VISUALIZATION WITH GGPLOT2
LECTURE: UNSUPERVISED LEARNING AND EVOLUTIONARY COMPUTATION USING R

Jakob Bossek

MALEO Group, Department of Computer Science, Paderborn University, Germany

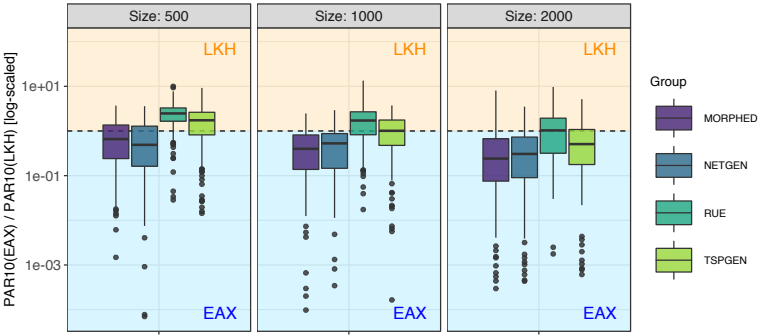
28th Oct, 2024

Table of Contents

Gallery

Gallery

Examples of `ggplot2` visualizations from my research:



Introduction

Introduction

What is ggplot2 and why should I use it?

- Powerful R package for data visualization
- Based on the *Grammer of Graphics*[1] by Leland Wilkinson (Wilkinson 2005)
- Easy to learn and full of features
- Active development (steady implementation of new features, bugfixes)
- Active and helpful community (mailing list, stack overflow)
- In the meanwhile de-facto standard for visualization in R
- Using `ggplot2` is fun!

[1] Extended to the *layered Grammer of Graphics* by Hadley Wickham.

Sorry, I hate R!

No worries! You can translate what you learn today (grammer of graphics) to other languages:

Libraries inspired by `ggplot2`

- `gadfly` for the Julia language[2]
- Python implementation ggpy[3]
- ggramm for Matlab
- GGPlot for Perl
- etc.

[2] Very young (2009), high-performance general-purpose language with focus on numerical calculations and computational science.

[3] Alternative: call R functions directly from Python, e.g., with `rpy2`.

Advantages vs disadvantages

Advantages ☺

- High level of abstraction
- Produces high-quality images
- Sticks to essential graphics design rules
- Easy to generate "new", outstanding visualizations
- Basics not that difficult to learn
- Build complex visualizations (given some effort)

Disadvantages ☹

- Data in data frame ~~Data in data frame~~

  Not a disadvantage in my eyes!
- No support for 3D data

  Unfortunately no support planned, but there are similar alternatives: `rayshader` or `plotly`!
- No graph theory stuff

  ~~No graph theory stuff~~

  Actually not true anymore! See packages `ggnet2`, `geomnet` or `ggnetwork` Tyner, Briatte, and Hofmann 2017

Prerequisite: tidy data

Unsurprinsingly, as `ggplot2`'s creator and main developer is Hadely Wickham, `ggplot2` operates on tidy data.

Recall: Rectangular data is tidy if ...

- Each column is a variable
- Each row is an observation
- Each observational unit has its own table

Use `tidyverse` funtionality to tidy data!

Basic concepts

Grammer of Graphics

Hadley (Wickham 2009) describes the idea as follows:

> *. . . the grammar tells us that a statistical graphic is a mapping from data to aesthetic attributes (colour, shape, size) of geometric objects (points, lines, bars). The plot may also contain statistical transformations of the data and is drawn on a specific coordinate system . . .*

- Abstraction of graphics ideas and objects
- Allow "theoretical" discussion of how (new) graphics are composed
- Much like in spoken language it allows for extension and adapation to new (previously unseen) situations

Grammer of Graphics

- Introduced by Leland Wilkinson (2005) to give an answer to the question: *What is a statistical graphic?*
- Core idea: graphic is composed of of different layers
- In each layer data is mapped to different aesthetics attributes (e.g., colour) of geometric objects (e.g., points)
- Abstraction of low-level plots
- $\rightsquigarrow$ no named methods like plot, hist or scatterplot

Are you confused?

Does not matter! You can generate all types of basic plots without a deep understanding of the underlying principles ☺

Basic vocabulary

data The actual data (always a R data frame)

aesthetics Visual properties *mapped* to variables of the data (i.e., columns of the data frame)

- Map categorical variable `sex` to colour: male → red, female → blue
- Also possible: map continuous variable `temperature` to colour

geoms Short version of *geometric objects*; actual type of object to display (e.g., point, boxplot, . . .)

facets Use multiple panels to plot subsets of the data

Starting with ggplot

CRAN version[4]

```
> install.packages("ggplot2")
> library(ggplot2)
```

Development version

Useful to check out and experiment with upcoming features:

```
> install.packages("devtools")
> devtools::install_github("tidyverse/ggplot2")
> library(ggplot2)
```

[4] Current version number is 3.3.5

Starting with ggplot (cont.)

Data set diamonds

Should be familiar: data on $\approx 54\,000$ diamonds:

```
> require(ggplot2, quiet = TRUE)
> data(diamonds)
> ds = subset(diamonds, color %in% c("F", "G", "H", "I"))
> set.seed(123)
> ds = ds[sample(1:nrow(ds), size = 200L, replace = FALSE), ]
> head(ds, n = 6L)

## # A tibble: 6 x 10
##   carat cut     color clarity depth table price     x     y     z
##   <dbl> <ord>   <ord> <ord>   <dbl> <dbl> <int> <dbl> <dbl> <dbl>
## 1  1    Good    H     SI2      63.2    60  3740  6.27  6.3   3.97
## 2  0.3  Ideal   H     VS1      61.6    55   526  4.27  4.3   2.64
## 3  0.52 Ideal   H     VVS1     61      56  1748  5.17  5.21  3.17
## 4  0.9  Premium G     SI1      61.9    59  3669  6.18  6.13  3.81
## 5  0.3  Ideal   F     VS2      61.4    57   605  4.34  4.36  2.67
## 6  0.98 Premium I     I1       59.6    60  2064  6.43  6.3   3.79
```

Starting with ggplot2 (cont.)

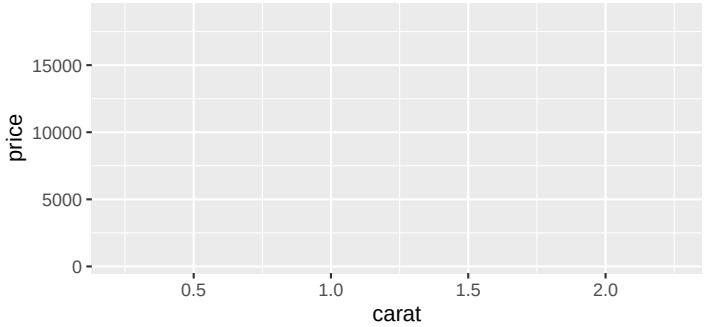
We want a scatterplot of carat vs price

```
> ggplot(ds) # empty plot
```

Starting with ggplot2 (cont.)

We want a scatterplot of carat vs price

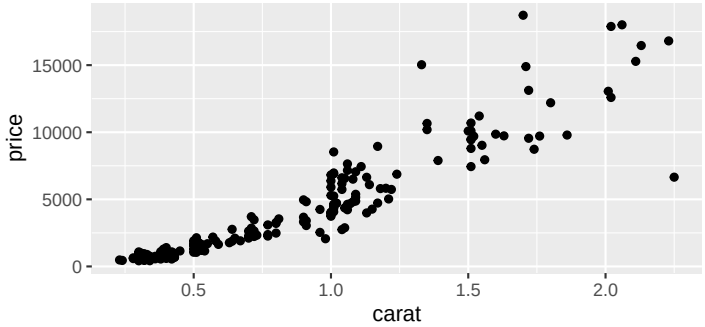
```
> ggplot(ds, aes(x = carat, y = price)) # map aesthetics
```



Starting with ggplot2 (cont.)

We want a scatterplot of carat vs price

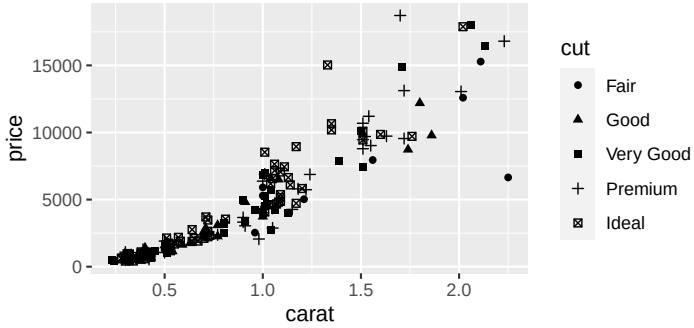
```
> ggplot(ds, aes(x = carat, y = price)) + geom_point() # add objects
```



Starting with ggplot2 (cont.)

Now we want the points to be shaped by `cut`:

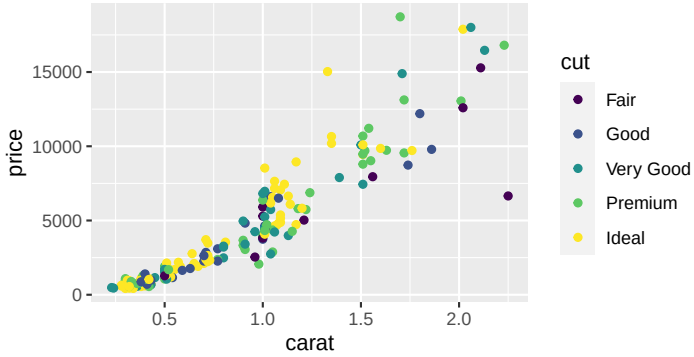
```
> g = ggplot(ds, aes(x = carat, y = price, shape = cut))
> g + geom_point()
```



Starting with ggplot2 (cont.)

Alternatively let's map `cut` to the colour aesthetic:

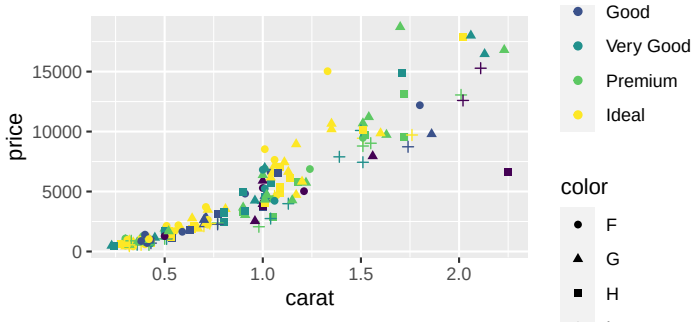
```
> g = ggplot(ds, aes(x = carat, y = price, colour = cut))
> g + geom_point()
```



Starting with ggplot2 (cont.)

Now we want to distinguish between `cut` and `color`.

```
> g = ggplot(ds, aes(x = carat, y = price, colour = cut, shape = color))
> g + geom_point()
```



Starting with ggplot2 (cont.)

Let's dive in the syntax of ggplot2

- Use the ggplot command to pass *data* and set *aesthetics*

```
> g = ggplot(data = ds, mapping = aes(x = carat, y = price, colour = cut))
```

- Produces **plot object**, i.e., special R object with class attribute *ggplot*
- First parameter is the source data to display
- Second parameter is the aesthetics mapping, i.e., binding variables to visual properties
- Cannot be displayed without adding at least one **layer**

Starting with ggplot2 (cont.)

Let's dive in the syntax of ggplot2 (cont.)

- Add (*geometric* or *statistical*) layers to the base, e.g.,

```
> g = g + geom_point()
> g = g + geom_point(colour = "tomato", size = 2.1)
```

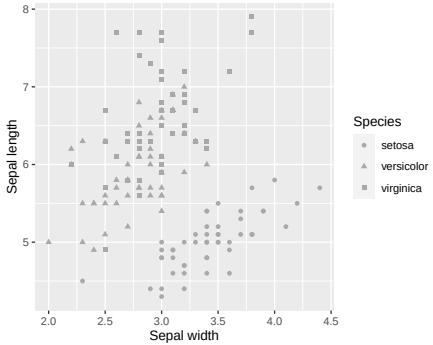
- The $+$ is here of course an overloaded version of the plus operation for objects of type *ggplot*
- There is a vast number of possible geoms, e.g., lines, bars, polygons, text, ...
- Each geometric layer can take its own aesthetics mapping (valid just for this layer)

Exercises

1. Install the `ggplot2` package on your system
2. Have a look at the `iris` dataset (`data(iris)`) and check its documentation. Generate a scatterplot of `Sepal.Width` vs. `Sepal.Length`
3. Change the colour of the points to gray
4. Find out how to change the axis labels
5. Assign distinct shapes to the points by `Species`

Sample solutions

```
> data(iris) # access docs with ?iris
> g = ggplot(iris, aes(x = Sepal.Width, y = Sepal.Length))
> g = g + geom_point(aes(shape = Species), color = "darkgray")
> g + labs(x = "Sepal width", y = "Sepal length")
```



Facetting

Starting with ggplot2 - Facets (cont.)

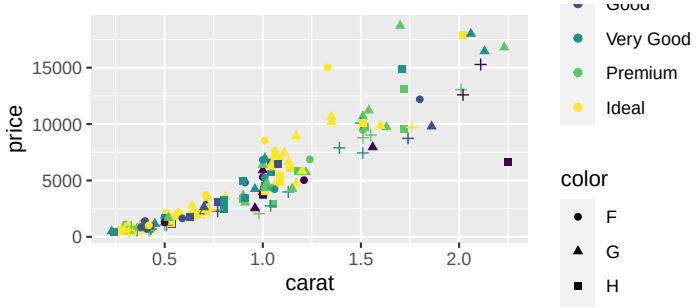
Facets

- Split data into subsets by one or two categorical variable(s)
- Render a seperate plot for each subset
- Function `facet_grid(formula, ...)` for crossing of one grouping variable
- Function `facet_wrap(formula, ...)` for crossing two grouping variables
- Keep in mind: for categorical variables with n and m respectivly factors levels you get a $m \times n$ matrix of panels

Starting with ggplot2 (cont.)

Remember that plot?

```
> g = ggplot(ds, aes(x = carat, y = price, colour = cut, shape = color))
> g + geom_point()
```

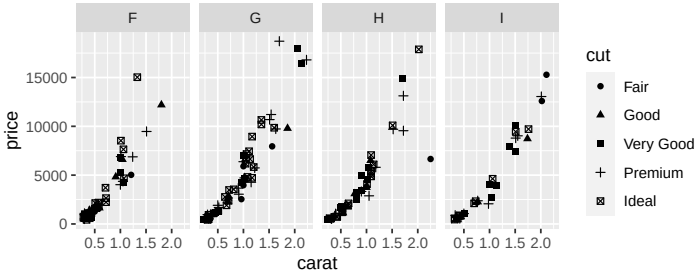


Confusing to recognize some structure here: too many colors and symbols.

Starting with ggplot2 - Facets

So let's try **facetting** and split our data according to color:

```
> g = ggplot(ds, aes(x = carat, y = price, shape = cut))
> g + geom_point() + facet_grid(. ~ color)
```

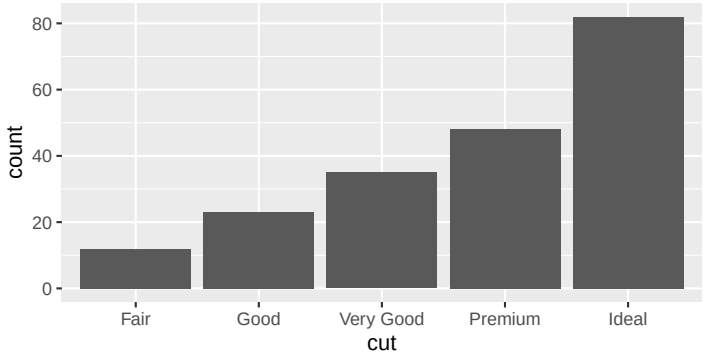


Basic plots

Basic plots - barplot

Check out the number of different *cuts* in the diamonds dataset:

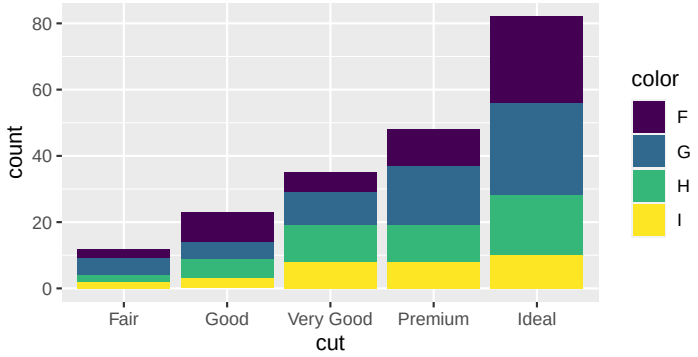
```
> ggplot(ds, aes(x = cut)) + geom_bar()
```



Starting with ggplot (cont.)

What about *cuts* and *color*?

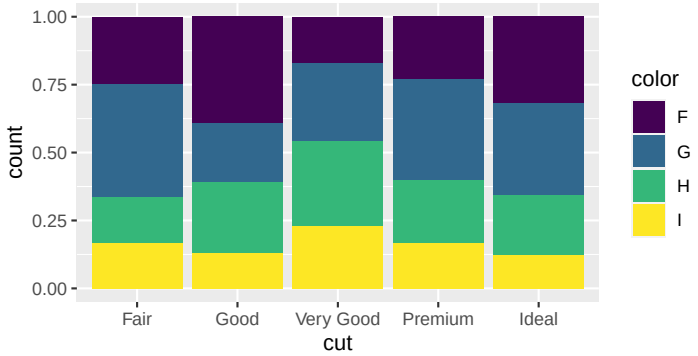
```
> ggplot(ds, aes(x = cut, fill = color)) + geom_bar()
```



Starting with ggplot (cont.)

Want the proportions instead of the absolute values?

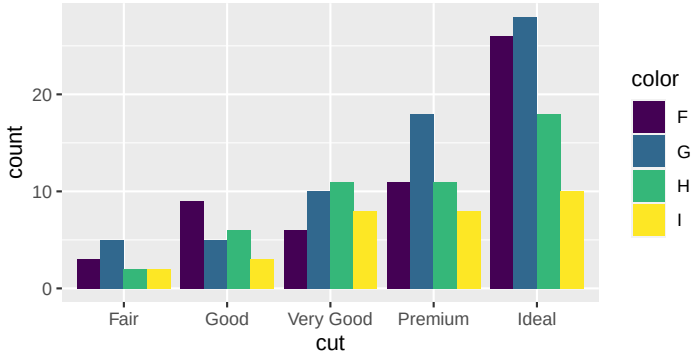
```
> ggplot(ds, aes(x = cut, fill = color)) + geom_bar(position = "fill")
```



Starting with ggplot (cont.)

Maybe we prefer to draw the bars side by side?

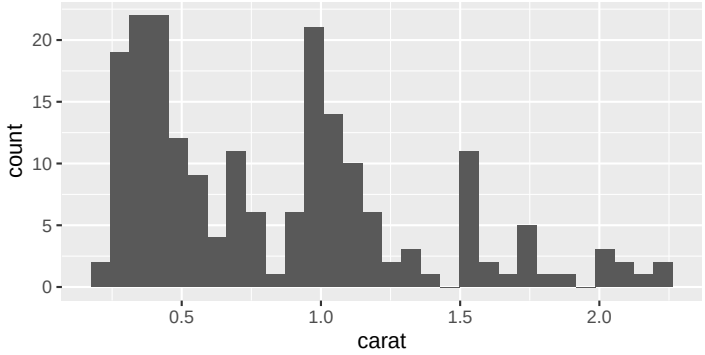
```
> ggplot(ds, aes(x = cut, fill = color)) + geom_bar(position = "dodge")
```



Basic plots - Histogram

Check out the distribution of the *carat* in the diamonds dataset:

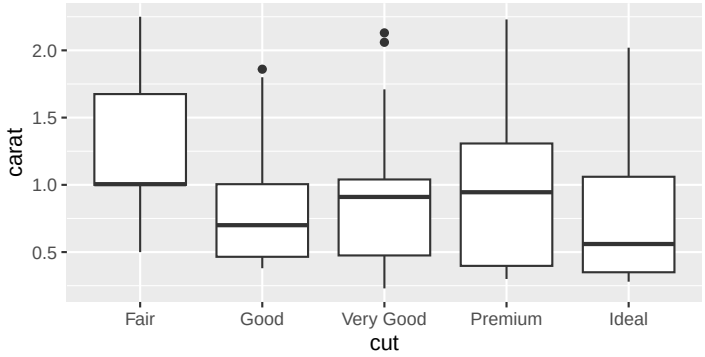
```
> ggplot(ds, aes(x = carat)) + geom_histogram()

## `stat_bin()` using `bins = 30`.  Pick better value with `binwidth`.
```



Basic plots - Histogram

Check out the distribution of *carat* by *cut*:

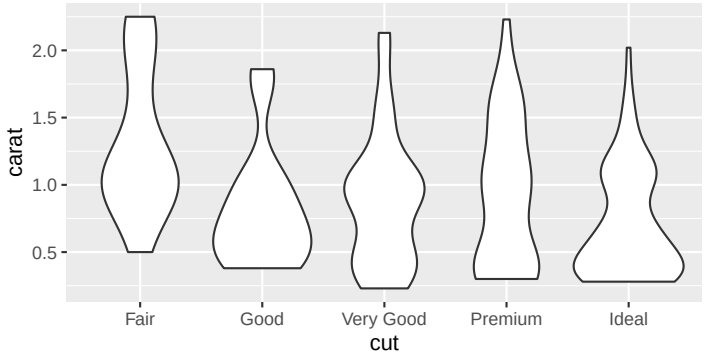
```
> ggplot(ds, aes(x = cut, y = carat)) + geom_boxplot()
```



Basic plots - Histogram

Check out the distribution of *carat* by *cut*:

```
> ggplot(ds, aes(x = cut, y = carat)) + geom_violin()
```



Exercises

1. Visualize the entire `price` distribution of `diamonds` with a density curve (`geom_density()`). Add a blue vertical dashed line indicating the mean value of the entire sample (`geom_vline()`)

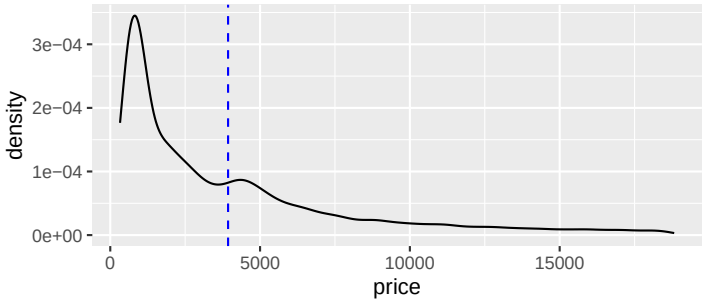
2. Now draw individual density curves splitting the data by `cut`. Try to draw vertical dashed lines indicating the mean value per group

3. Next, draw individual density curves splitting the data by `cut`, `color` and/or `clarity` (use facetting and mapping to colors). Hint: you might want to use only a subset of the data

Sample solutions i

1. Visualize the entire `price` distribution of `diamonds` with a density curve (`geom_density()`). Add a blue vertical dashed line indicating the mean value of the entire sample (`geom_vline()`)

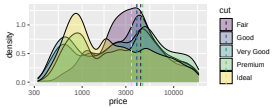
```
> g = ggplot(diamonds, aes(x = price)) + geom_density()
> g + geom_vline(xintercept = mean(diamonds$price), linetype = "dashed", color = "blue")
```



Sample solutions ii

2. Now draw individual density curves splitting the data by `cut`. Try to draw vertical dashed lines indicating the mean value per group.

```
> means = diamonds %>%
+   group_by(cut) %>%
+   summarize(price = mean(price)) %>%
+   ungroup()
> g = ggplot(diamonds, aes(x = price))
> g = g + geom_density(aes(fill = cut), alpha = 0.3)
> g = g + scale_x_log10() # transform x-axis
> g + geom_vline(data = means, mapping = aes(xintercept = price, color = cut),
+   linetype = "dashed")
```



Sample solutions iii

3. Next, draw individual density curves splitting the data by `cut`, `color` and/or `clarity` (use facetting and mapping to colors).

```
> # plot gets really large and is thus not diplayed here
> g = ggplot(
+   filter(diamonds, color %in% c("E", "I") & clarity %in% c("SI1", "SI2")))
> g = g + geom_density(aes(x = price, fill = cut), alpha = 0.3)
> g = g + facet_grid(color ~ clarity)
>
> # alternative: use interaction to "link" factors
> g = ggplot(
+   filter(diamonds, color %in% c("E", "I") & clarity %in% c("SI1", "SI2")))
> g = g + geom_density(aes(x = price, fill = cut), alpha = 0.3)
> g = g + facet_grid(. ~ interaction(color, clarity, sep = " / "))
```

Themes

Themes

`ggplot2` offers reasonable defaults for as good as every aspect of a plot, but ...

- sometimes you need to stick to a specific style-guide (e.g. black & white)
- you want to fine-tune e.g. the axis breaks, legend position, ...
- you want to increase the axis label size
- need to increase plot/panel margins
- you do not like the default colors and want to apply you own colour palette
- etc.

Themes (cont.)

Themes

- **Themes** control the *non-data parts* of your plots
- They are composed of multiple elements of different types, e.g plot.title [text], legend.background [rect]
- Two possible approaches (which can be combined)
  - **Apply predefined theme**: e.g. `theme_bw()` or `theme_grey()`

```
> # change every aspect of the rendering
> last_plot() + theme_bw()
```

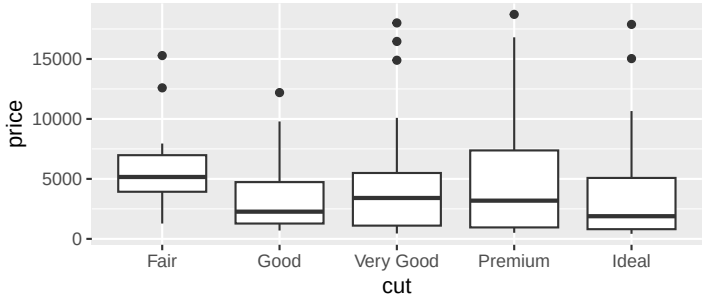
  - **Change only specific parts**: e.g.

```
> # change position of the legend and the colour of the plot title
> last_plot() + theme(
+   legend.position = "top",
+   plot.title = element_text(colour = "tomato"))
```

Themes (cont.)

Basic theme

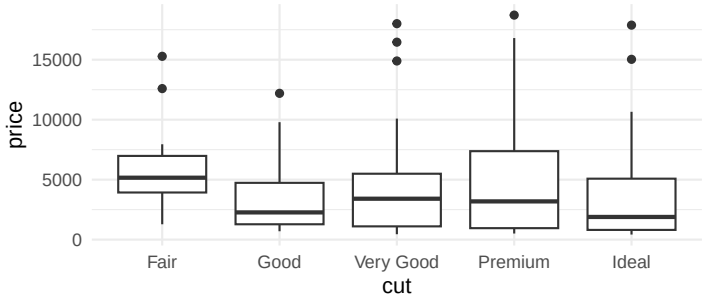
```
> g = ggplot(ds, aes(x = cut, y = price)) + geom_boxplot()
> g
```



Themes (cont.)

Predefined minimalistic theme

```
> last_plot() + theme_minimal()
```



Themes (cont.)

Specific theming

```
> last_plot() +
+   labs(title = "Distribution of prices") +
+   theme(plot.title = element_text(colour = "gray", size = 13))
```

Themes (cont.)

Creating a custom theme

If there is no theme that fits your imagination (or style-guide), build your own:

```
> my_theme = function() {
+   theme(
+     legend.position = "top",
+     panel.background = element_rect(fill = NA, colour = NA),
+     plot.background = element_rect(colour = NA, fill = NA)
+     #, ...
+   )
+ }
```

Set it globally for the entire session:

```
> theme_set(my_theme())
```

How to save a plot

Here comes ggsave(...)

- Convenient function for saving a plot (wrapper for graphic device driver)
- Only mandatory argument to ggsave is the **file name**[5]
- By default saves the last generated plot (determined via `last_plot()`)

Example

Save plot myplot in the current working directory

```
> ggsave("figure.pdf", plot = myplot)
```

[5] Other stuff like image size is guessed in a reasonable way.

How to save a plot

More examples

- Save the last plot generated (maybe the one on your screen)

```
> ggsave("figure.pdf")
```

- Save arbitrary ggplot object myplot in memory

```
> ggsave("figure.pdf", plot = myplot)
```

- Select device driver which should be used

```
> ggsave("figure.png")
> ggsave("figure.eps")
```

  - Device is determined by the file extension figure.**eps**
  - build-in support for all common graphic types, i. e., pdf, eps, png, jpeg, svg, . . .)

- see ?ggsave for more information

Case study

Case study 1

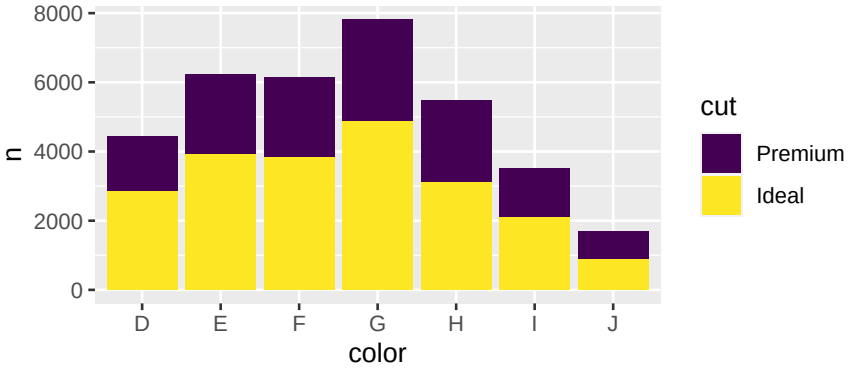
Q: What is the number of diamonds per `color` for the two best `cut` values?
First, let's do the aggregation:

```
> data(diamonds)
> X = diamonds %>%
+   filter(cut %in% c("Ideal", "Premium")) %>%
+   group_by(cut, color) %>%
+   summarize(n = n()) %>%
+   ungroup() %>%
+   mutate(perc = n / sum(n))

## `summarise()` has grouped output by 'cut'.  You can override using the `.groups`
## argument.

> print(X, n = 4)

## # A tibble: 14 x 4
##   cut     color     n   perc
##   <ord>   <ord> <int>  <dbl>
## 1 Premium D      1603 0.0454
## 2 Premium E      2337 0.0661
```

Case study 1 (cont.)

Now let's generate a basic bar plot and refine it iteratively:

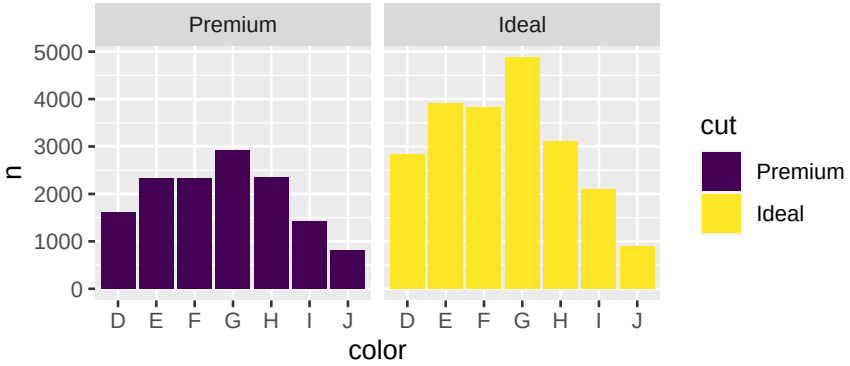
```
> g = ggplot(X) + aes(x = color, y = n, fill = cut) + geom_col()
> g
```



Case study 1 (cont.)

Now let's generate a basic bar plot and refine it iteratively:

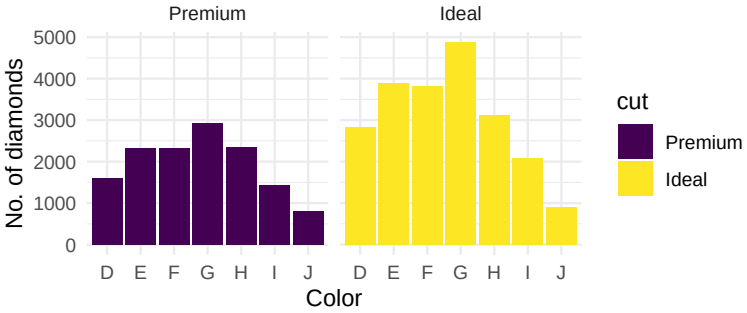
```
> g = g + facet_grid(. ~ cut)
> g
```



Case study 1 (cont.)

Now let's generate a basic bar plot and refine it iteratively:

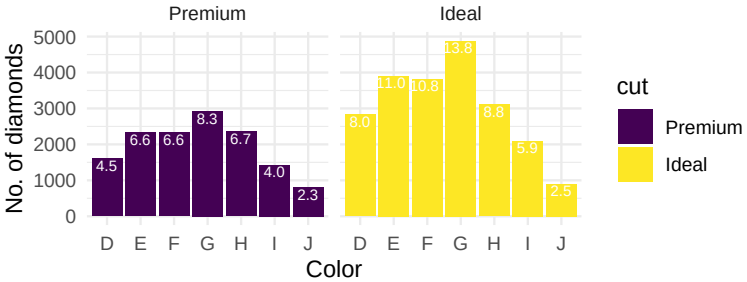
```
> g = g + theme_minimal() + labs(x = "Color", y = "No. of diamonds")
> g
```



Case study 1 (cont.)

Now let's generate a basic bar plot and refine it iteratively:

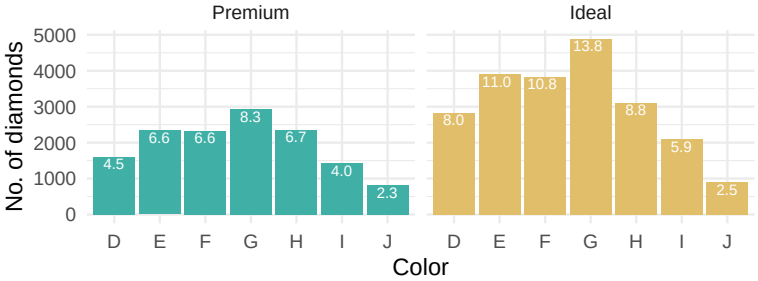
```
> g = g + geom_text(
+   mapping = aes(label = format(100 * perc, digits = 2)),
+   size = 2.5, vjust = 1.15, hjust = 0.6, color = 'white')
> g = g + labs(caption = "Percentage of total no. of diamonds in bars.")
> g
```



Case study 1 (cont.)

Now let's generate a basic bar plot and refine it iteratively:

```
> g = g + scale_fill_manual(
+   values = c("Ideal"  = "#E1BE6A", "Premium" = "#40B0A6")) +
+   theme(legend.position = "none")
> g
```



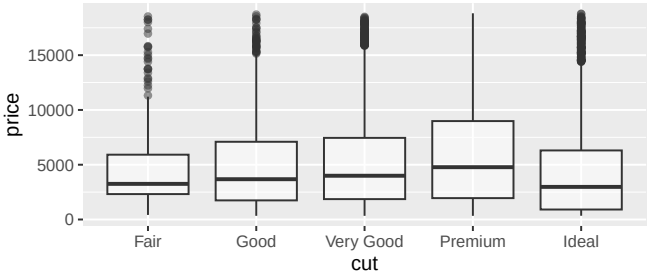
Percentage of total no. of diamonds in bars.

Case study 2

Q: What is the distribution of the `price` for all diamonds with `color` I or J separated by `cut`?

Again, first we generate a basic plot:

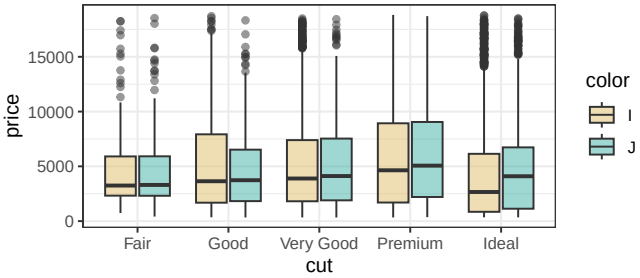
```
> g = ggplot(filter(diamonds, color %in% c("I", "J")))
> g = g + aes(x = cut, y = price) + geom_boxplot(alpha = 0.5)
> g
```



Case study 2 (cont.)

Now let's refine:

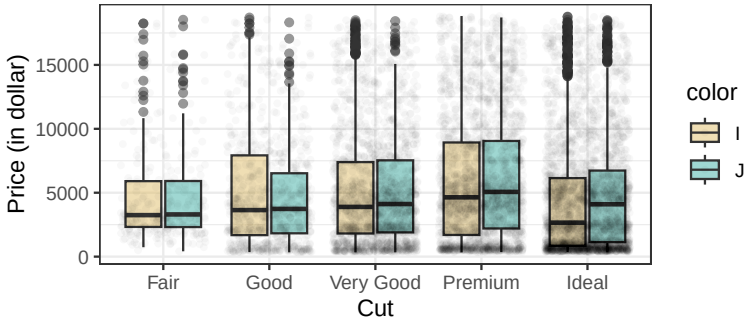
```
> g = g + aes(fill = color)
> g = g + theme(legend.position = "top") + theme_bw()
> g = g + scale_fill_manual(values = c("I"   = "#E1BE6A", "J" = "#40B0A6"))
> g
```



Case study 2 (cont.)

Let's add the actual observations:

```
> g = g + geom_jitter(aes(fill = NULL), alpha = 0.03, size = 1)
> g = g + xlab("Cut") + ylab("Price (in dollar)")
> g
```



Quick plots

Quick plots

Shortcut and consistent interface for users familiar with base R's `plot()` function:

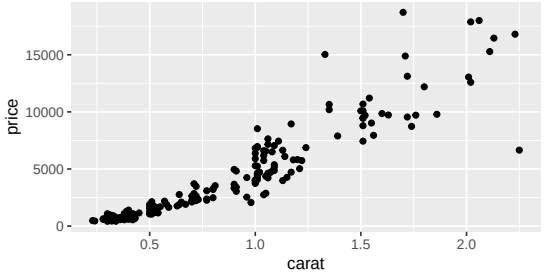
```
> # qplot has some more arguments, but these are the most important ones
> qplot(x, y, data, facets = NULL, geom = "auto",
+   xlim = c(NA, NA), ylim = c(NA, NA),
+   main = NULL, xlab = NULL, ylab = NULL)
```

x, y	Aesthetics passed into each layer
data	Optional dataframe (if none is passed it is generated internally).
facets	Faceting formula (passed down to `facet_grid()` or `facet_wrap()`)
geom	Geometric as a string, e.g., "boxplot" or "density"
xlim, ylim	*x*- and *y*-axis limits
main, xlab, ylab	Title and axis labels

Quick plots

Let's look at some examples:

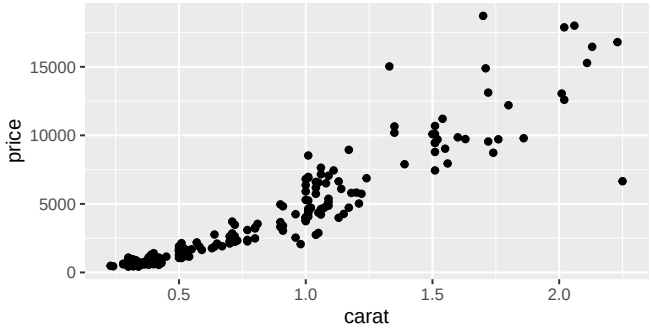
```
> qplot(carat, price, data = ds, geom = "point")

## Warning:  `qplot()` was deprecated in ggplot2 3.4.0.
## This warning is displayed once every 8 hours.
## Call `lifecycle::last_lifecycle_warnings()` to see where this warning was
## generated.
```



Quick plots

Quick plots makes an educated guess if no geom is specified.

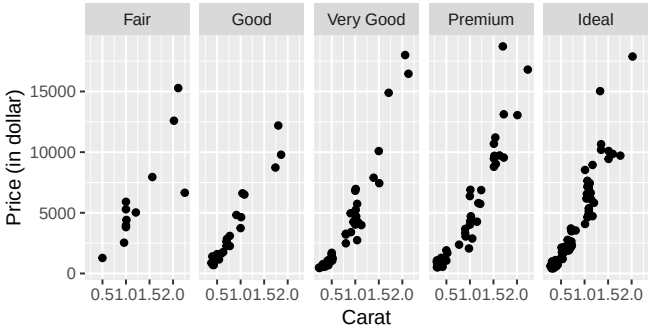
```
> qplot(carat, price, data = ds)
```



Quick plots

Facets are possible as well:

```
> qplot(carat, price, data = ds, facets = . ~ cut,
+   xlab = "Carat", ylab = "Price (in dollar)")
```



Clean visualizations

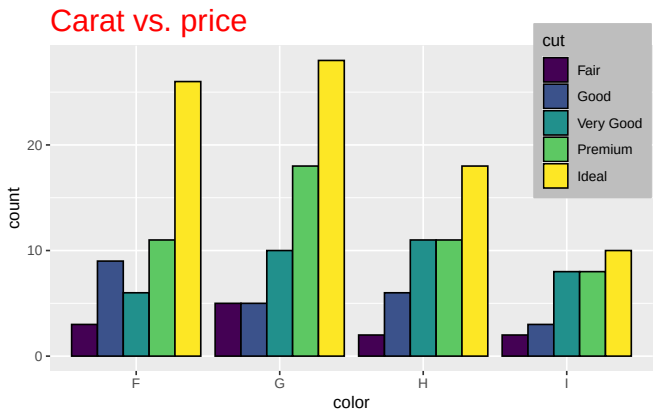
Awesome graphics focus on data

How does a "good" (statistical) plot look like?

- Focus on actually visualizing data
- Get rid of **chart junk**, i. e., every non-data aspect which obscures the data
- Be as minimalistic as possible (but not too minimalistic)
- Use color-blind colour palettes
- Be understandable/readable even when printed in black & white (grayscale)
- Fit in the overall picture

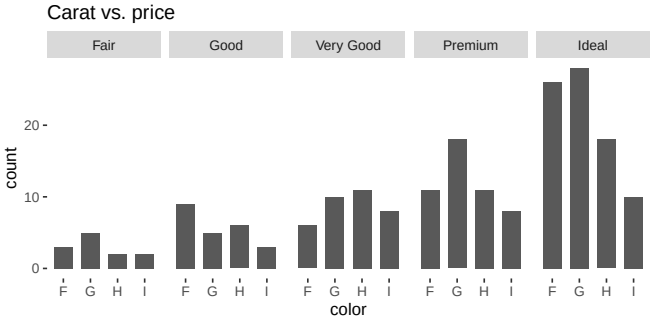
Awesome graphics focus on data (cont.)

Example of a really bad graphic



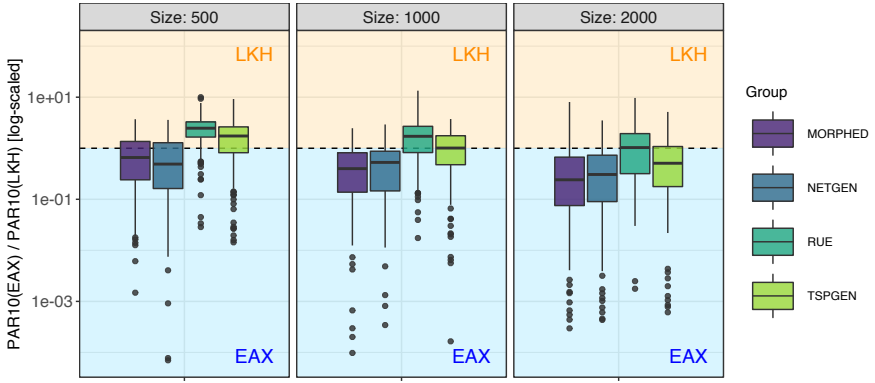
Awesome graphics focus on data (cont.)

Much cleaner with faceting



Example

Remember that one from the beginning?



Example

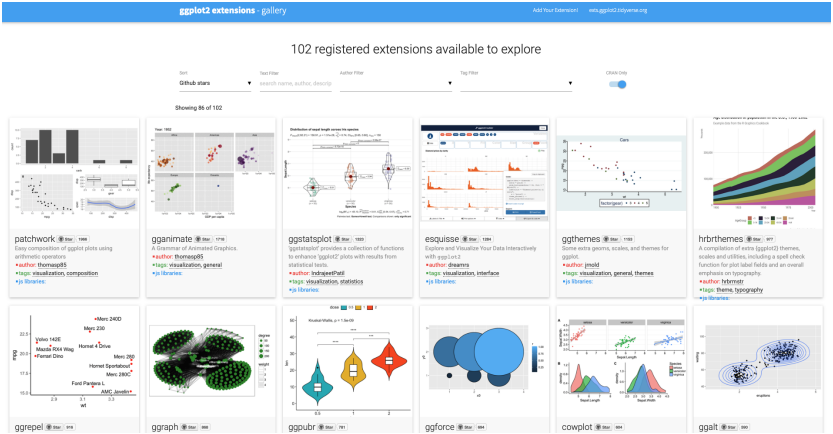
Code can get lengthy if you aim to fine-tune many details! ☺

```
> g = ggplot(tmp.df, aes(x = duel, y = ratio, fill = as.factor(group)))
> g = g + geom_blank()
> g = g + annotate("rect", xmin = -Inf, xmax = Inf, ymin = 1, ymax = Inf, alpha = 0.15, fill = "orange")
> g = g + annotate("rect", xmin = -Inf, xmax = Inf, ymax = 1, ymin = 0, alpha = 0.15, fill = "deepskyblue")
> g = g + geom_hline(yintercept = 1, linetype = "dashed")
> g = g + geom_boxplot(alpha = 0.825)
> g = g + scale_y_log10() #limits = c(1/15000, 100)
> g = g + theme_bw()
> g = g + geom_text(data = data.frame(x = c(1.2, 0.7), y = c(1/20000, 700), label = c("EAX", "LKH"), group = NA),
+   mapping = aes(x = x, y = y, label = label), color = c("blue", "darkorange"), size = 5)
> g = g + labs(
+   x = "Solver duel", y = "PAR10(EAX) / PAR10(LKH) [log-scaled]",
+   fill = "Group")
> g = g + viridis::scale_fill_viridis(discrete = TRUE, begin = 0.1, end = 0.85)
> g = g + facet_wrap(. ~ Size, nrow = 1L, labeller = label_both)
> g = g + theme(
+   legend.position = "right",
+   axis.title.y = element_text(size = 12), axis.text.y = element_text(size = 12),
+   axis.title.x = element_blank(), axis.text.x = element_blank(),
+   strip.text = element_text(size = 12),
+   legend.key = element_rect(color = NA, fill = NA), legend.key.size = unit(1.4, "cm"),
+   legend.title = element_text(size = 12),
+   legend.text = element_text(size = 12))
> g = g + guides(fill = guide_legend(nrow = 5))
```

Take away message

- `ggplot2` is a powerful tool for applied data analysis
- Implementation of the *Grammer of Graphics*
- Build complex graphics with ease
- Highly customizable via *themes*
- Very similar implementations available for other languages
- Definitely worth the learn effort! ☺

ggplot2 **is huge!**



Further reading

- **Hadley's book** (Wickham 2009)[6] (printed book is nice to have, but almost instantly outdated ☺)
- **Official documentation**[7]
- **Extension library**[8] (my personal favourites: `gganimate`, `geomnet`, `plotly`, `patchwork`, `cowplot`)
- Chapter on *Exploratory Data Analysis* (EDA) in (Wickham and Grolemund 2017)[9]

[6] `https://ggplot2-book.org`
[7] `https://ggplot2.tidyverse.org`
[8] `https://exts.ggplot2.tidyverse.org`
[9] `https://r4ds.had.co.nz/exploratory-data-analysis.html`

What comes next?

Overview of the upcoming week:

Date	Content	Speaker
04 Nov.	`ggplot2`	Jakob
05 Nov.	Tutorial on `tidyverse`	Raphael
11 Nov.	Exploratory Data Analysis (EDA)	Raphael[10]
12 Nov.	Tutorial on `ggplot2`	Raphael
18 Nov.	Hierarchical Clustering and k-means	Jakob
19 Nov.	Tutorial on EDA	Raphael
⋮	⋮	⋮

[10] Jakob will be at the TU Dresden.

Wrap-Up

Wrap-Up

Todays content

Grammer of Graphics and its implementation in `ggplot2`

Your task(s)

- Again, we just scratched the surface here! Work through the data transformation chapter in (Wickham and Grolemund 2017)
- Work on exercise sheet
- Ideally search for more material online

References I

Wilkinson, Leland (2005). *The Grammar of Graphics (Statistics and Computing)*. Berlin, Heidelberg: Springer-Verlag. ISBN: 0387245448.

Tyner, Sam, François Briatte, and Heike Hofmann (2017). "Network Visualization with ggplot2". In: *The R Journal* 9.1, pp. 27–59. DOI: 10.32614/RJ-2017-023.

Wickham, Hadley (2009). *ggplot2: elegant graphics for data analysis*. Springer New York. ISBN: 978-0-387-98140-6.

Wickham, Hadley and Garrett Grolemund (Jan. 2017). *R for Data Science: Import, Tidy, Transform, Visualize, and Model Data*. 1st ed. O'Reilly Media. ISBN: 1491910399.