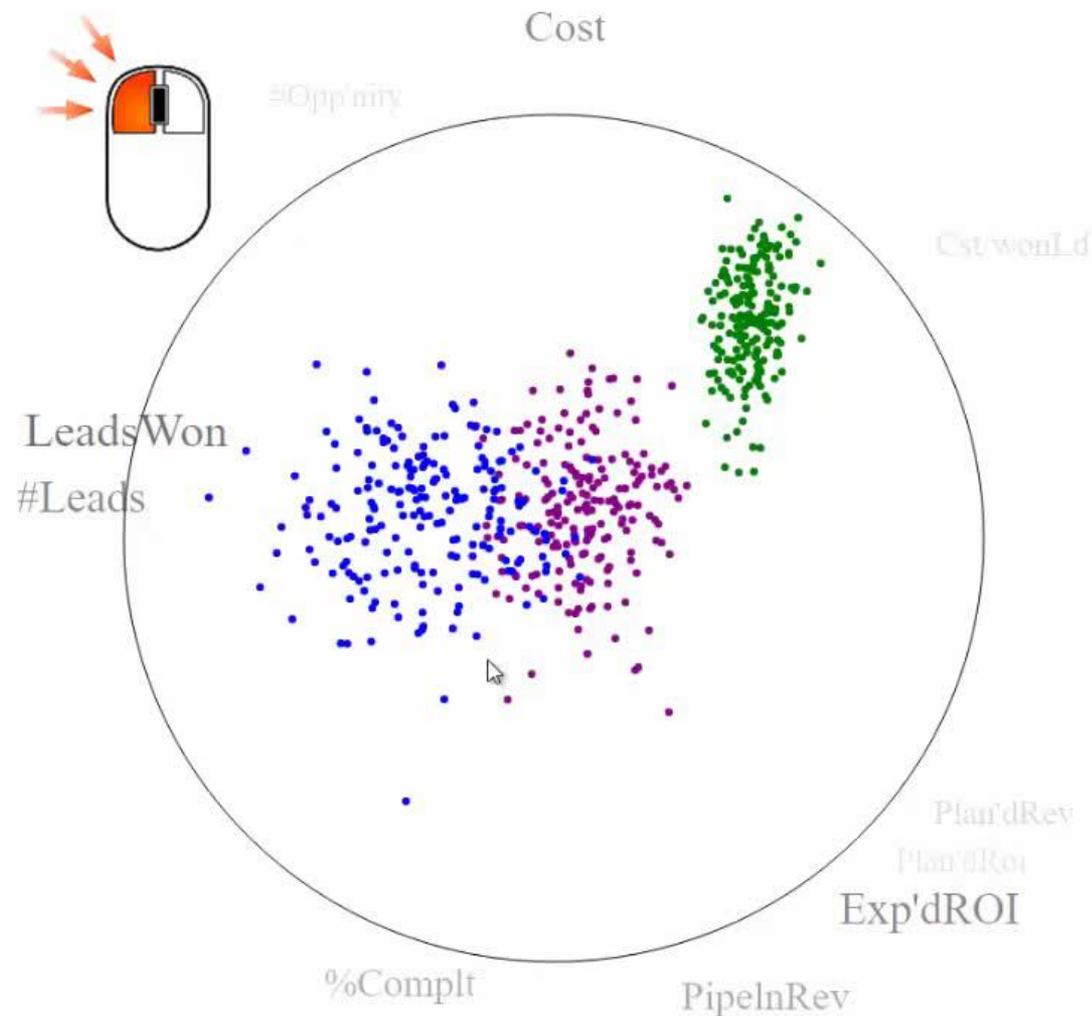
Decomposes high-D data spaces into lower-D subspaces by

- clustering
- classification
- reducing clusters to intrinsic dimensionality via local PCA

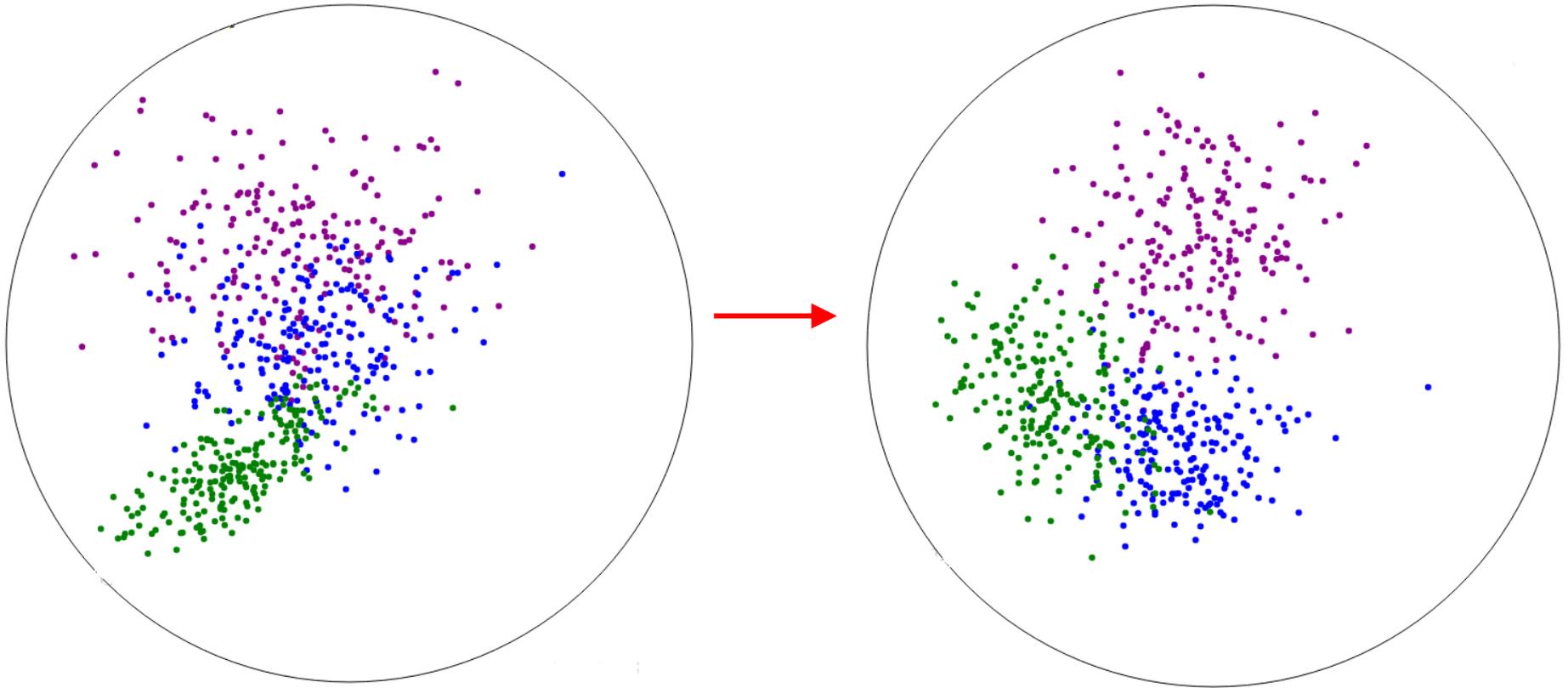
Allows users to interactively explore these lower-D subspaces

- explore them as a chain of 3D subspaces
- transition seamlessly to adjacent 3D subspaces on demand
- save observations as you go (and return to them just as well)

# TRACKBALL-BASED CLUSTER EXPLORATION

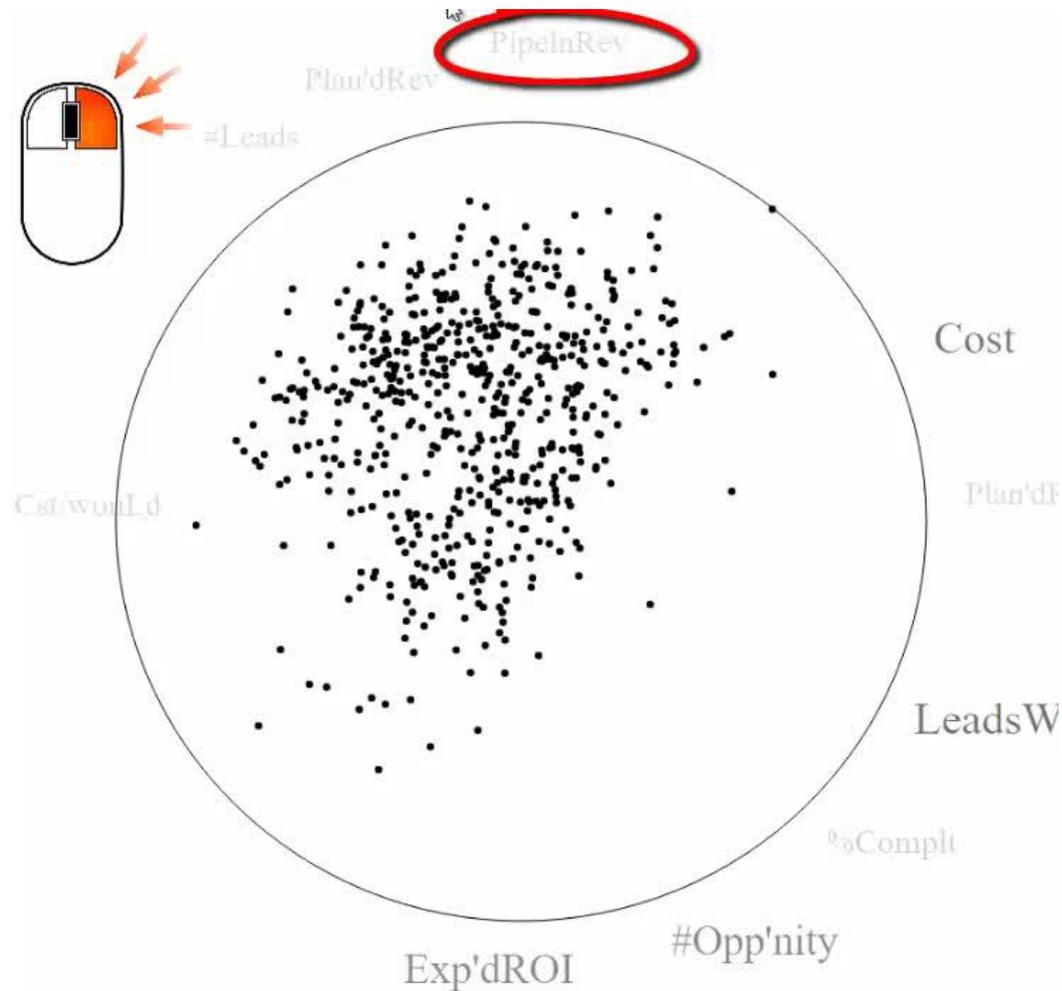


# INTERACTIVE VIEW OPTIMIZER



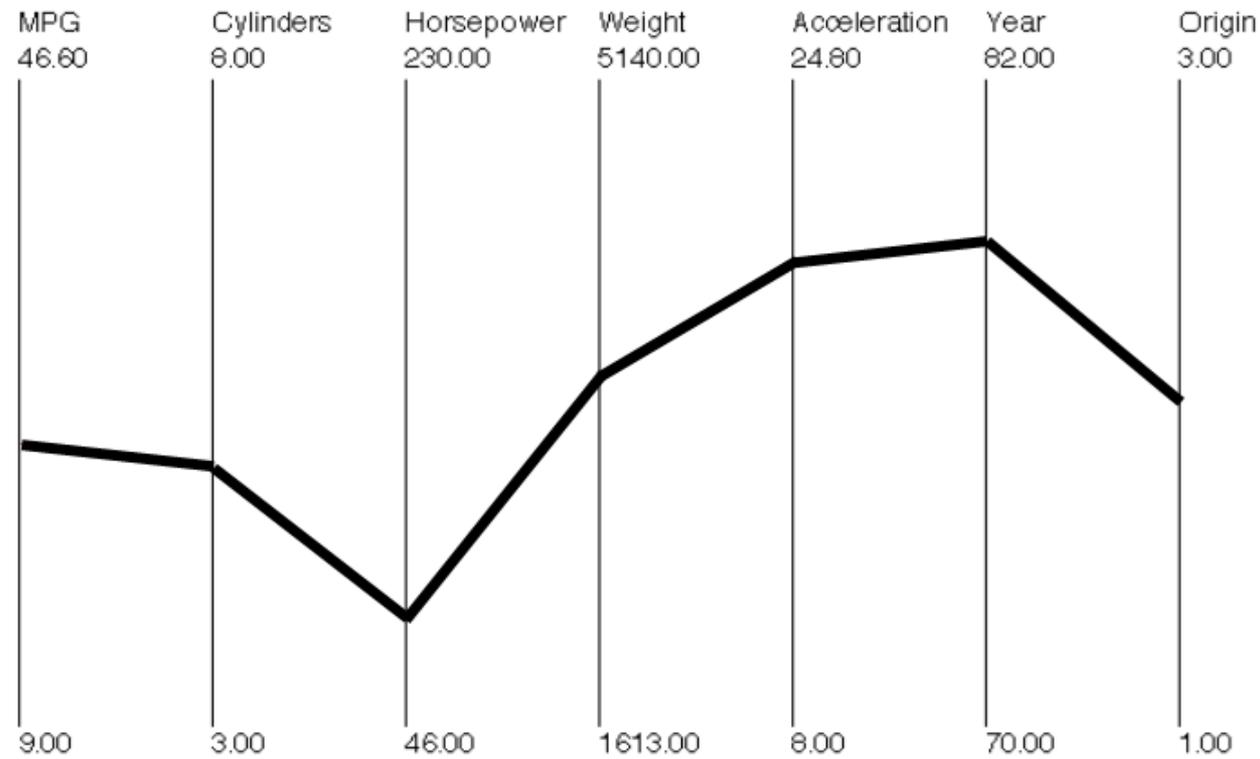
Uses genetic-algorithm driven projection pursuit  
Several view quality metrics are available

# CHASE INTERESTING CLUSTERS – TRANSITION TO ADJACENT 3D SUBSPACES



# PARALLEL COORDINATES

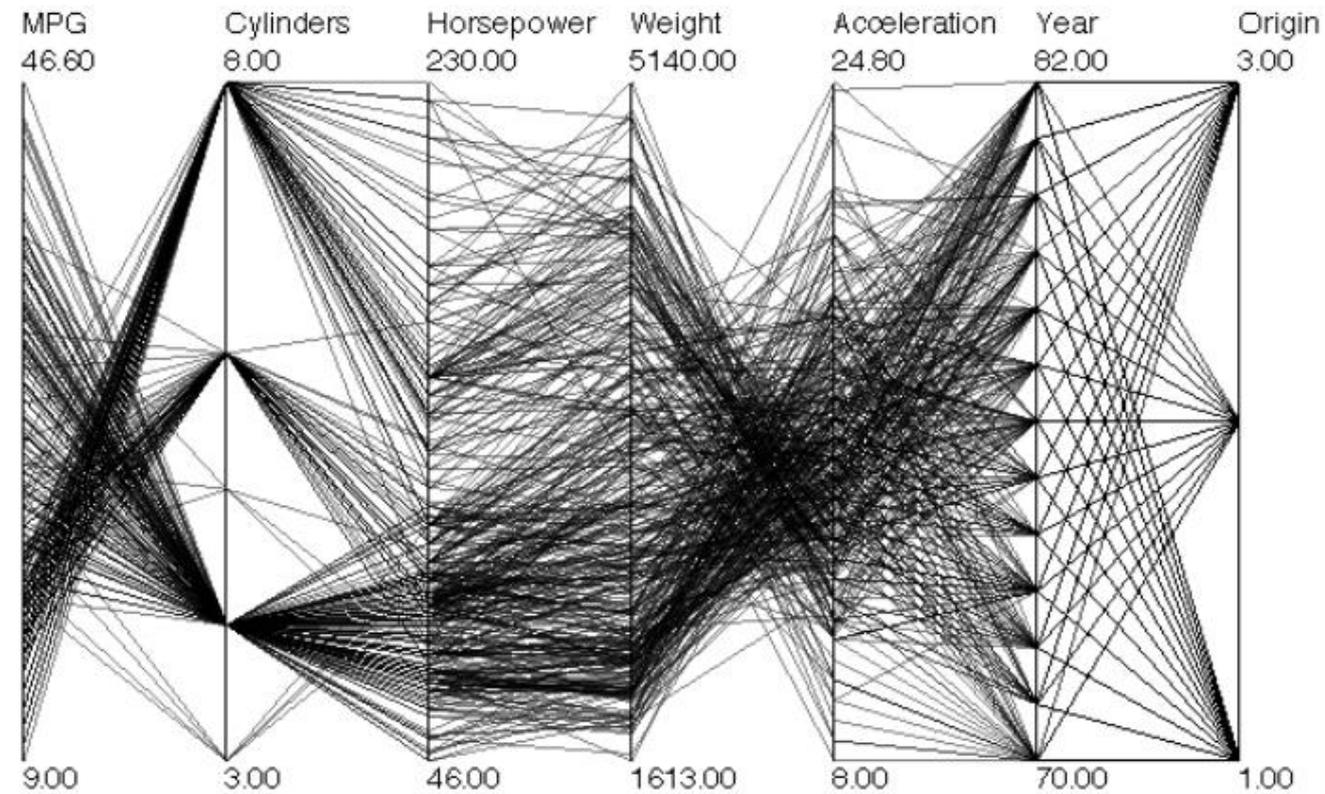
# PARALLEL COORDINATES – 1 CAR



The  $N=7$  data axes are arranged side by side

- in parallel

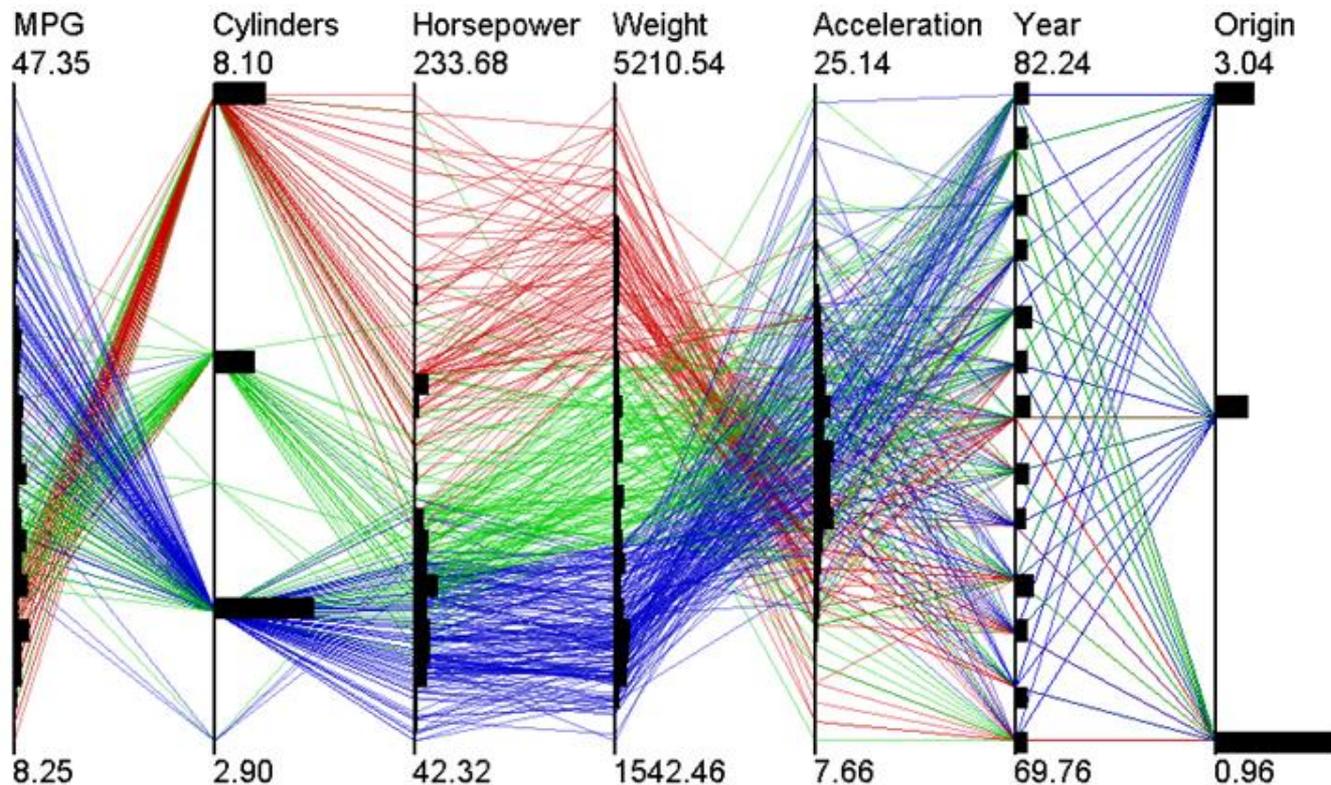
# PARALLEL COORDINATES – 100 CARS



Hard to see the individual cars?

- what can we do?

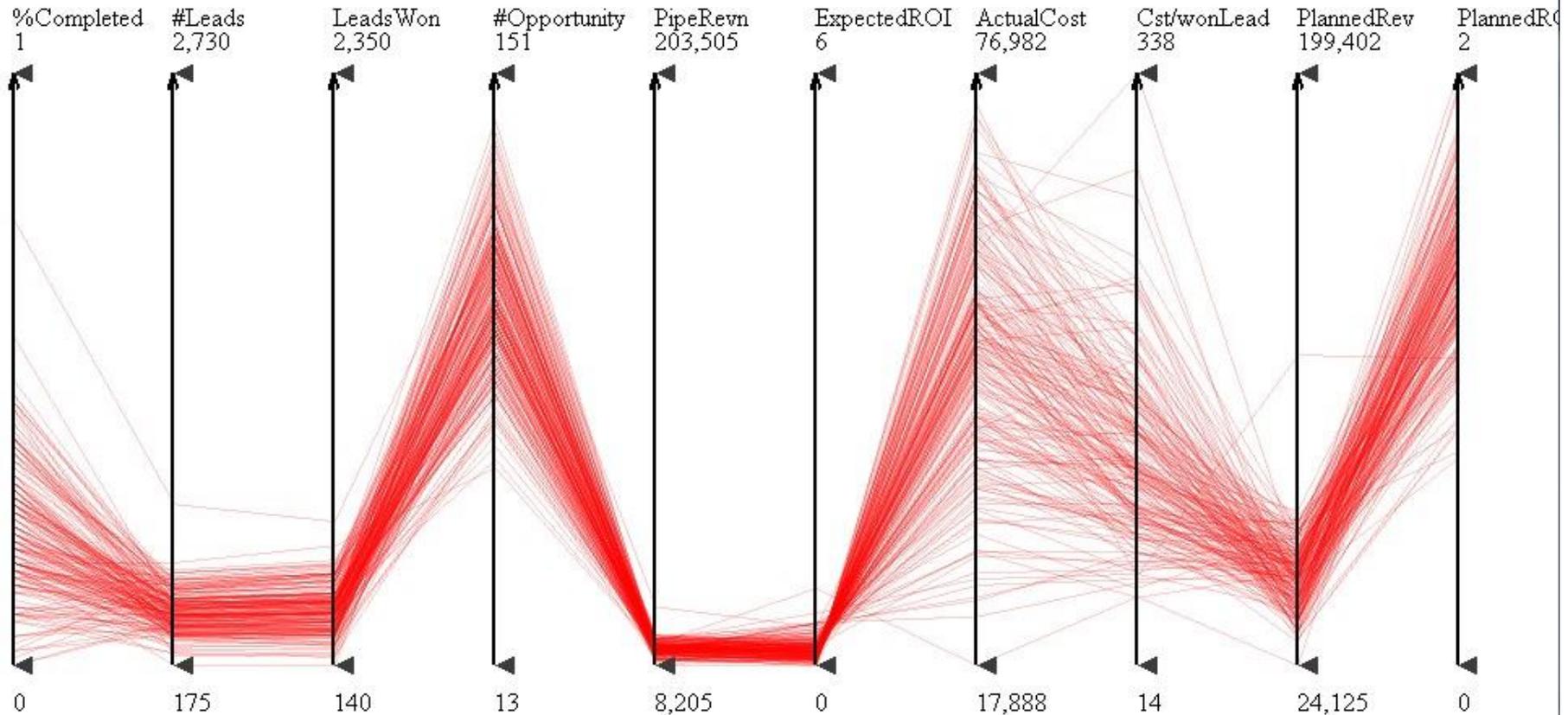
# PARALLEL COORDINATES – 100 CARS



Grouping the cars into sub-populations

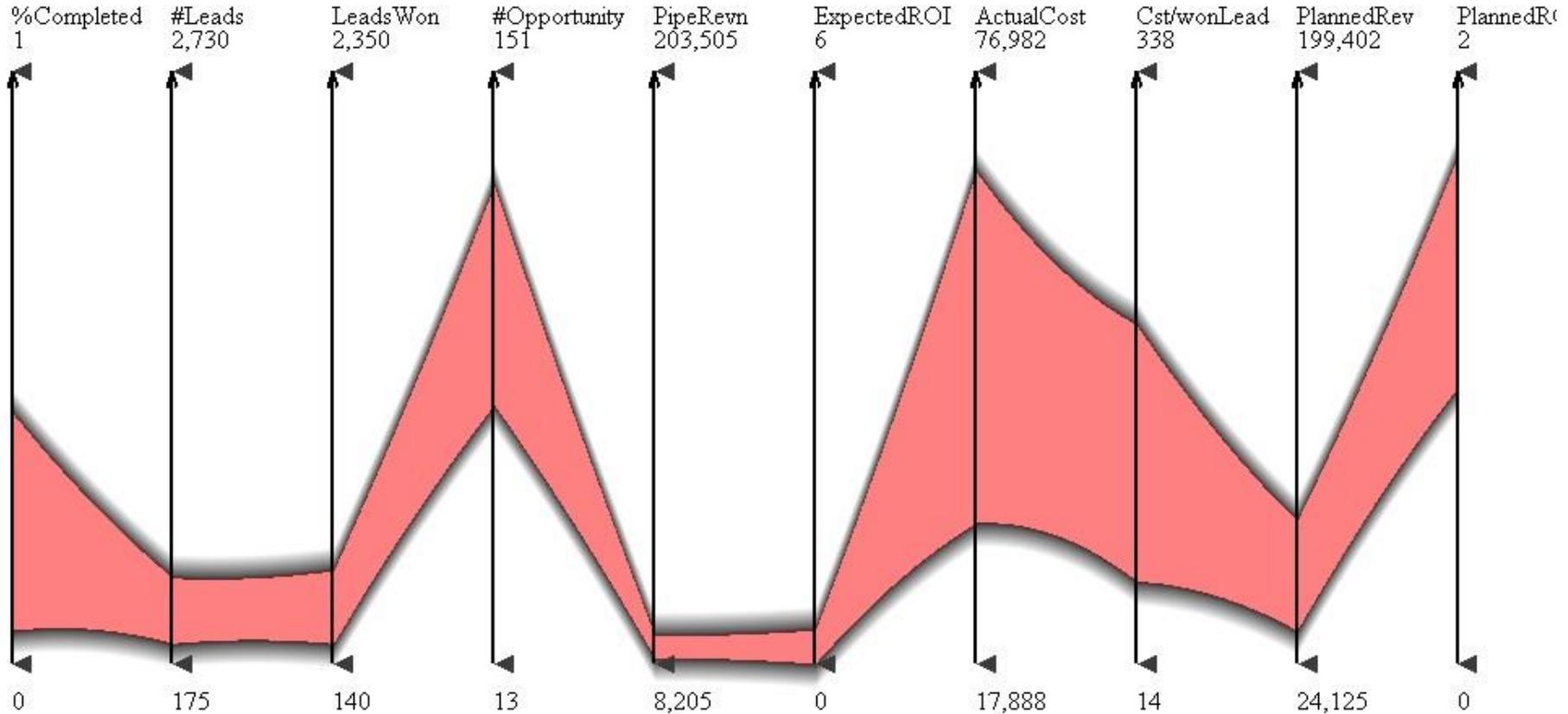
- we perform clustering
- can be automated or interactive (put the user in charge)

# PC With Illustrative Abstraction



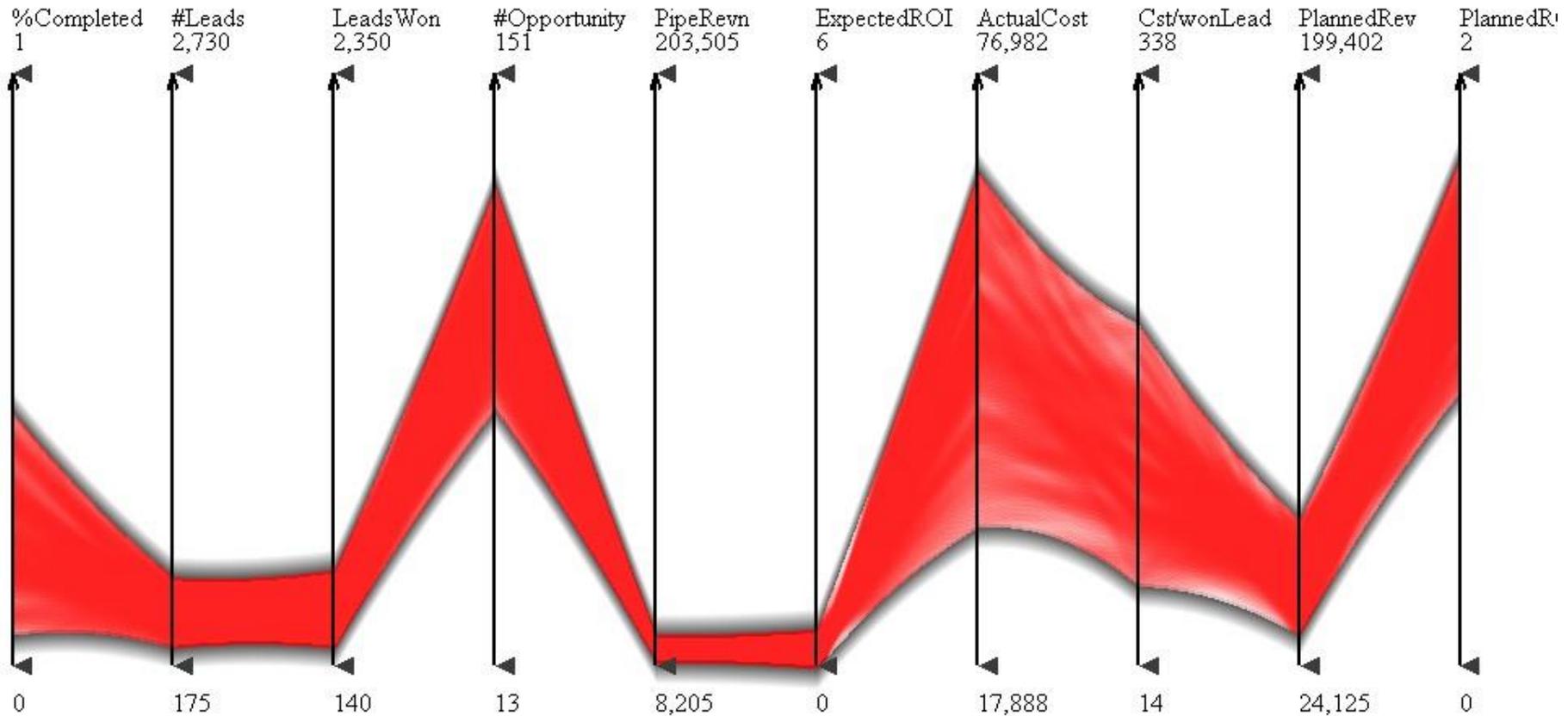
individual polylines

# PC With Illustrative Abstraction



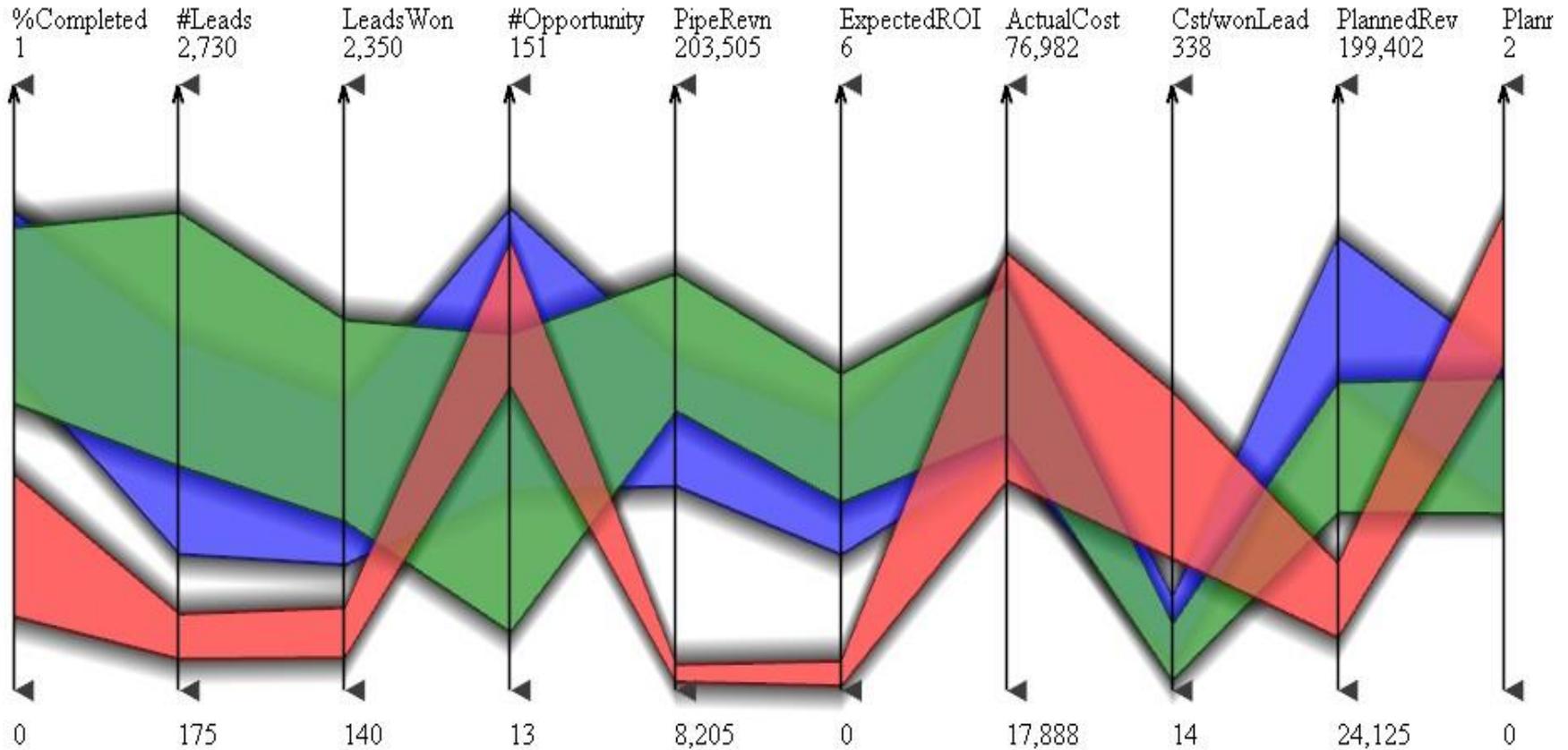
completely abstracted away

# PC With Illustrative Abstraction



blended partially

# PC With Illustrative Abstraction



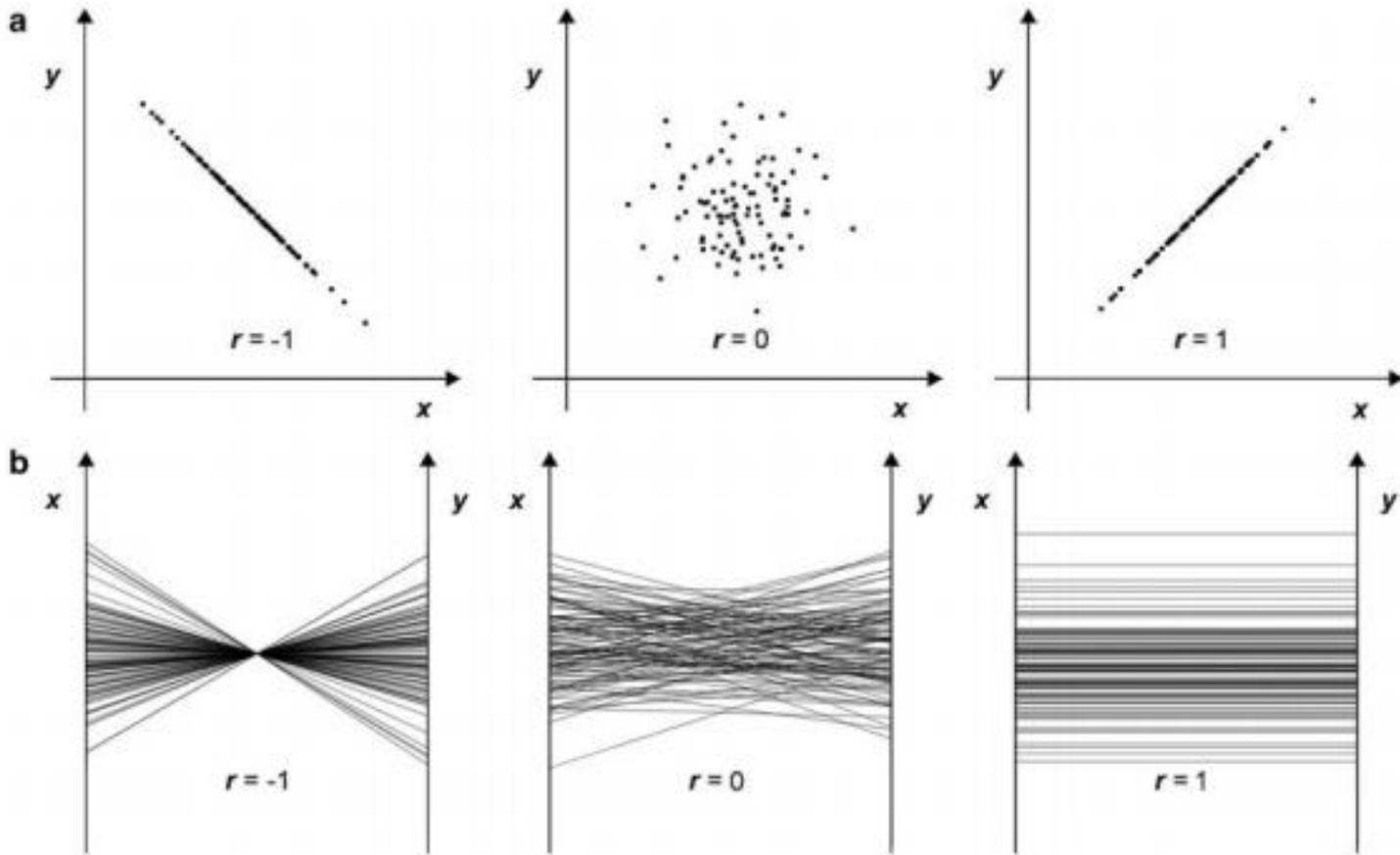
all put together – three clusters

[McDonnell and Mueller, 2008]

# Interaction is Key

Interaction in Parallel Coordinate

# PATTERNS IN PARALLEL COORDINATES



correlation

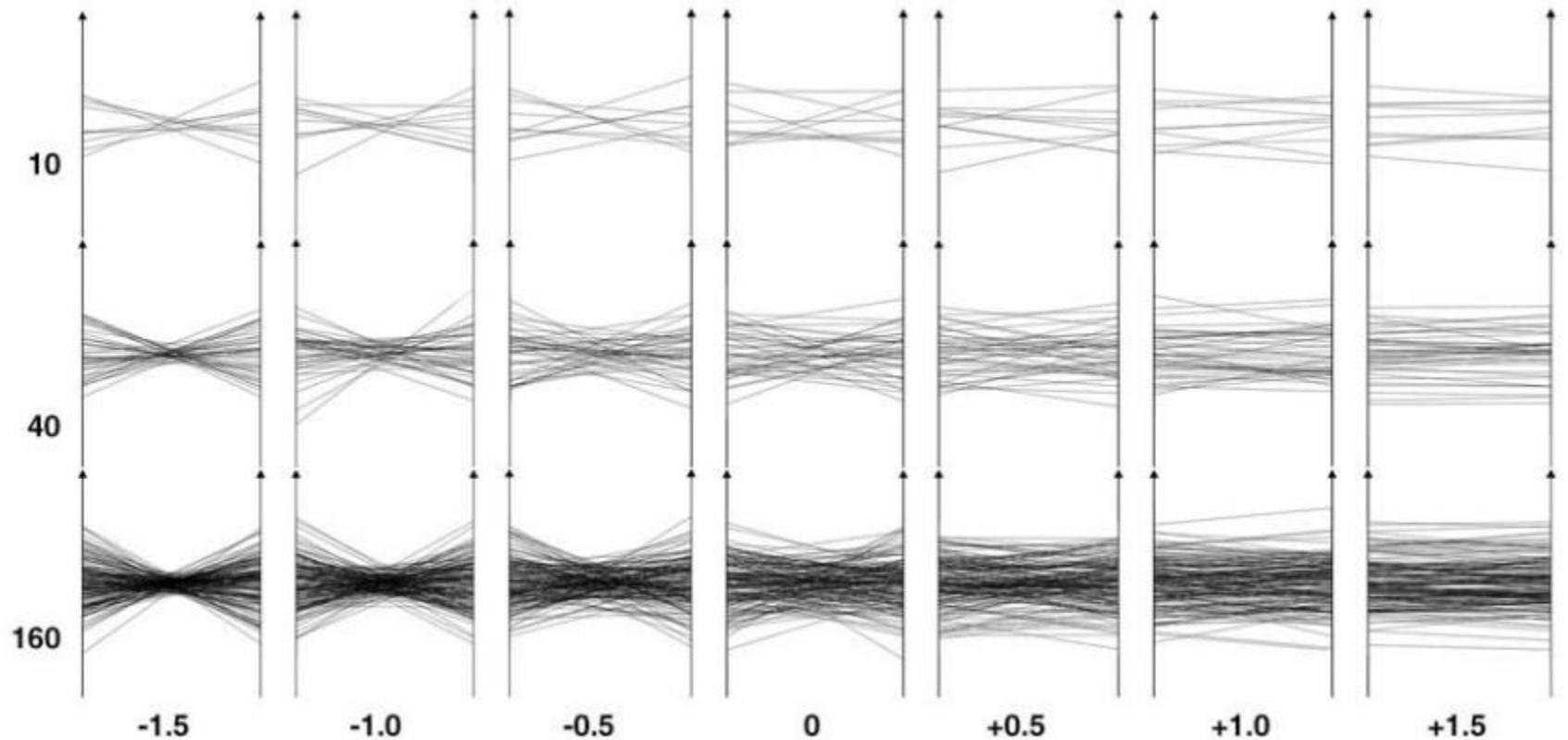
$r = -1.0$

$r = 0$

$r = 1.0$

# PATTERNS IN PARALLEL COORDINATES

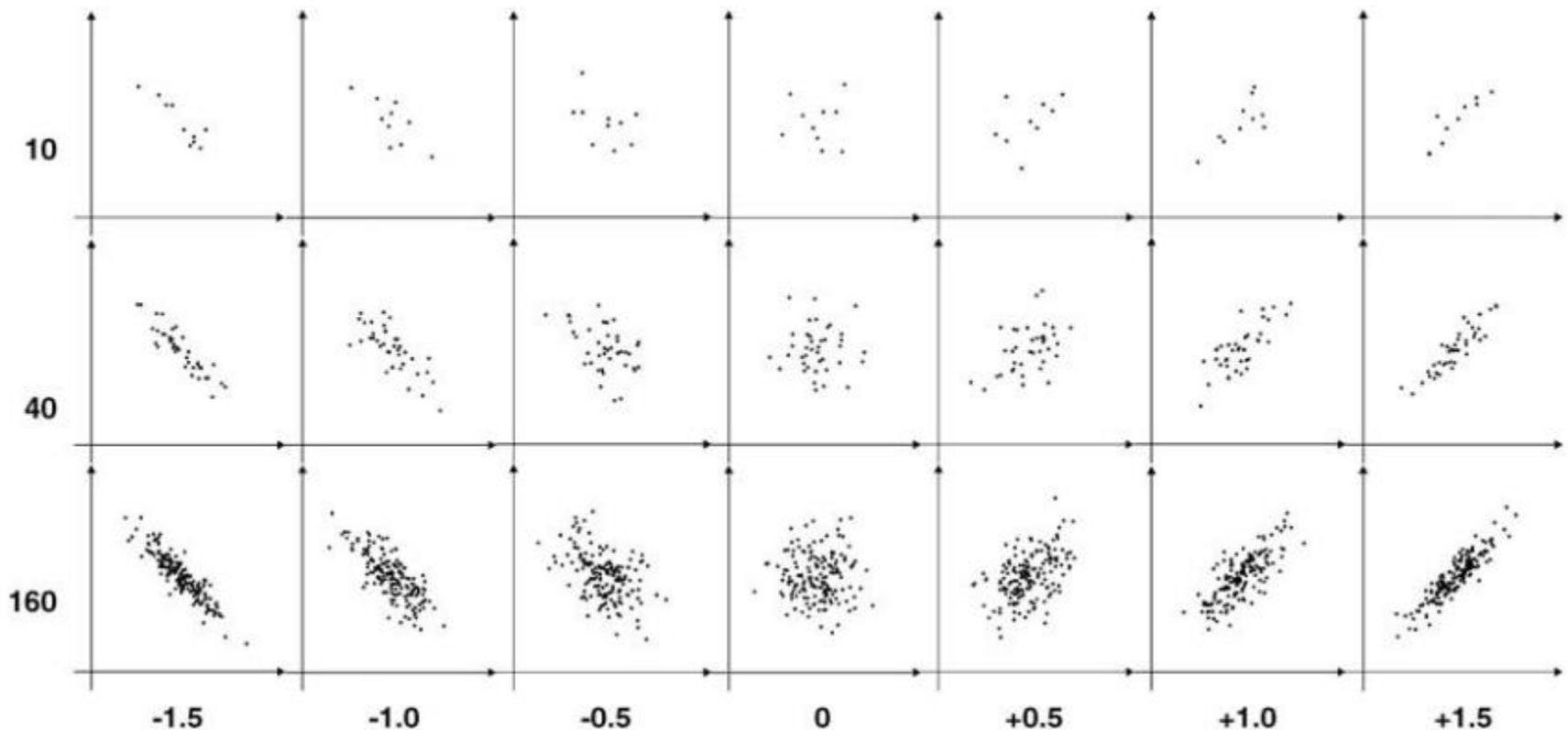
# points



Fisher-z (corresponding to  $\rho = 0, \pm 0.462, \pm 0.762, \pm 0.905$ )

# PATTERNS IN SCATTERPLOTS

# points



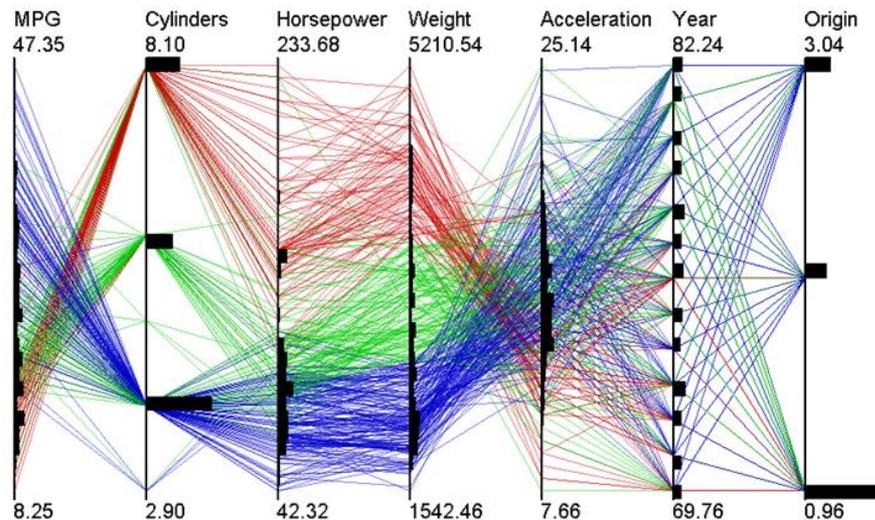
Fisher-z (corresponding to  $\rho = 0, \pm 0.462, \pm 0.762, \pm 0.905$ )

Li et al. found that twice as many correlation levels can be distinguished with scatterplots

# AXIS REORDERING PROBLEM

There are  $n!$  ways to order the  $n$  dimensions

- how many orderings for 7 dimensions?
- 5,040
- but since can see relationships across 3 axes a better estimate is  $n!/((n-3)! 3!) = 35$
- still a lot of axes orderings to try out → we need help

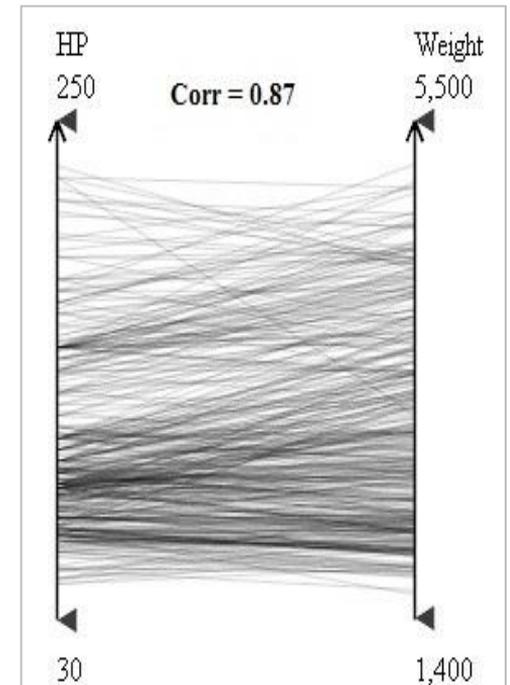
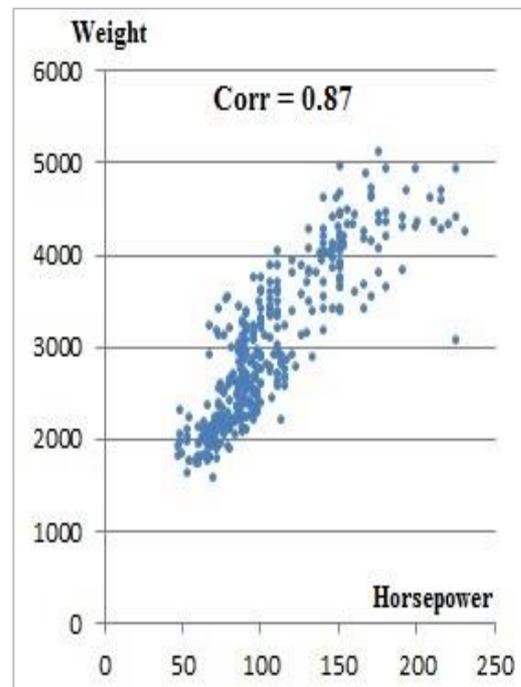


# WE NEED A MEASURE FOR RELATIONSHIPS

## Correlation

- a statistical measure that indicates the extent to which two or more variables fluctuate together

$$r_{xy} = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2 \sum_{i=1}^n (y_i - \bar{y})^2}}$$



# BUILDING THE CORRELATION MATRIX

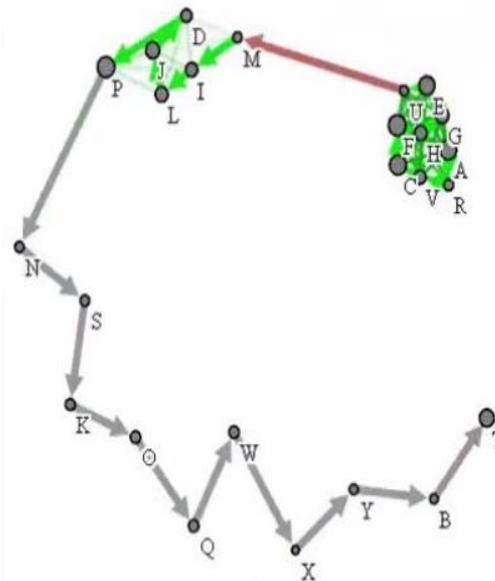
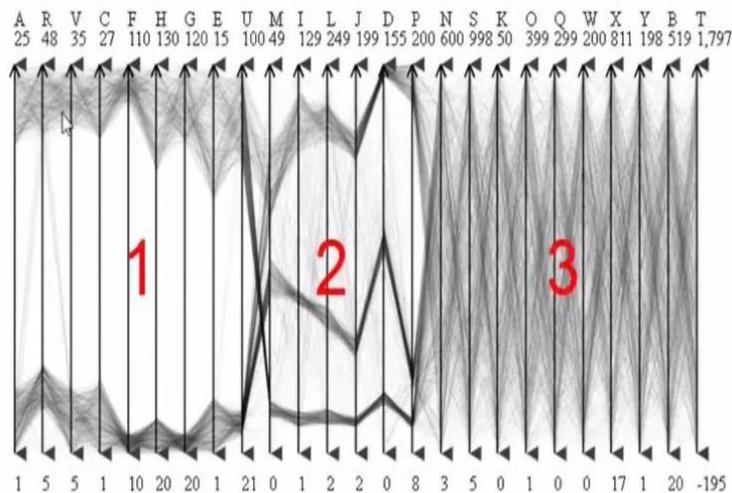
Create a correlation matrix

Run a mass-spring model

Run Traveling Salesman on the correlation nodes

Use it to order your parallel coordinate axes via TSP

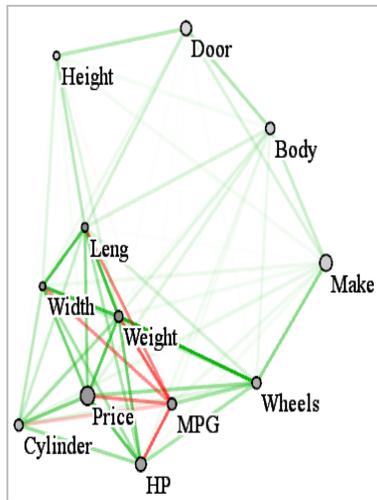
Z. Zhang, K. McDonnell, K. Mueller, "A Network-Based Interface for the Exploration of High-Dimensional Data Spaces," *IEEE Pacific Vis*, 2012



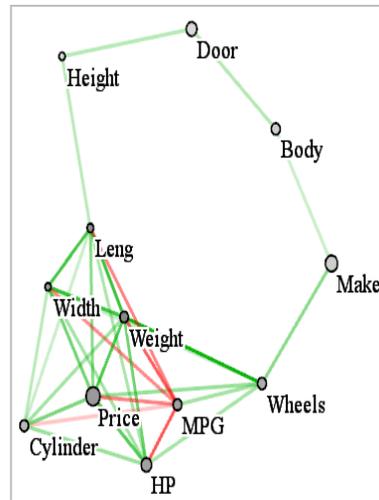
	MRK	MSFT	PFE	PG	T	TRV	UTX	VZ	WMT	XOM
MRK	1	0.39	0.72	-0.43	0.57	0.031	-0.26	0.61	-0.11	-0.25
MSFT	0.39	1	0.14	0.11	0.56	0.25	0.25	0.67	-0.074	0.24
PFE	0.72	0.14	1	-0.77	0.08	-0.37	-0.65	0.19	-0.077	-0.72
PG	-0.43	0.11	-0.77	1	0.25	0.68	0.92	0.086	0.072	0.9
T	0.57	0.56	0.08	0.25	1	0.65	0.46	0.87	-0.059	0.54
TRV	0.031	0.25	-0.37	0.68	0.65	1	0.83	0.43	-0.0067	0.81
UTX	-0.26	0.25	-0.65	0.92	0.46	0.83	1	0.27	-0.033	0.93
VZ	0.61	0.67	0.19	0.086	0.87	0.43	0.27	1	0.026	0.36
WMT	-0.11	-0.074	-0.077	0.072	-0.059	-0.0067	-0.033	0.026	1	0.832
XOM	-0.25	0.24	-0.72	0.9	0.54	0.81	0.93	0.36	0.832	1

# INTERACTION WITH THE CORRELATION NETWORK

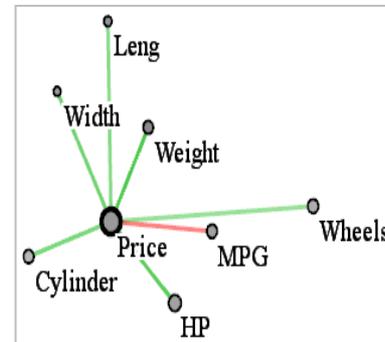
- Vertices are attributes, edges are correlations
  - vertex: size determined by  $\sum_{j=0}^D \frac{|\text{correlation}(i,j)|}{D-1} \quad j \neq i$
  - edge length is a measure of  $(1-|\text{correlation}|)$
  - edge: color/intensity  $\rightarrow$  sign/strength of correlation



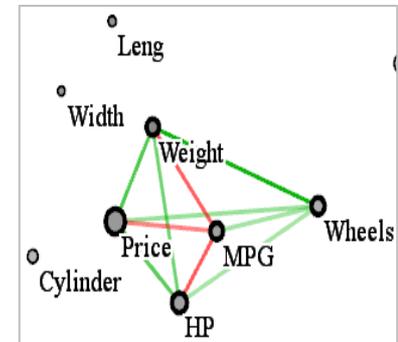
all edges



filtered by strength

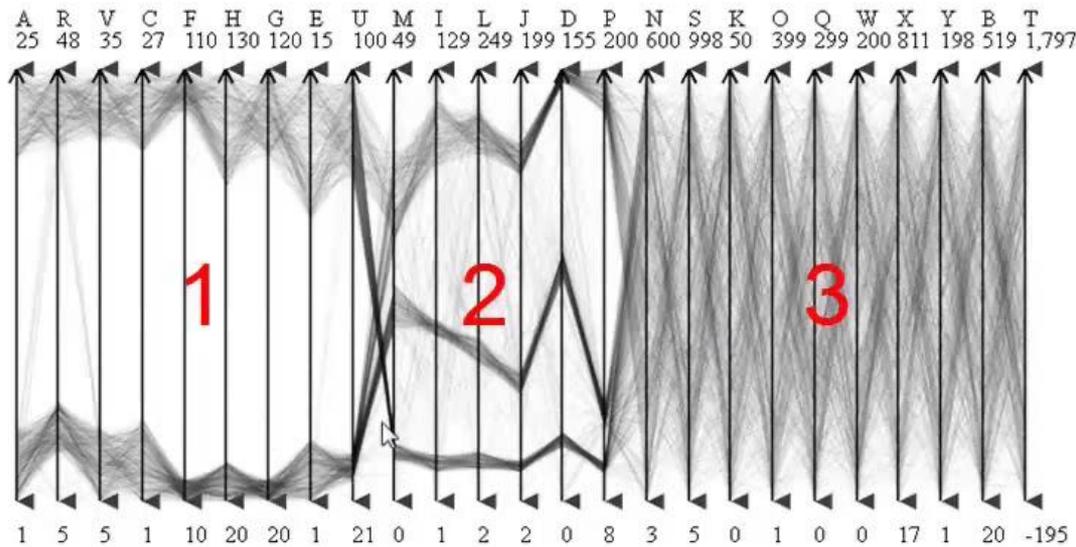


attribute centric

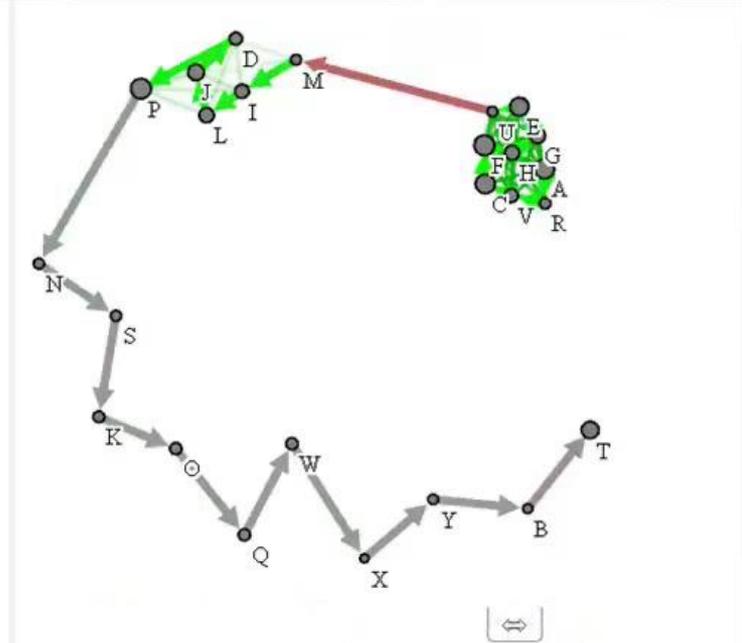


subset of attributes

# MULTISCALE ZOOMING



3 subspaces are well separated.



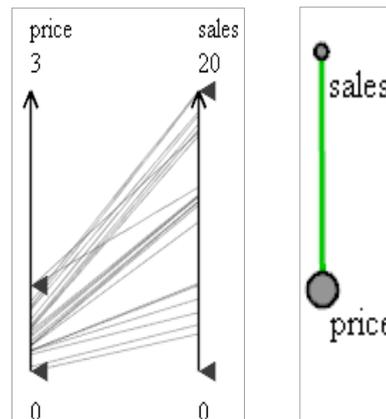
# BRACKETING AND CONDITIONING

Correlation strength can often be improved by constraining a variable's value range

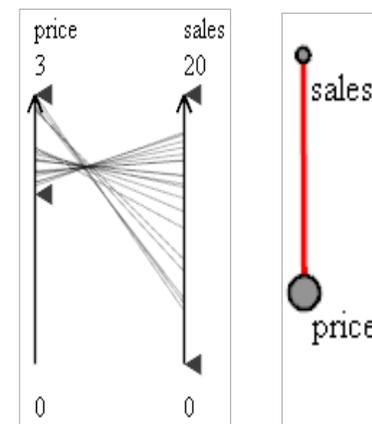
- this limits the derived relationships to this value range
- such limits are commonplace in targeted marketing, etc.



no bracketing



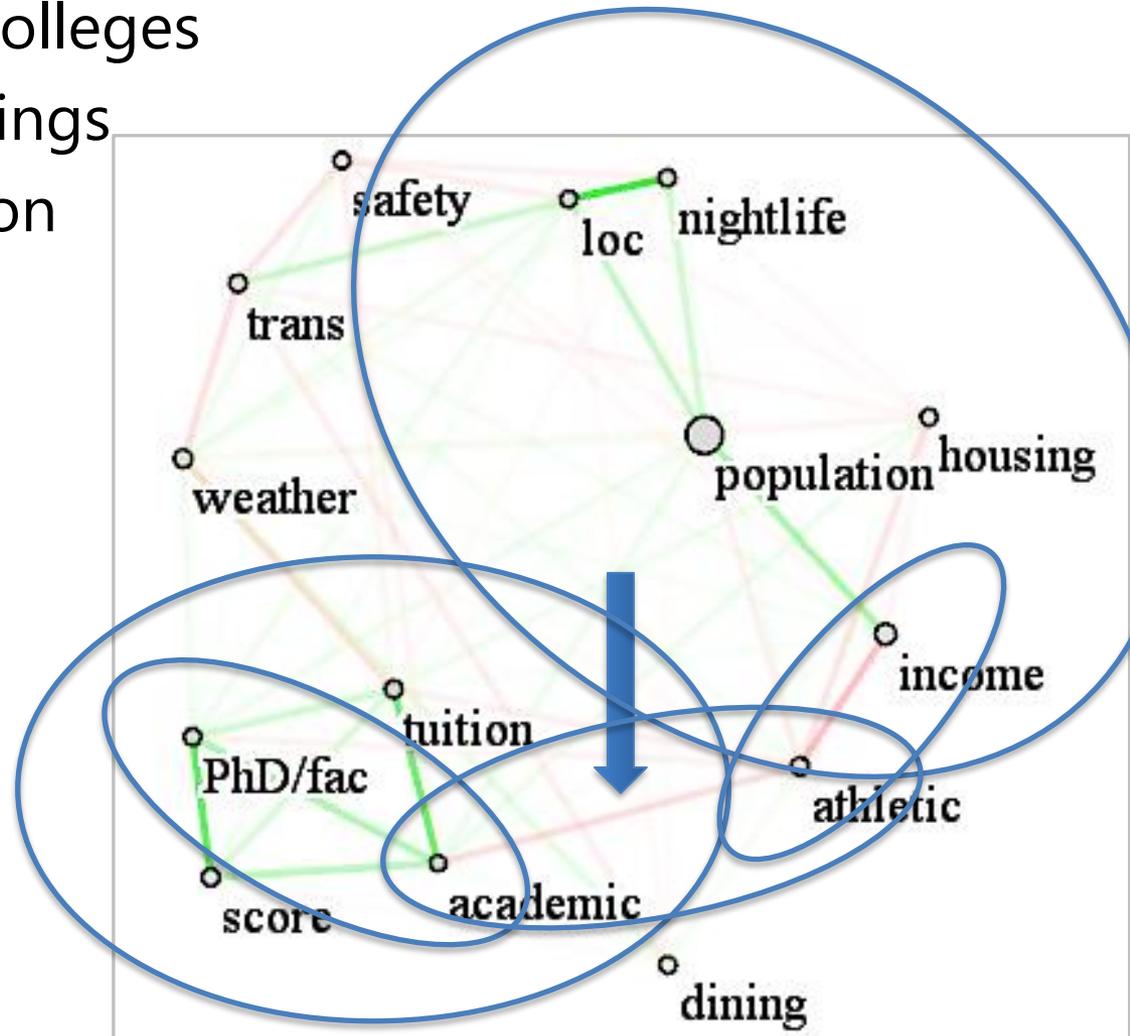
lower price range



higher price range

# CORRELATION PLOTS ARE POWERFUL

Fused dataset of 50 US colleges  
US News: academic rankings  
College Prowler: survey on campus life attributes

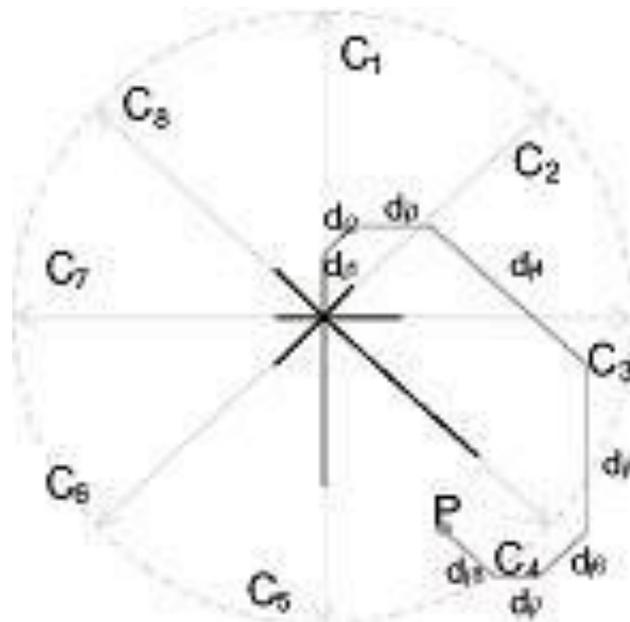


# RADIAL LAYOUTS

# STAR COORDINATES

Coordinate system based on axes positioned in a “star”, or circular pattern

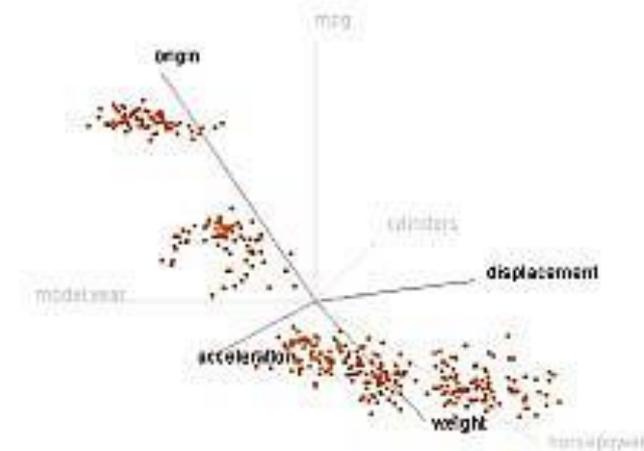
- no prior PCA and subsequent projection
- instead, a point P is plotted as a vector sum of all axis coordinates



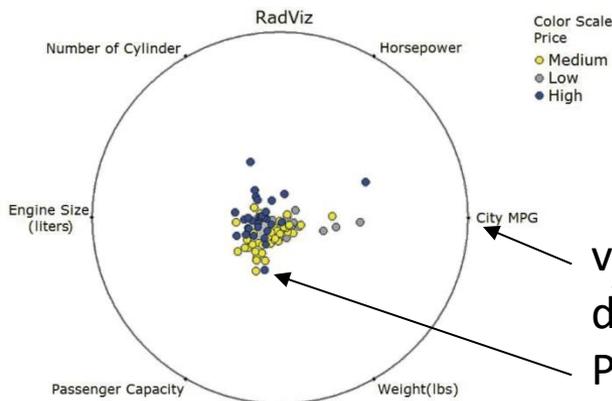
# STAR COORDINATES

## Operations defined on Star Coords

- scaling changes contribution to resulting visualization
- axis rotation can visualize correlations
- also used to reduce projection ambiguities



## Similar paradigm: RadViz



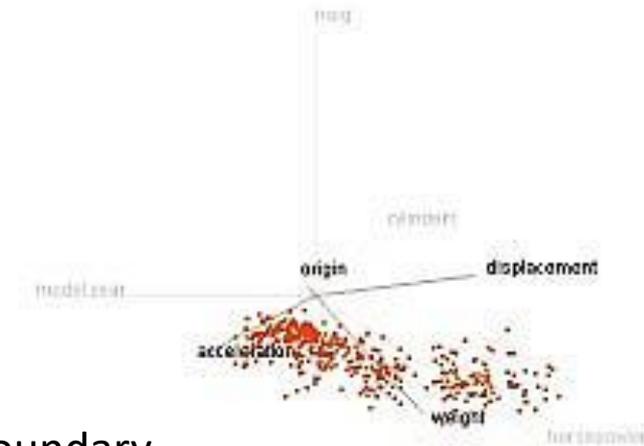
$$P = \sum_{i=1}^n w_j v_j$$

$$w_i = d_j / \sum_{k=1}^n d_k$$

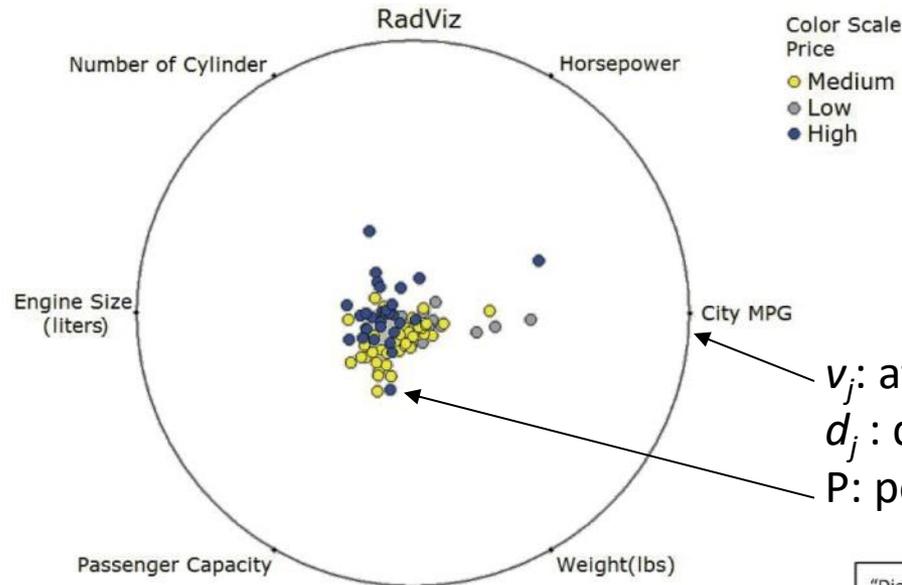
$v_j$ : attribute coordinates on disk boundary

$d_j$ : data vector values

$P$ : point location in RadViz disk



# RADVIZ

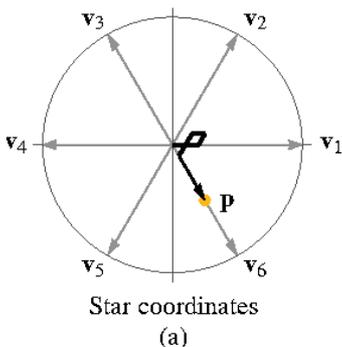


$$P = \sum_{i=1}^n w_j v_j$$

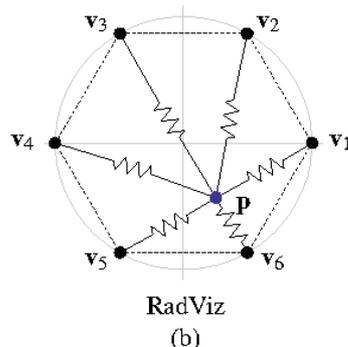
$$w_i = d_j / \sum_{k=1}^n d_k$$

$v_j$ : attribute coordinates on disk boundary  
 $d_j$ : data vector values  
 $P$ : point location in RadViz disk

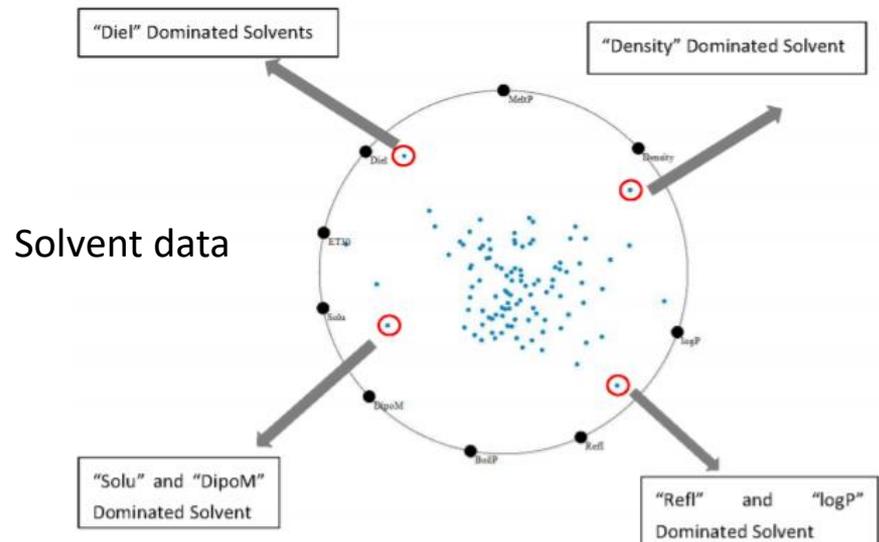
$$\frac{x}{\sum x} = (0.2, 0.1, 0, 0.1, 0.2, 0.4)$$



$$x = (0.5, 0.25, 0, 0.25, 0.5, 1)$$



Comparison with Star-coordinates



# RADAR CHART

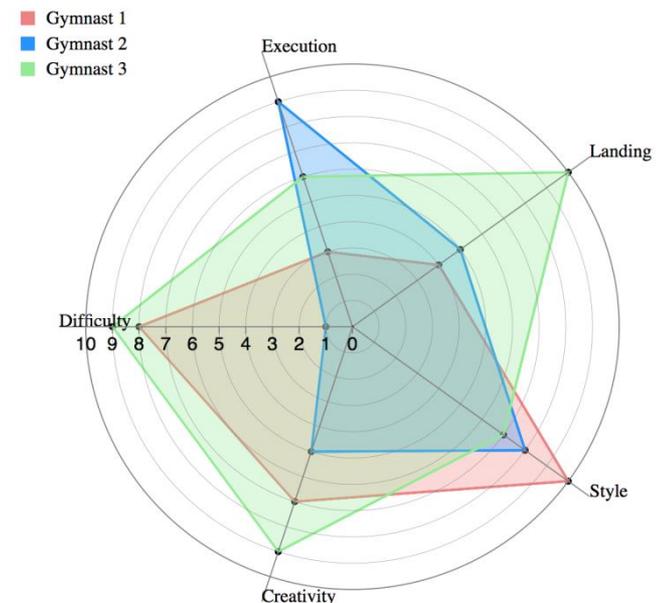
Equivalent to a parallel coordinates plot, with the axes arranged radially

- each star represents a single observation
- can show outliers and commonalities nicely

## Disadvantages

- hard to make trade-off decisions
- distorts data to some extents when lines are filled in

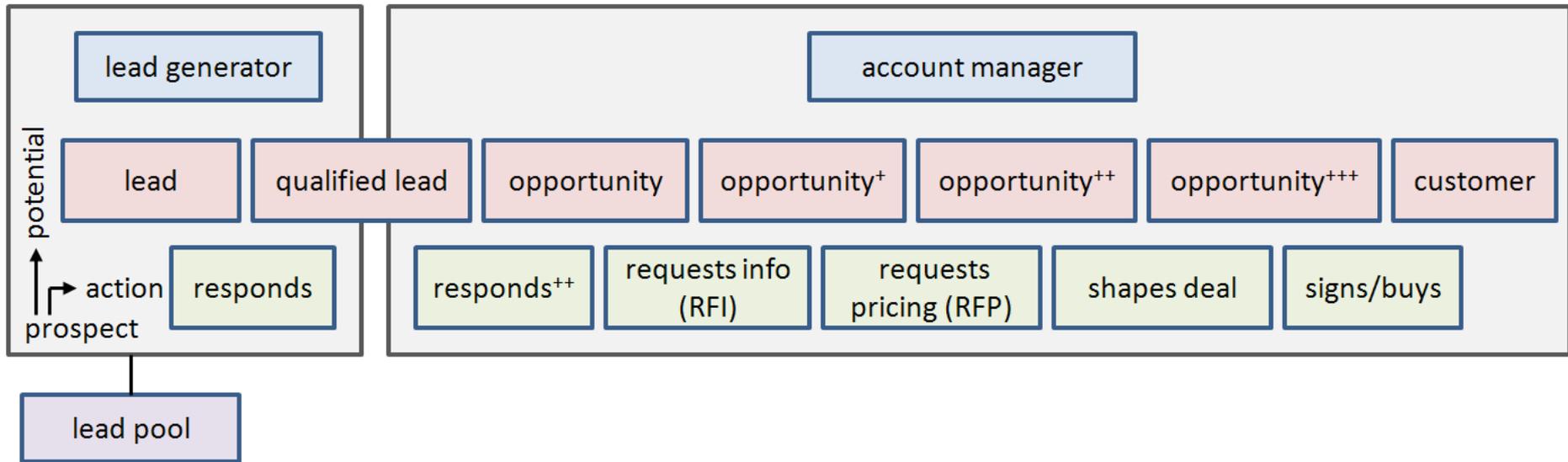
Gymnast Scoring Radar Chart



# TELLING STORIES WITH PARALLEL COORDINATES

EXAMPLE: SALES STRATEGY ANALYSIS

# ANATOMY OF A SALES PIPELINE



# THE SETUP

## Scene:

- a meeting of sales executives of a large corporation, Vandelay Industries

## Mission:

- review the strategies of their various sales teams

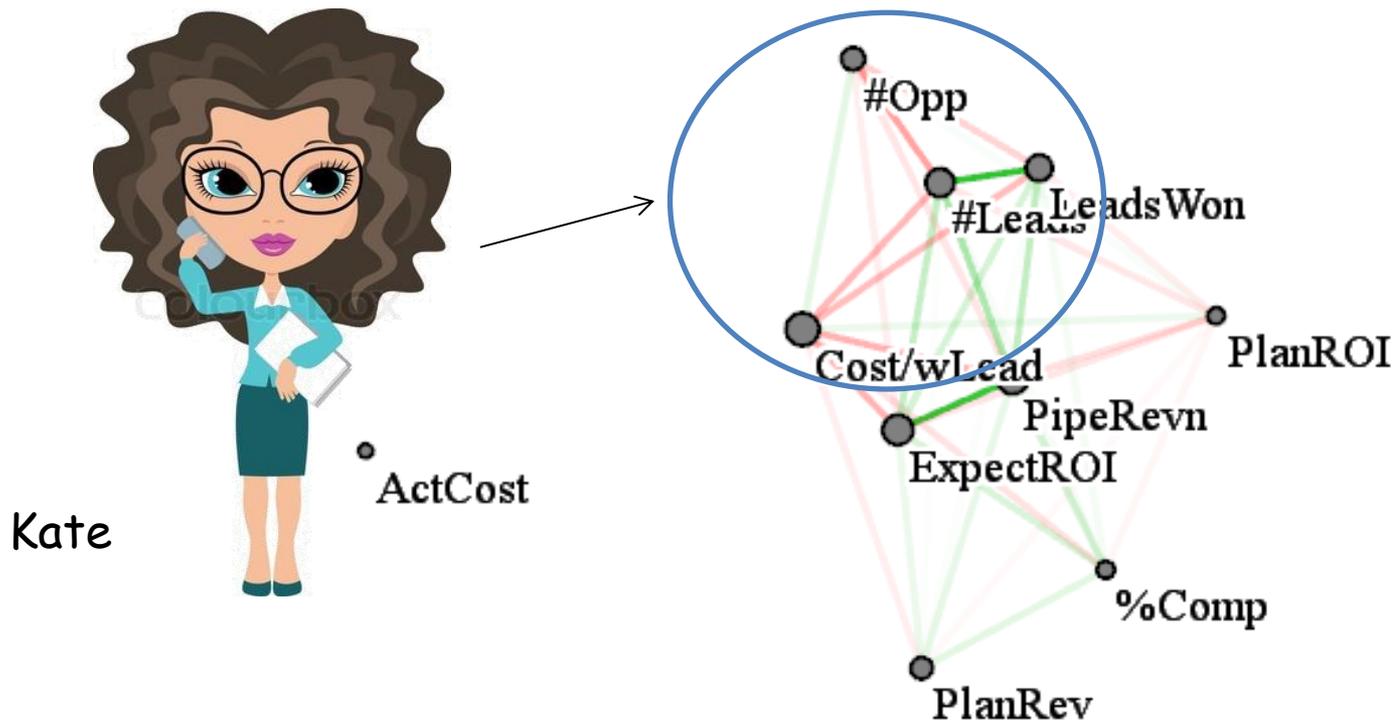
## Evidence:

- data of three sales teams with a couple of hundred sales people in each team

# KATE EXPLAINS IT ALL

Meet Kate, a sales analyst in the meeting room:

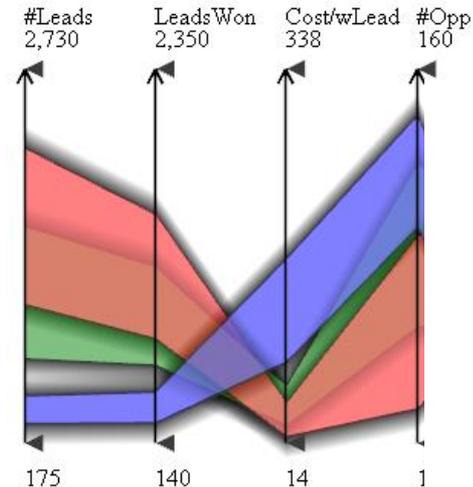
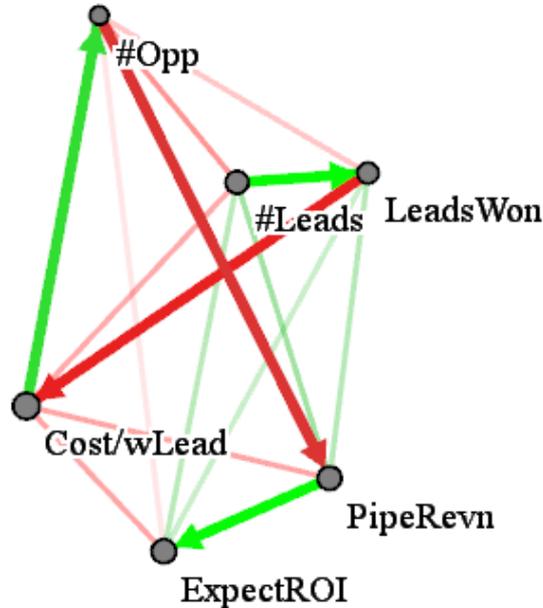
“OK...let’s see, cost/won lead is nearby and it has a positive correlation with #opportunities but also a negative correlation with #won leads”



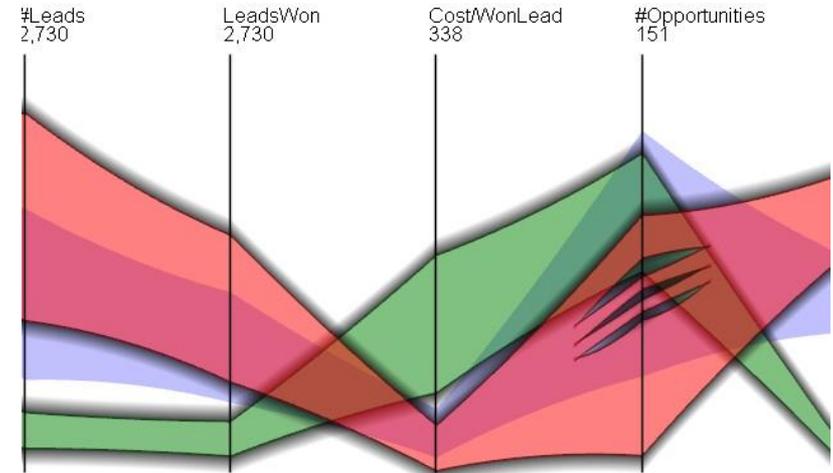
# KATE DESIGNS THE NARRATION

“Let’s go and make a revealing route!”

- she uses the mouse and designs the route shown
- she starts explaining the data like a story ...



# FURTHER INSIGHT



Kate notices something else:

- now looking at the red team
- there seems to be a spread in effectiveness among the team
- the team splits into three distinct groups

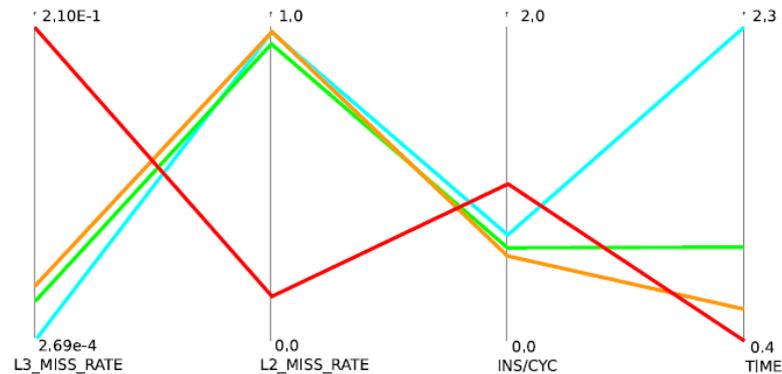
She recommends: "Maybe fire the least effective group or at least retrain them"

# HOW TO TEACH MAINSTREAM USERS

# RECENT REVIEWER COMMENT

From a paper sent to a software visualization conference:

Figure 8

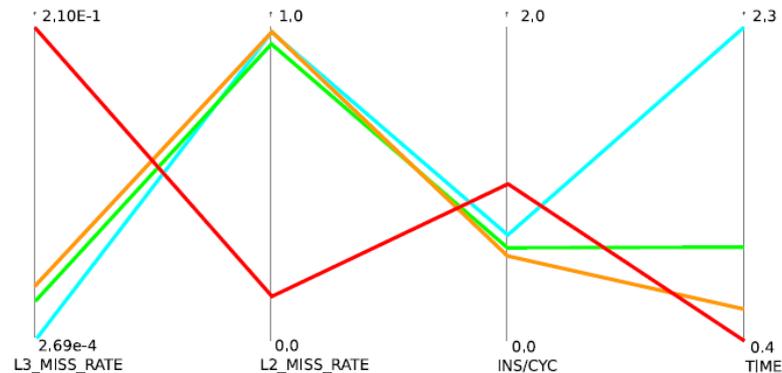


- Multiple visualizations appear to present categorical data as line graphs, which seems a strange choice.

# RECENT REVIEWER COMMENT

From a paper sent to a software visualization conference:

Figure 8

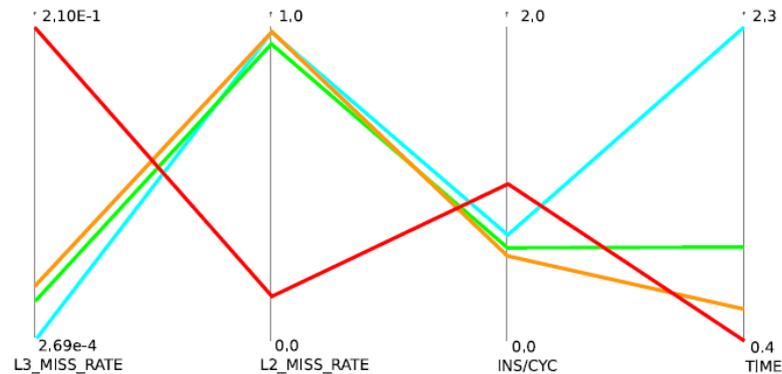


- Multiple visualizations appear to present categorical data as line graphs, which seems a strange choice. Figure 8, for example, at first sight appeared to be showing a change over time, but in fact further inspection shows that the different x-coordinates are almost entirely unrelated to one another and in no particular order.

# RECENT REVIEWER COMMENT

From a paper sent to a software visualization conference:

Figure 8



- Multiple visualizations appear to present categorical data as line graphs, which seems a strange choice. Figure 8, for example, at first sight appeared to be showing a change over time, but in fact further inspection shows that the different x-coordinates are almost entirely unrelated to one another and in no particular order. This is such an unusual choice that I'm not sure that I am understanding the role of the graphs correctly.

# Learning Visualizations by Analogy

Puripant Ruchikachorn and Klaus Mueller



Stony Brook  
University

<https://www.youtube.com/watch?v=mdolkHA-RpA>

# USER STUDIES

## Encode user responses based on task complexities

- none (0): cannot report any findings
- low (1): understand representation visual encoding
- medium (2): identify groups and outliers
- high (3): recognize correlations and trends

# USER STUDIES – CAR DATASET

## Visual understanding:

- (1) The MPG of the orange-highlighted car is ~40% of its range
- (2) There is just one line at the top of the acceleration scale
- (3) Heavier cars are faster

## Data Understanding:

- (1) The number of cylinders of the orange-highlighted car is 4, one fifth between 3 and 8.
- (2) Many cars have the same numbers of cylinders, mostly even numbers particularly 4 and 8.
- (3) Heavier cars have more cylinders and hence more horsepower and speed.

# RESULTS

<i>Participants</i>		V1	V2	V3	V4	V5	V6	V7	V8	V9	V10	V11
Parallel Coordinates Plot	Before	3	0	0	0	1	0	2	1	0	3	3
	After	3	2	2	1	2	2	3	2	1	3	3
	Diff.	0	2	2	1	1	2	1	1	1	0	0

D1	D2	D3	D4	D5	D6	D7	D8	D9	D10	D11
0	2	3	1	1	3	1	1	2	0	3
2	3	3	3	1	3	2	2	3	2	3
2	1	0	2	0	0	1	1	1	2	0

NEXT LECTURE:  
NON-LINEAR PROJECTION  
TECHNIQUES (EMBEDDINGS)