R Fundamentals and Best Practices for Mass Spectrometry Data Analysis

Sunday, November 8 (12:00-3:15pm Eastern)

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Module #3: Basic data cisualization with ggplot2

Module #4: Data preparation for visualization & extended ggplot2

Data Visualization

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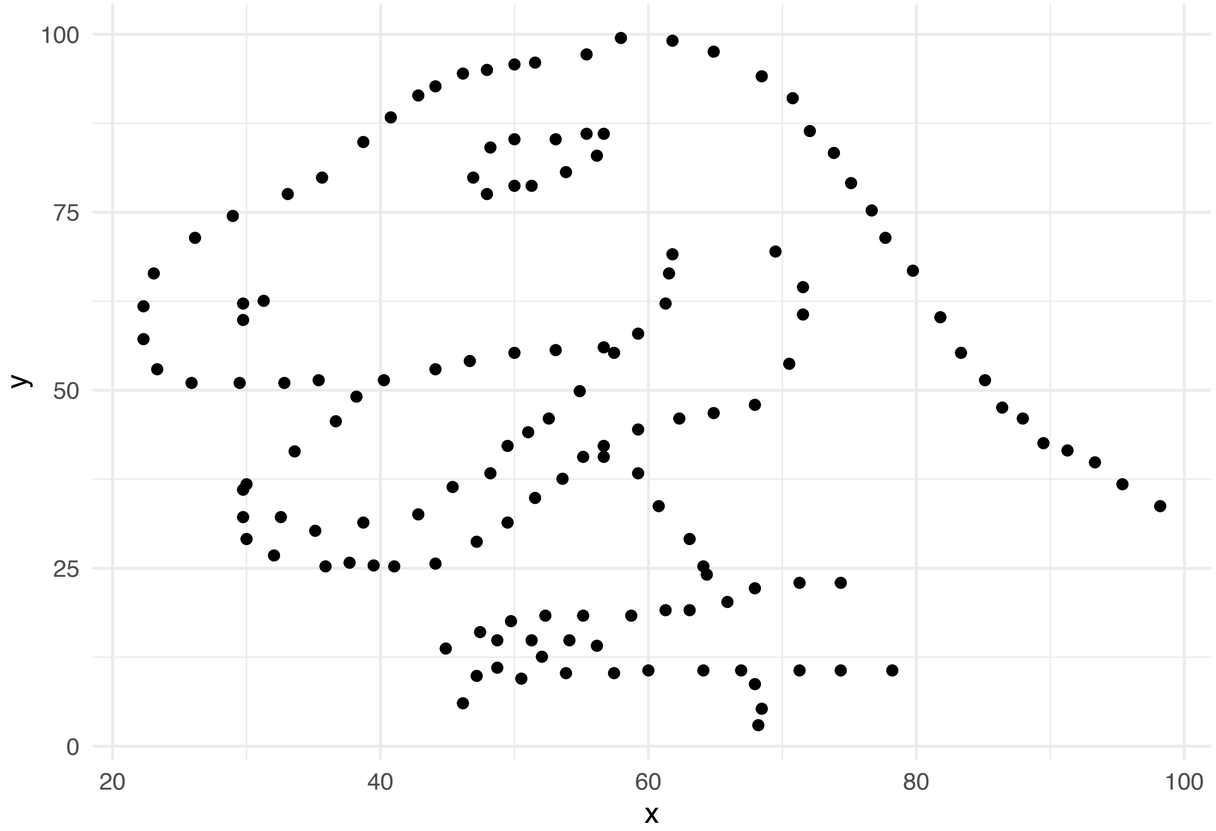
STATISTICAL GRAPHICS: WHY WE LOOK AT DATA

Why do we look at data?

Dataset #1:



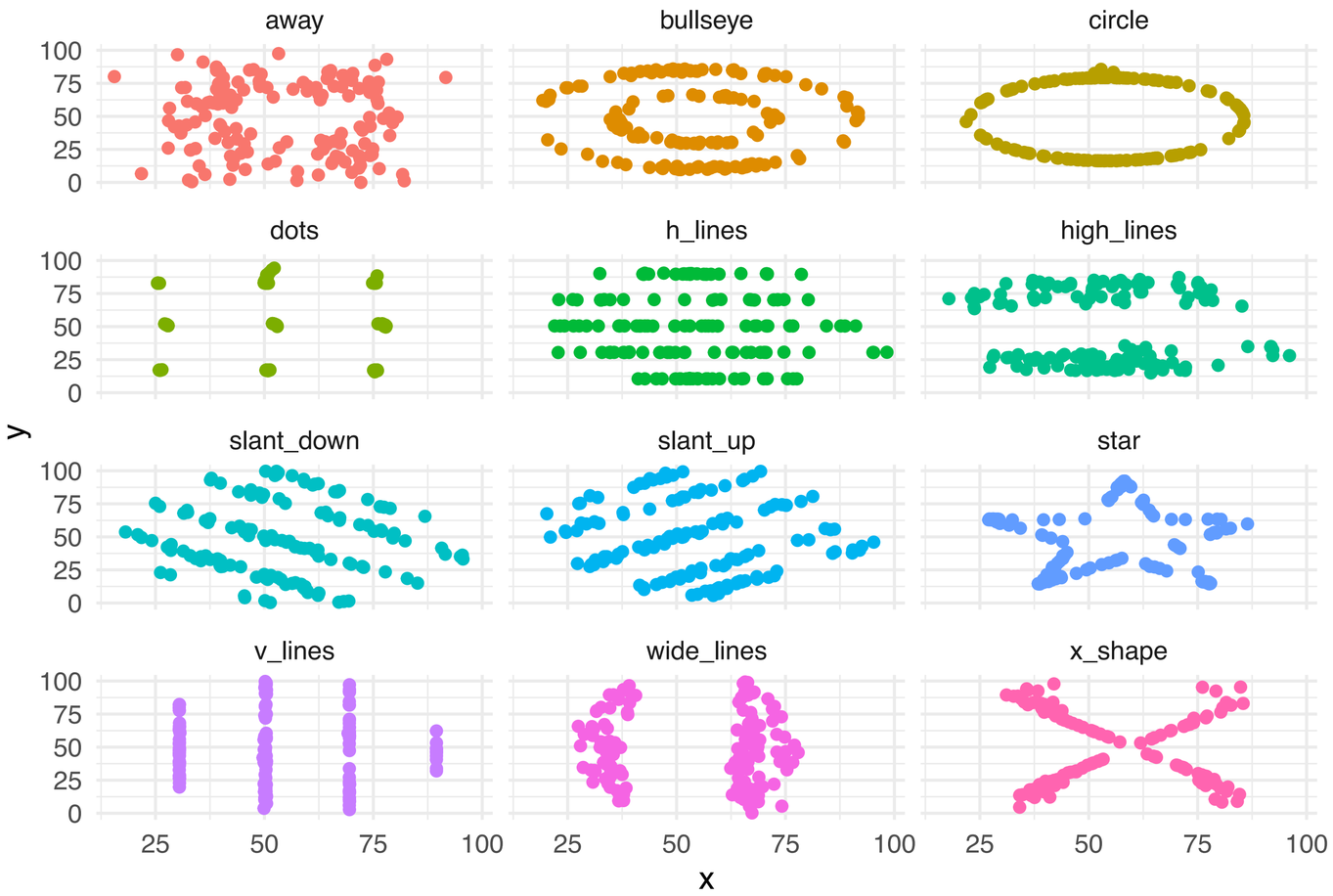
How similar are the other 12 datasets?

13 datasets with same statistics:

X mean	54.26
Y mean	47.83
X std. dev	16.76
Y std. dev	26.93
Correlation	-0.06

Why we look at data

Datasets #2-13:



X mean	54.26
Y mean	47.83
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"The Datasaurus Dozen": https://www.autodeskresearch.com/publications/samestats

Looking at data is important

- Summary statistics don't tell whole story
- Easily find patterns
- Identify potential outliers
- Check model assumptions
- Intuitively display results

What are some common ways of looking at data?

Some common statistical graphics

- Scatter plot
- Line plot
- Box-and-whisker plot
- Histogram
- Bar plot

Roles of statistical graphics

One variable

- Histogram
- Bar plot
- Box plot
- Pie chart

Two or more variables

- Scatter plot
- Line plot
- Box plot
- Faceting

Roles of statistical graphics

Distributions

- Histogram
- Bar plot
- Box plot
- Pie chart

Relationships

- Scatter plot
- Line plot
- Box plot
- Faceting

A GRAMMAR OF GRAPHICS

How do we plot data?

- By using the "name" of graphic?
  - Scatter plot
  - Box plot
  - Histogram
- Using "base" R (and similar approaches):
  - `plot()` - scatter plot
  - `boxplot()` - box plot
  - `hist()` - histogram

Is there a better way?

What are some common ingredients of statistical graphics?

Recipes for common statistical graphics

- Scatter plot
  - Maps variables to x- and y- axes
  - Uses points to represent observations
- Line plot
  - Maps variables to x- and y- axes
  - Uses lines to connect observations
- Box plot
  - Maps 5-number summary to x- or y-axis
  - Uses boxes and whispers to show this
- Histogram
  - Maps bins to x-axis and binned counts to y-axis
  - Uses bars+length to represent counts
- Bar plot
  - Maps categories to x-axis and counts to y-axis
  - Uses bars+length to represent counts
- Pie chart
  - Maps categories to color and proportion to angle
  - Uses wedges+area to represent proportions

Key ingredients for statistical graphics

- Some kind of data
- Encodings from data to aspects of the plot
  - Marks ("**geometric objects**", e.g., points and lines)
  - Channels ("**aesthetics**", e.g., color and size)
- Statistical transformations
- Coordinate system
- Scales and annotations

Building a plot

Consider a simple dataset:

A	*B*	*C*	*D*
2	3	4	a
1	2	1	a
4	5	15	b
9	10	80	b

http://vita.had.co.nz/papers/layered-grammar.pdf

How do we create a scatter plot of A versus C?

What if we want to include D?

Building a plot

We map the x-axis to **A**, the y-axis to **C**, and shape to **D**

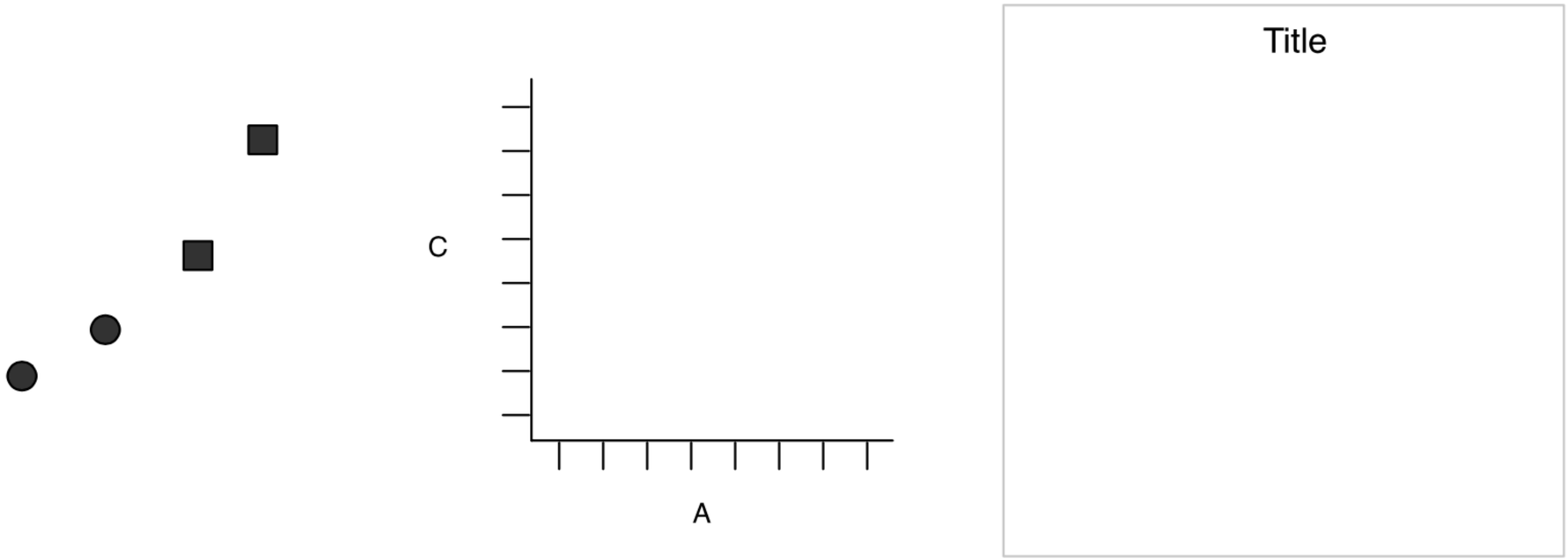
x	*y*	Shape
2	4	circle
1	1	circle
4	15	square
9	80	square

http://vita.had.co.nz/papers/layered-grammar.pdf

This is the "aesthetic mapping" of the plot

Building a plot

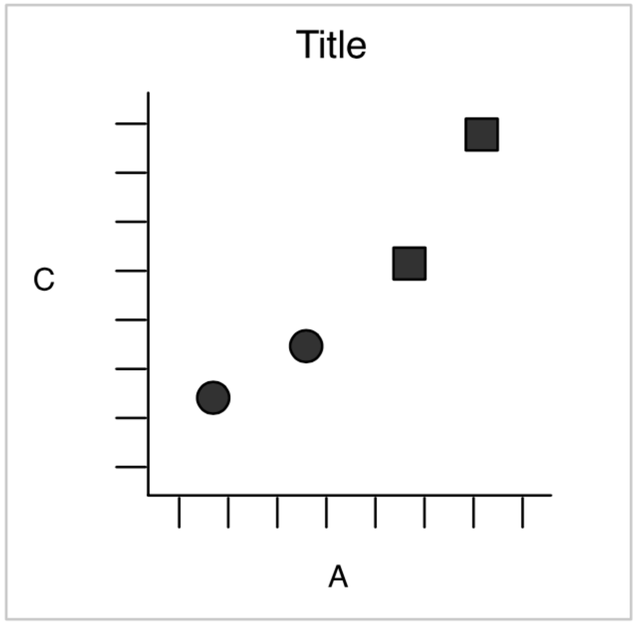
We have (1) marks or **geometric objects**, (2) **scales** and a **coordinate system**, and (3) plot **annotations**



http://vita.had.co.nz/papers/layered-grammar.pdf

Building a plot

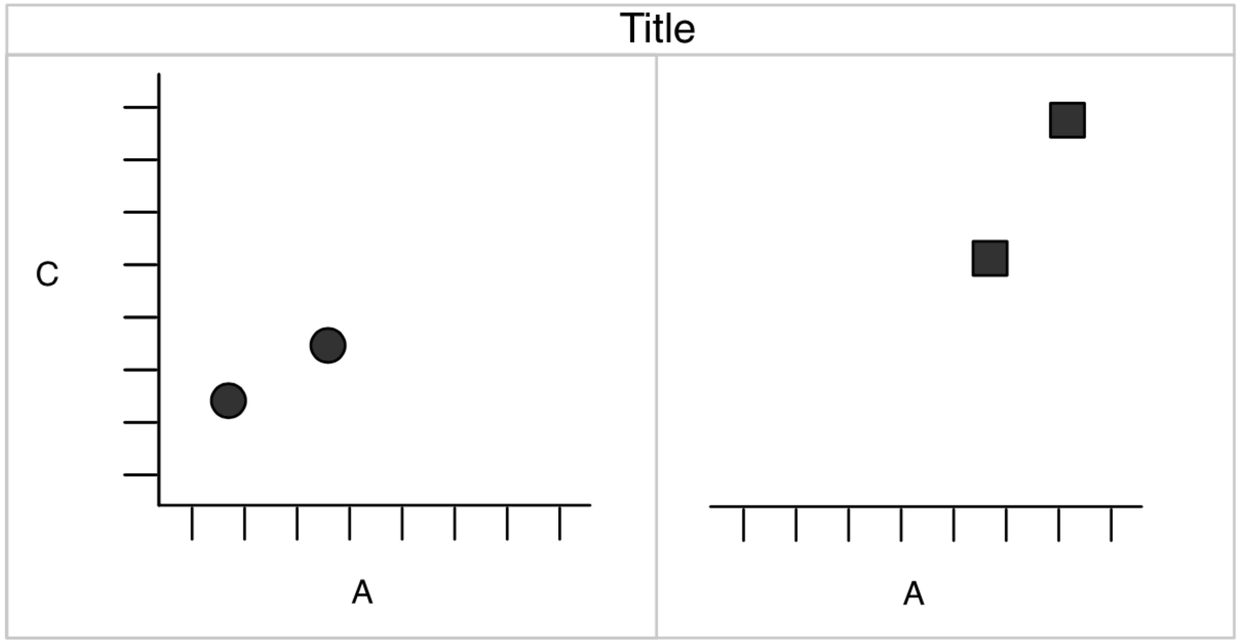
Putting the ingredients together, we have a plot:



http://vita.had.co.nz/papers/layered-grammar.pdf

Building a plot

If we want to compare the relationship between **A** and **C** for each level of **D**, we can facet on **D**



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Faceting splits the data into subsets and creates sub-plots for each subset

Building a vocabulary

We can build more complicated plots by adding to our vocabulary:

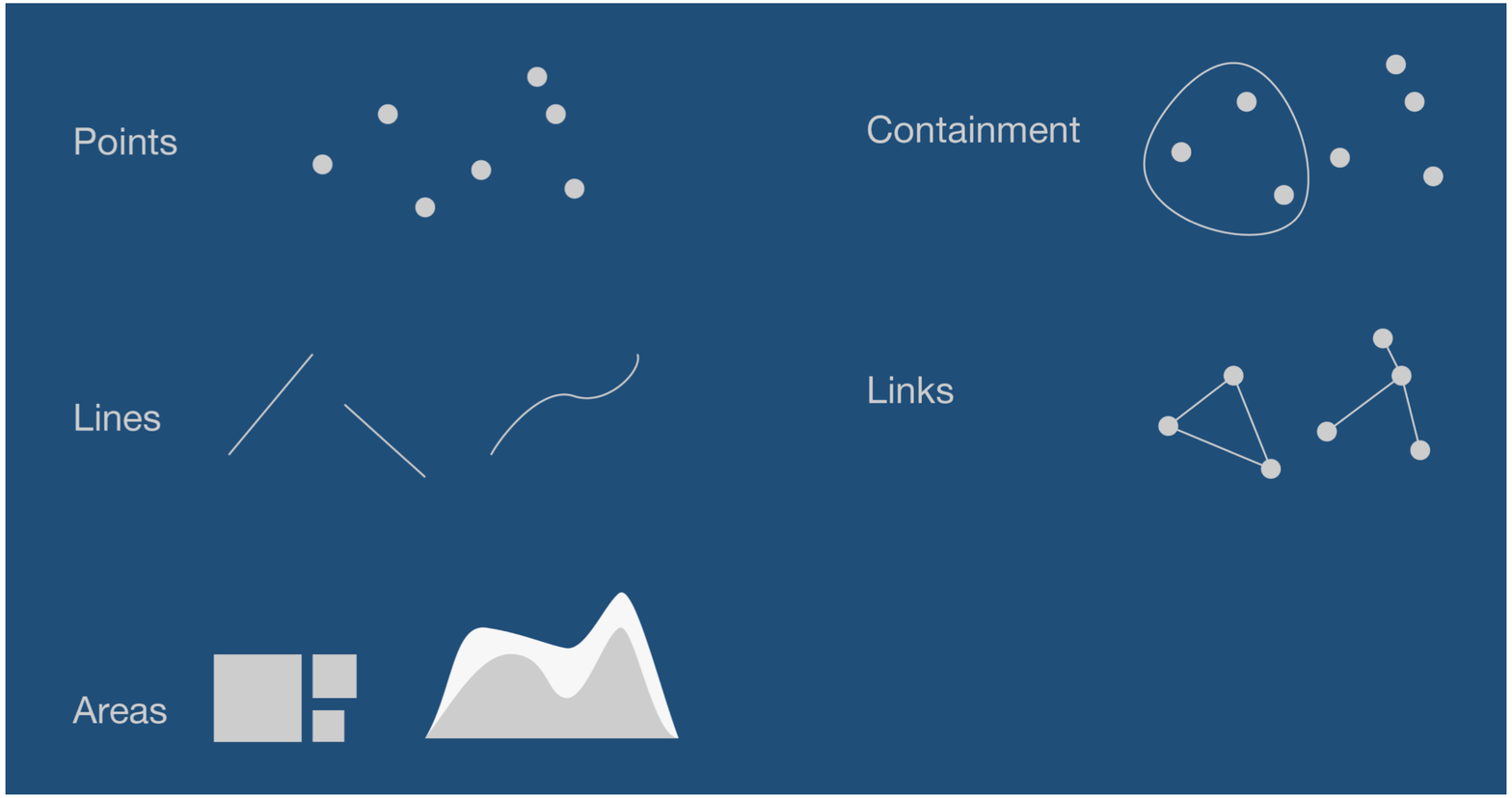
- Layers to overlay plots on top of each other
- Multiple datasets on the same plot
- Apply statistical transformations (e.g., binning)
- Apply position adjustments (e.g., jitter)
- *A way to build such plots programmatically*

A layered grammar of graphics

- Default dataset
- Default set of mappings from variables to graphical aesthetics
- One or more layers, each having:
  - Mark, or geometric object
  - Statistical transformation
  - Position adjustment
  - (Optionally) new dataset
  - (Optionally) new set of aesthetic mappings
- Scale for each mapped aesthetic
- Facet specification

Visual encodings: Marks

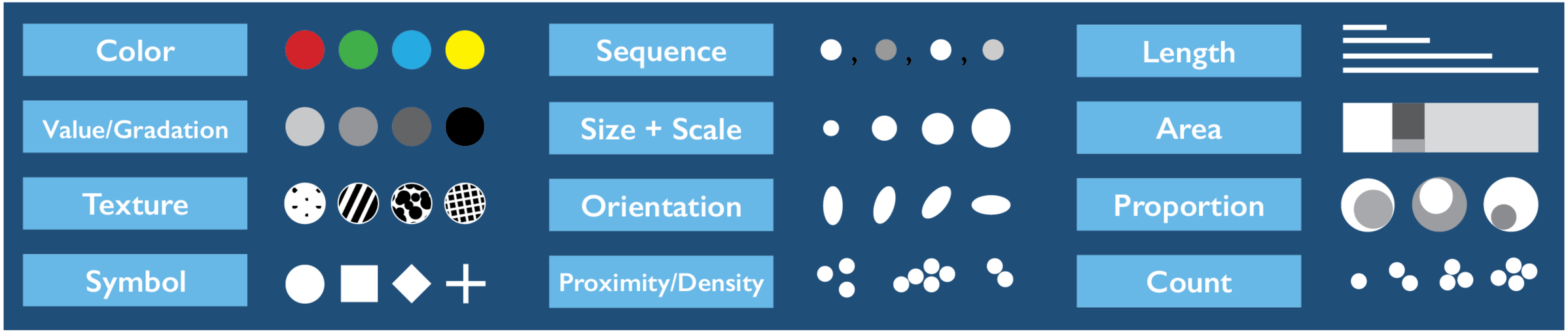
Marks, or **geometric objects**, draw the graphic



Courtesy of Steven Braun, CAMD Art + Design

Visual encodings: Channels

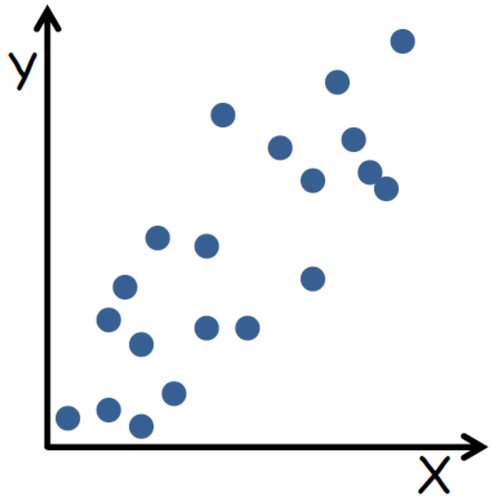
Channels, or **aesthetics** + **scales**, encode values



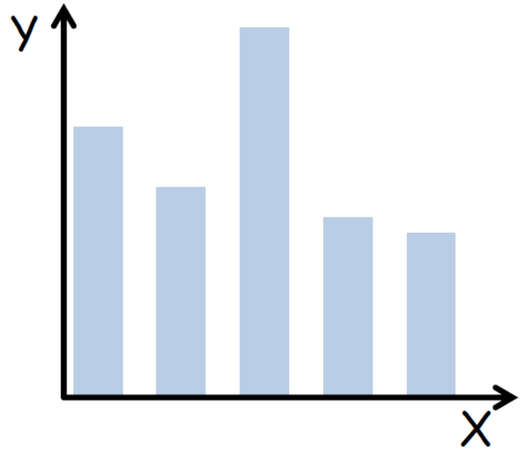
Courtesy of Steven Braun, CAMD Art + Design

Choosing visual encodings

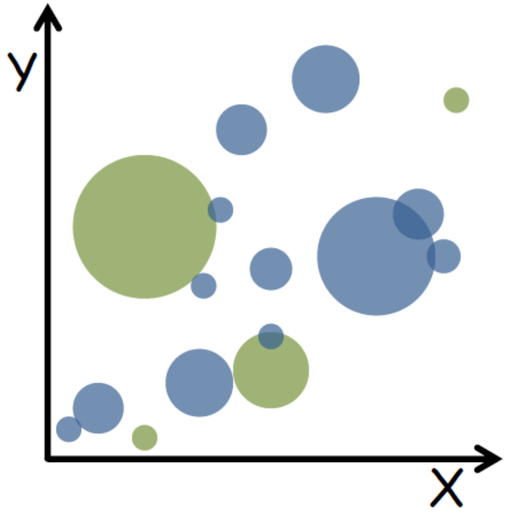
Your choice of **geometric objects,**
aesthetic mappings, and **scales** define the graphic



Marks: points
Channels: position



Marks: lines
Channels: length, position



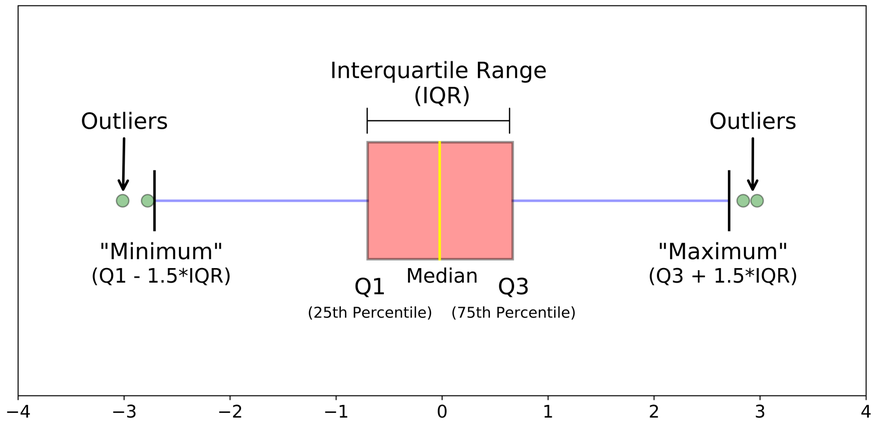
Marks: points
Channels: position, size, color

Courtesy of Steven Braun, CAMD Art + Design

Statistical transformations

Many statistical graphics utilize **statistical transformations**:

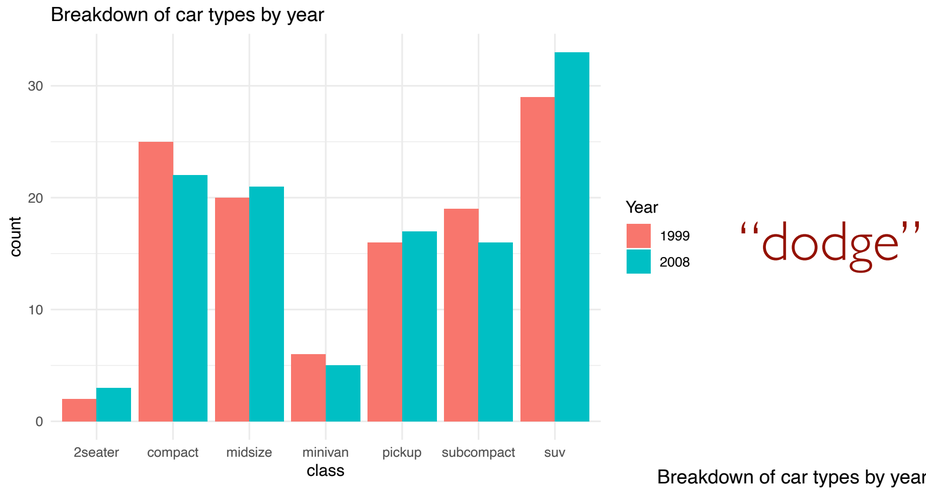
- Box plot
  - Five-number summary + outliers
- Histogram
  - Binning
- Bar plot
  - Counting



Position adjustments

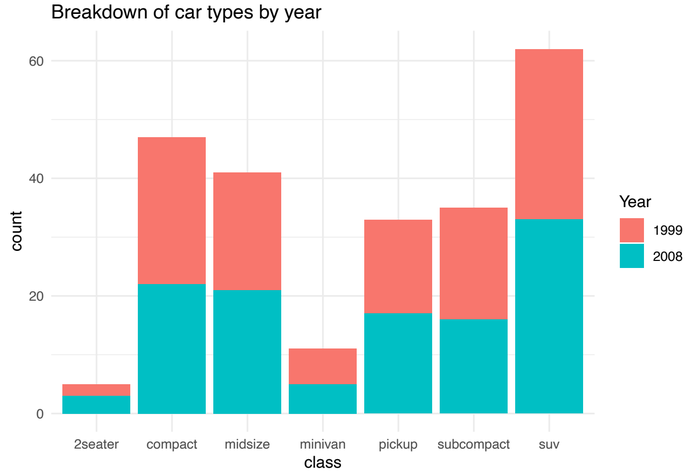
Many statistical graphics require **position adjustments**

- Scatter plot
  - Jitter
- Bar plot
  - Dodge
  - Stack



"dodge"

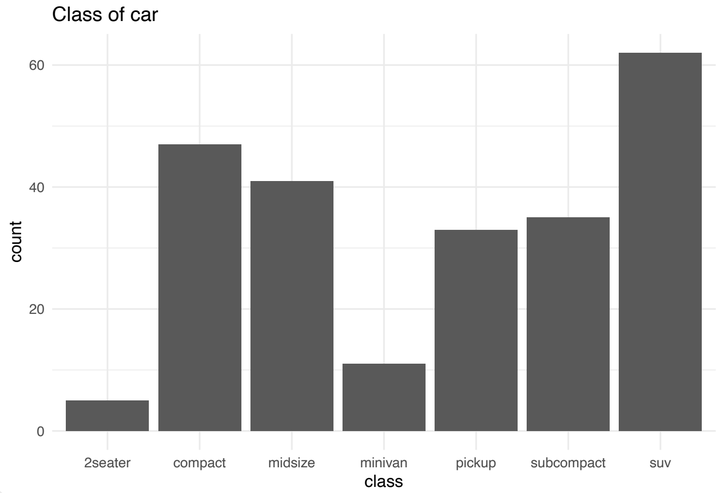
"stack"

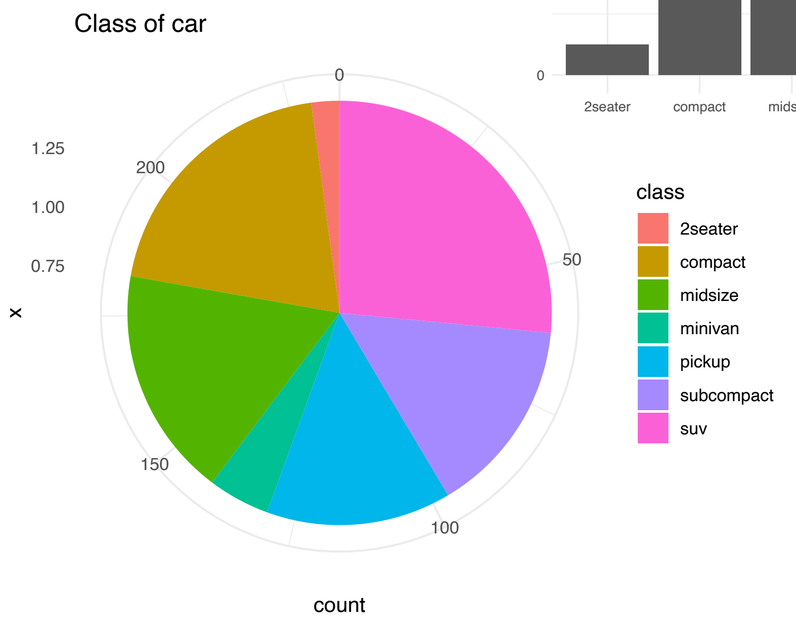


Coordinate systems

Some graphics may require different **coordinate systems**

- Cartesian
- Polar
- Map





Implementing a grammar of graphics

A version of the "layered grammar of graphics" is implemented in **ggplot2**:


```
ggplot(data = <DATASET>,
       mapping = aes(<MAPPINGS>)) +
  layer(geom = <GEOM>,
        stat = <STAT>,
        position = <POSITION>) +
  <SCALE_FUNCTION>() +
  <COORDINATE_FUNCTION>() +
  <FACET_FUNCTION>()
```

or, more simply:

```
ggplot(data = <DATASET>,
       mapping = aes(<MAPPINGS>)) +
  <GEOM_FUNCTION>()
```

Recipes for common statistical graphics

- Scatter plot
  - Geom = "point"
  - Stat = "identity"
- Line plot
  - Geom = "line"
  - Stat = "identity"
- Box plot
  - Geom = "boxplot"
  - Stat = "boxplot"
- Histogram
  - Geom = "bar"
  - Stat = "bin"
- Bar plot
  - Geom = "bar"
  - Stat = "count"
- Pie chart
  - Geom = "bar"
  - Stat = "count"

+ coords = "polar"

GGPLOT2

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Gopalika Shama
Rishabh Rajesh Shanbhag
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Sara Taheri
Anuska Tak
Derrie Susan Varghese
Amrutha Vempati

Video of the presentation: https://www.youtube.com/channel/UCnbUMFlIRLaY7fwfSintWuQ/