Lecture 8

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Iterating

Exploratory Data Analysis

Exploratory analyses

Base R graphics

`grid` graphics

`ggplot2` basics

Iterating

Iterating

- Reference: Iteration chapter of R for Data Science by Wickham and Grolemund.
  - Published book: Chapter 17
  - Online book: Chapter 21: http://r4ds.had.co.nz/iteration.html
- The use of `lapply()` in the previous lecture is an example of iterating:
  - Our data is in a vector (list), and we want to perform the same operation on each element.
- Tools that we have discussed that are useful for iterating are `for()` and `while()` loops.
- Iteration is so common that special tools have been developed with the aim of reducing the amount of code (and therefore errors) required for common iterative tasks.
  - Tools in base R include the `apply()` family of functions.
  - A tidyverse package called `purrr` includes more.

Vectorizing to avoid iteration

- Before iterating, think about whether it is possible to use vectorization instead.
- Example:

```
f <- function(x) {
  n <- length(x); out <- vector(mode="numeric",length=n)
  for(i in 1:n) {
    if(x[i]>0) {
      out[i] <- log(x[i])
    } else {
      out[i] <- NA
    }
  }
  out
}
fvec <- function(x) {
  n <- length(x); out <- vector(mode="numeric",length=n)
  ind <- (x>0)
  out[ind] <- log(x[ind])
  out[!ind] <- NA # recycles NA
  out
}
```

Example data

- To illustrate iteration we simulate data and fit four regression models.

```
set.seed(42)
n <- 100
x1 <- rnorm(n); x2<-rnorm(n)
y1 <- x1 + rnorm(n,sd=.5); y2 <- x1+x2+rnorm(n,sd=.5)
y3 <- x2 + rnorm(n,sd=.5); y4 <- rnorm(n,sd=.5)
rr <- list(fit1 = lm(y1 ~ x1+x2),
  fit2 = lm(y2 ~ x1+x2),
  fit3 = lm(y3 ~ x1+x2),
  fit4 = lm(y4 ~ x1+x2))
```

Extracting the regression coefficient for x1

- Using a `for()` loop, we initialize an object to hold the **output**, loop along a **sequence** of values for an index variable, and execute the **body** for each value of the index variable.

```
beta1hat <- vector("double",length(rr))
for(i in seq_along(rr)) { # safer than 1:length(rr)
  beta1hat[i] <- coefficients(rr[[i]])["x1"]
}
beta1hat
```

```
## [1]  0.92814538  1.03114836  0.04316514 -0.01842827
```

Looping over elements of a set

- The index set in the `for()` loop can be general.
  - We might use this generality to loop over named components of a list.

```
fits <- paste0("fit",1:4)
for(ff in fits) {
  print(coefficients(rr[[ff]])["x1"])
}
```

```
##        x1
## 0.9281454
##       x1
## 1.031148
##         x1
## 0.04316514
##          x1
## -0.01842827
```

- Looping over a set makes it harder to save the results, though.

The body of a loop can be a small part of the code

- In our examples, most of the code is for setting up the output and looping, with very little to do with the body.
- To illustrate, consider a small change: instead of the estimated coefficient of `x1` we wanted the estimated coefficient of `x2`:

```
beta1hat <- vector("double",length(rr))
for(i in seq_along(rr)) { # safter than 1:length(rr)
  beta1hat[i] <- coefficients(rr[[i]])["x2"]
}
beta1hat
```

```
## [1]  0.04264659  1.00306653  0.93035180 -0.11630942
```

Using `lapply()`

- The intent of `lapply()` is to take care of the output and the loop, allowing us to focus on the body.

```
b1fun <- function(fit) { coefficients(fit)["x1"] } # body
bfun <- function(fit,cc) { coefficients(fit)[cc] } # body
lapply(rr,b1fun)  # or sapply(rr,b1fun) or unlist(lapply(rr,b1fun))
```

```
## $fit1
##        x1
## 0.9281454
##
## $fit2
##       x1
## 1.031148
##
## $fit3
##         x1
## 0.04316514
##
## $fit4
##          x1
## -0.01842827
```

```
lapply(rr,bfun,"x2")
```

Iterating with the `map()` functions from `purrr`

- The `purrr` package provides a family of functions `map()`, `map_dbl()`, etc. that do the same thing as `lapply()` but work better with other tidyverse functions.
  - `map()` returns a list, like `lapply()`.
  - `map_dbl()` returns a double vector, etc.

```
library(purrr)
map_dbl(rr,b1fun) # or rr %>% map_dbl(b1fun)
```

```
##         fit1         fit2         fit3         fit4
##  0.92814538  1.03114836  0.04316514 -0.01842827
```

Pipes and `map()` functions

- Suppose we want to record a model summary returned by the `summary()` function.
  - `summary()` is a generic function. When applied to an `lm()` object it computes regression summaries like standard errors and model R^2.

```
rr %>%
  map(summary) %>%
  map_dbl(function(ss) { ss$r.squared })
```

```
##       fit1       fit2       fit3       fit4
## 0.78845184 0.91430933 0.73684218 0.04087594
```

- Notice that we can define a function on-the-fly in the call to a `map()` function.
- `map()` functions have a short-cut for function definitions.

```
rr %>%
  map(summary) %>%
  map_dbl(~.$r.squared)
```

```
##       fit1       fit2       fit3       fit4
## 0.78845184 0.91430933 0.73684218 0.04087594
```

- In `~.` read `~` as "define a function" and `.` as "argument to the function"
  - Comment: This is a little too terse for my tastes, but I mention it in case you see it in practice.

Exploratory Data Analysis

Topics

- Exploratory data analysis, with emphasis on `ggplot2` graphics, using the gapminder data.
  - Suppose we want to use information on `continent`, `year`, `pop` and `gdpPercap` to predict `lifeExp`.
- Base R graphics *vs* grid graphics
- Introduction to `ggplot2`

Exploratory analyses

Exploratory analyses

- Univariate summaries, such as means/medians, sds/IQRs, histrograms, to examine distributions and identify possible measurement errors.
- Pair-wise correlations, to look for relationships between variables
- Pair-wise regression relationships and added-variable-plots
    - Trends over time deserve special attention
- Illustrate with the `gapminder` data set.

```
library(gapminder)
data(gapminder)
```

Univariate Summaries

- Different summaries are appropriate for categorical and quantitative variables
  - Tabulate categorical variables
  - Five number summary for quantitative variables

```
summary(gapminder)
```

```
##         country        continent        year         lifeExp
##  Afghanistan:  12   Africa  :624   Min.   :1952   Min.   :23.60
##  Albania    :  12   Americas:300   1st Qu.:1966   1st Qu.:48.20
##  Algeria    :  12   Asia    :396   Median :1980   Median :60.71
##  Angola     :  12   Europe  :360   Mean   :1980   Mean   :59.47
##  Argentina  :  12   Oceania : 24   3rd Qu.:1993   3rd Qu.:70.85
##  Australia  :  12                  Max.   :2007   Max.   :82.60
##  (Other)    :1632
##       pop              gdpPercap
##  Min.   :6.001e+04   Min.   :   241.2
##  1st Qu.:2.794e+06   1st Qu.:  1202.1
##  Median :7.024e+06   Median :  3531.8
##  Mean   :2.960e+07   Mean   :  7215.3
##  3rd Qu.:1.959e+07   3rd Qu.:  9325.5
##  Max.   :1.319e+09   Max.   :113523.1
##
```

Comments on summaries

- Observations in `pop` and `gdpPercap` differ by orders of magnitude
  - May be more informative to consider transformations of these variables.
  - For example, a log-10 transformation: one-unit differences correspond to 10-fold increases.
- Aside: Which country has per-capita GDP of $113,523? Or more generally, which observations are in, say, the top 0.1%?

```
library(dplyr)
filter(gapminder,gdpPercap > quantile(gdpPercap,0.999))
```

```
## # A tibble: 2 x 6
##   country continent  year lifeExp    pop gdpPercap
##   <fct>   <fct>     <int>   <dbl>  <int>     <dbl>
## 1 Kuwait  Asia       1957    58.0 212846   113523.
## 2 Kuwait  Asia       1972    67.7 841934   109348.
```

Unviariate summaries by grouping variable

- May be of interest to do summaries of some variables stratified by a grouping variable.

```
oldops <- options(tibble.width=Inf, tibble.print_max=Inf)
gm_byContinent <- group_by(gapminder,continent)
summarize(gm_byContinent,min(lifeExp),median(lifeExp),
          IQR(lifeExp),mean(lifeExp),sd(lifeExp),max(lifeExp))
```

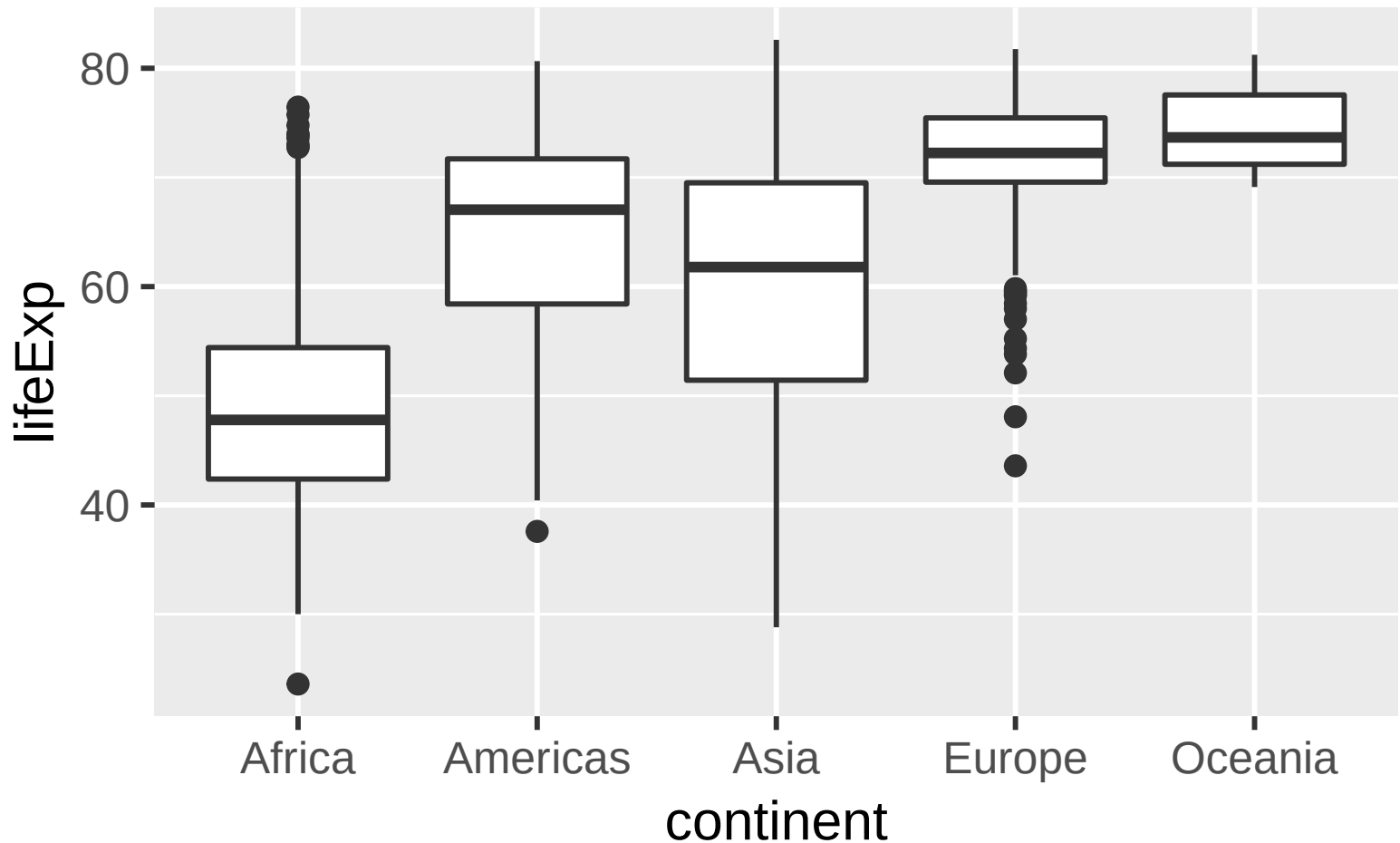
```
## # A tibble: 5 x 7
##   continent `min(lifeExp)` `median(lifeExp)` `IQR(lifeExp)`
##   <fct>              <dbl>             <dbl>          <dbl>
## 1 Africa              23.6              47.8          12.0
## 2 Americas            37.6              67.0          13.3
## 3 Asia                28.8              61.8          18.1
## 4 Europe              43.6              72.2           5.88
## 5 Oceania             69.1              73.7           6.35
##   `mean(lifeExp)` `sd(lifeExp)` `max(lifeExp)`
##             <dbl>         <dbl>          <dbl>
## 1            48.9          9.15           76.4
## 2            64.7          9.35           80.7
## 3            60.1         11.9            82.6
## 4            71.9          5.43           81.8
## 5            74.3          3.80           81.2
```

```
options(oldops)
```

Boxplots

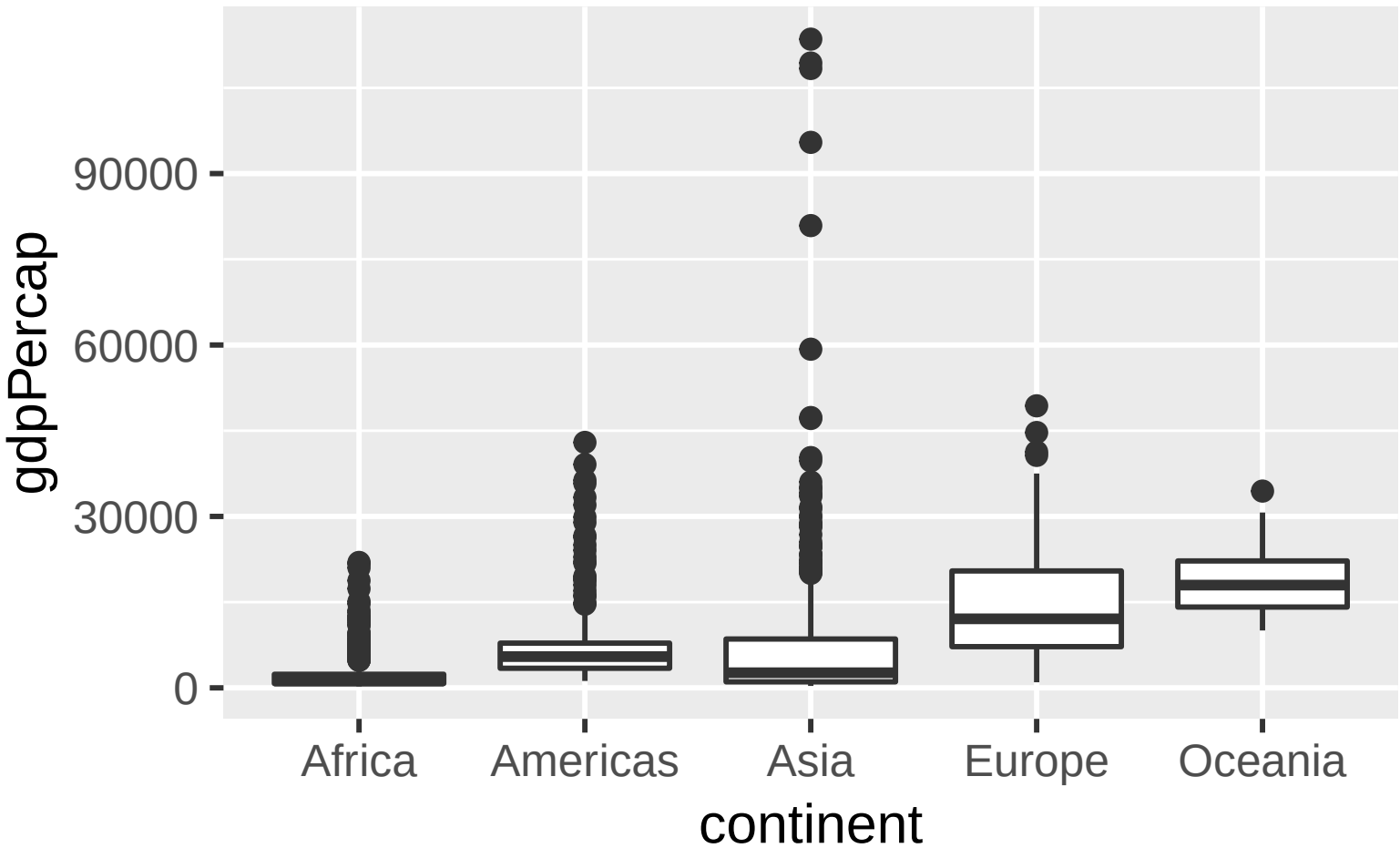
- Graphical representation of the five number summary for grouped data

```
library(ggplot2)
ggplot(gapminder,aes(x=continent, y=lifeExp)) + geom_boxplot()
```



Boxplots, cont.

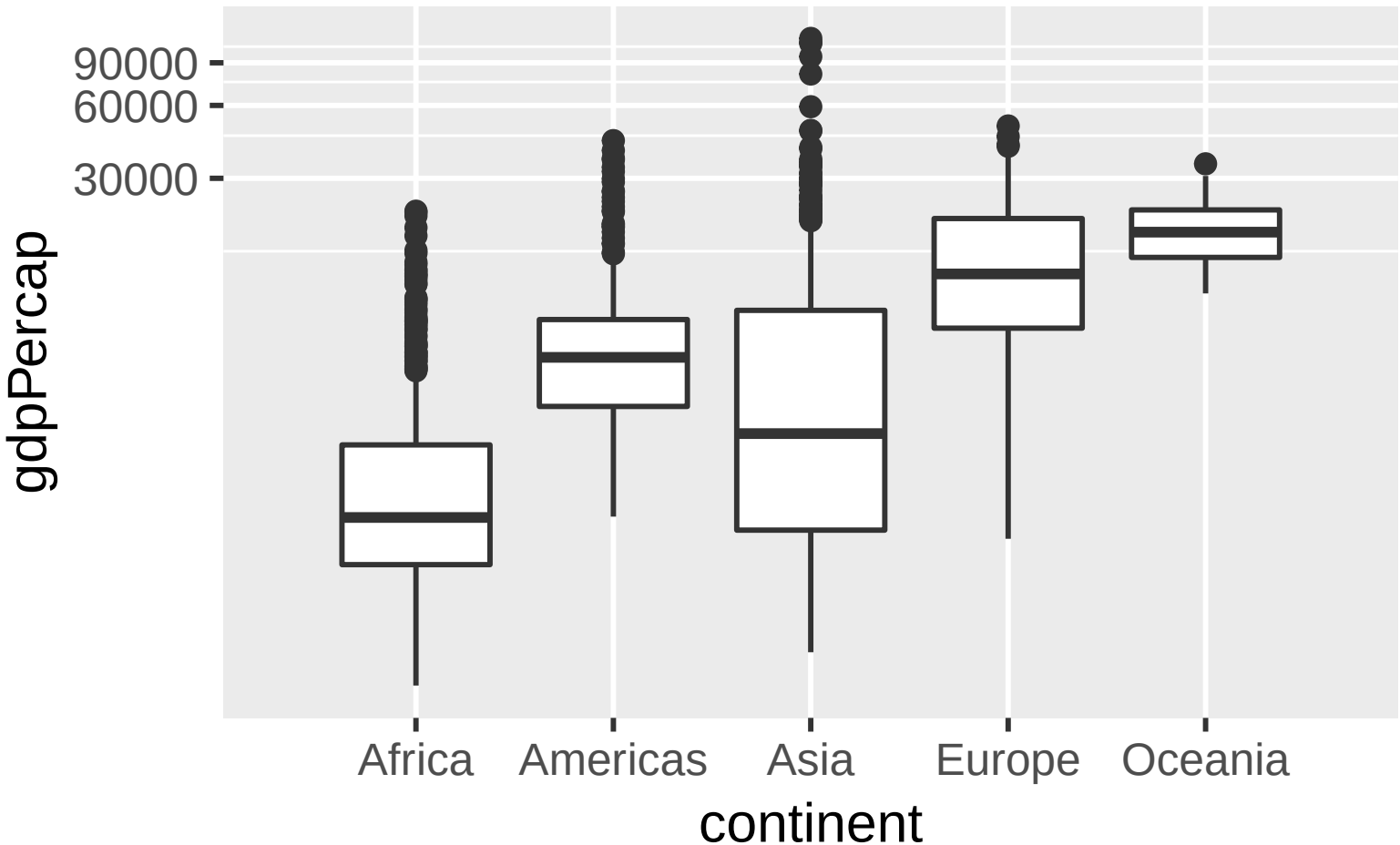
```
ggplot(gapminder,aes(x=continent, y=gdpPercap)) + geom_boxplot()
```



- Distribution of log-transformed data may be more informative.

Boxplots, cont.

```
ggplot(gapminder,aes(x=continent, y=gdpPercap)) +
  coord_trans(y="log10") + geom_boxplot()
```



Adding transformed variables to a dataset

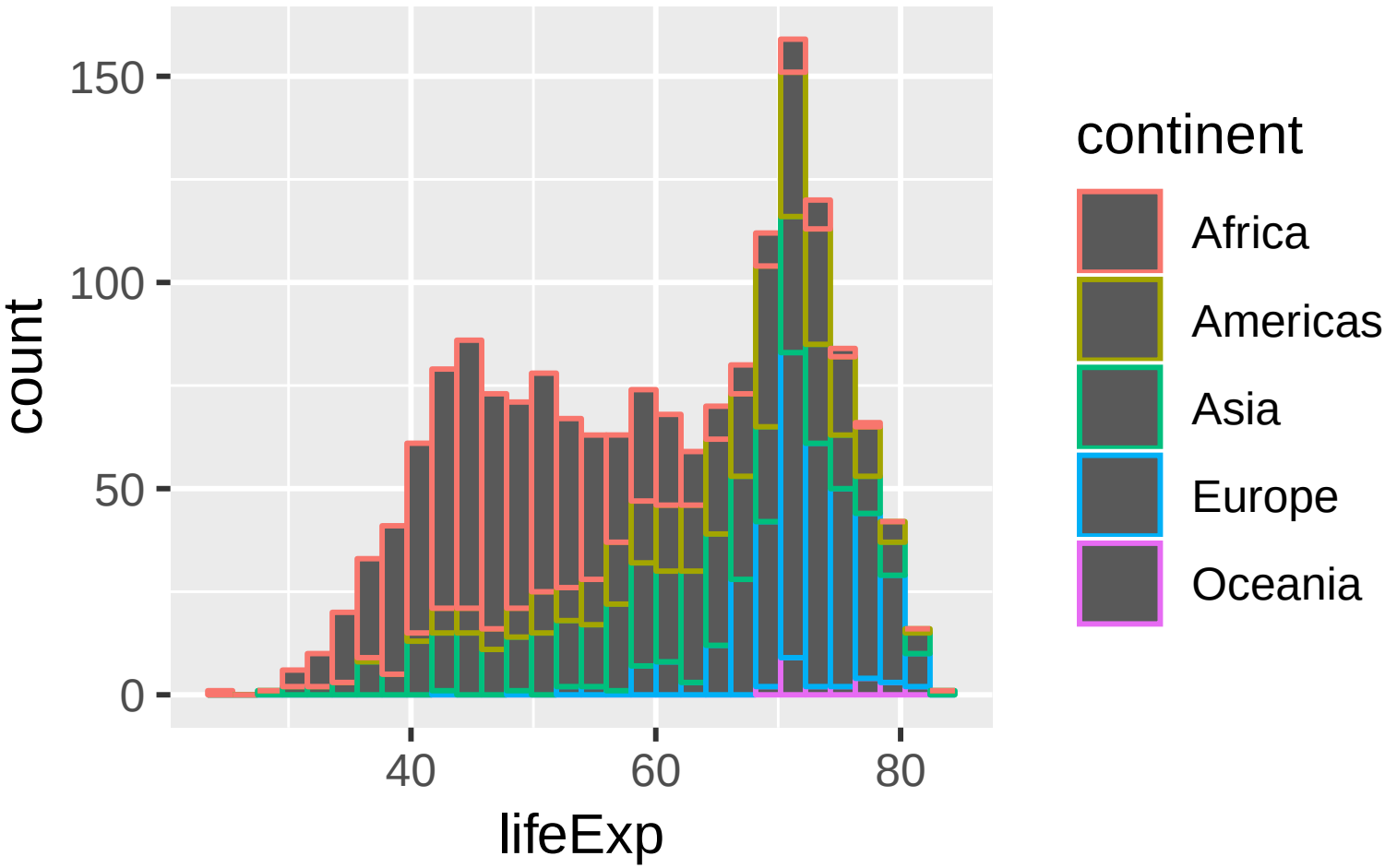
- Above suggests we add log of gdpPercap to the dataset.
- A similar exploration of the pop variable suggests we include log of pop too.
- Will use log-base-10.

```
gapminder <- mutate(gapminder,
                    log10Pop = log10(pop),
                    log10GdpPercap = log10(gdpPercap))
```

Histograms

- Shows the shape of distributions and can suggest possible outliers
- Stacked histograms:

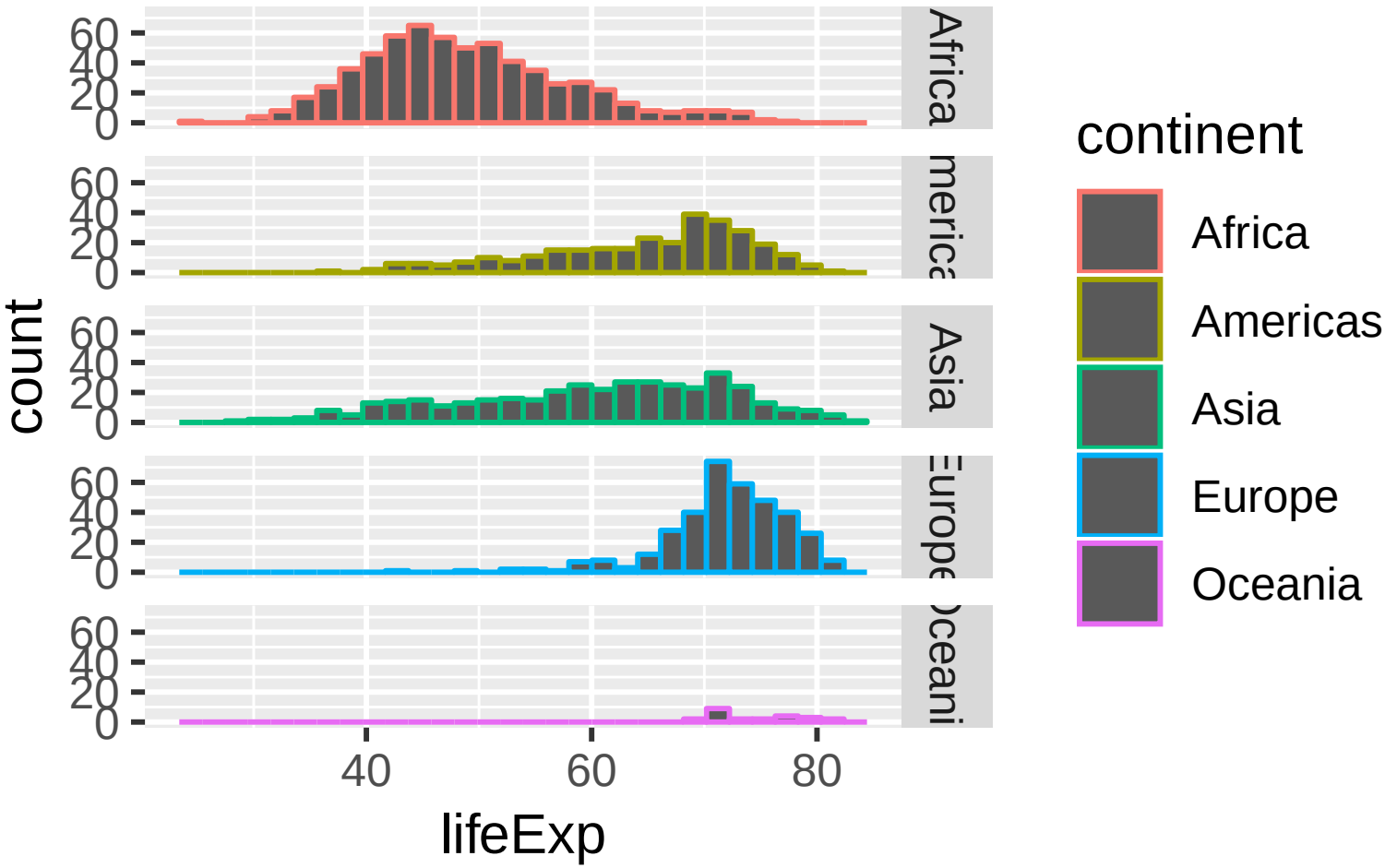
```
ggplot(gapminder,aes(x=lifeExp, color=continent)) + geom_histogram()
```



Histograms, continued

- Histograms in different plot panels, or "facets":

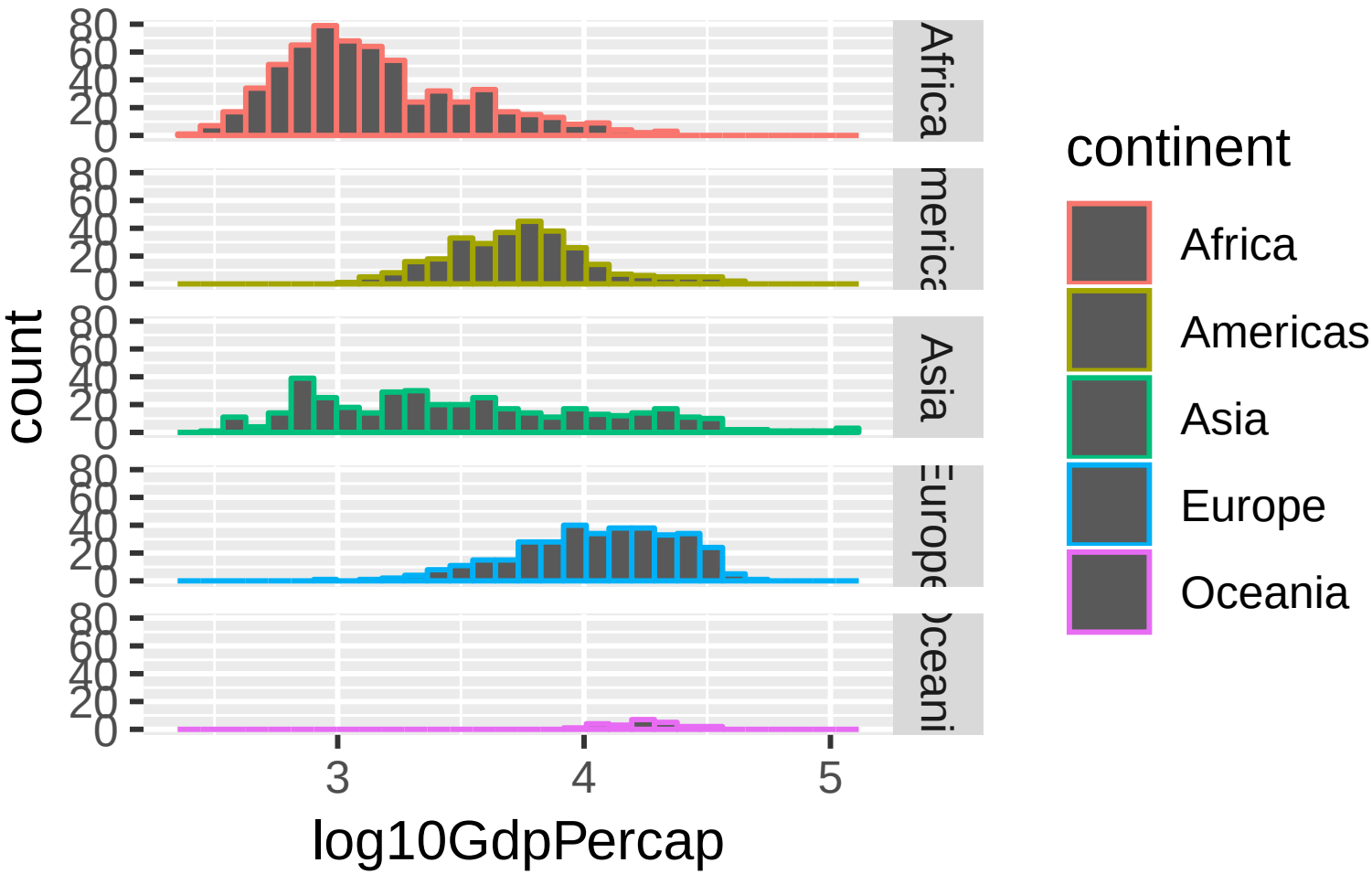
```
ggplot(gapminder,aes(x=lifeExp, color=continent)) +
  geom_histogram() + facet_grid(continent ~ .)
```



Histograms of the explanatory variables

- May also be of interest

```
ggplot(gapminder,aes(x=log10GdpPercap, color=continent)) +
  geom_histogram() + facet_grid(continent ~ .)
```

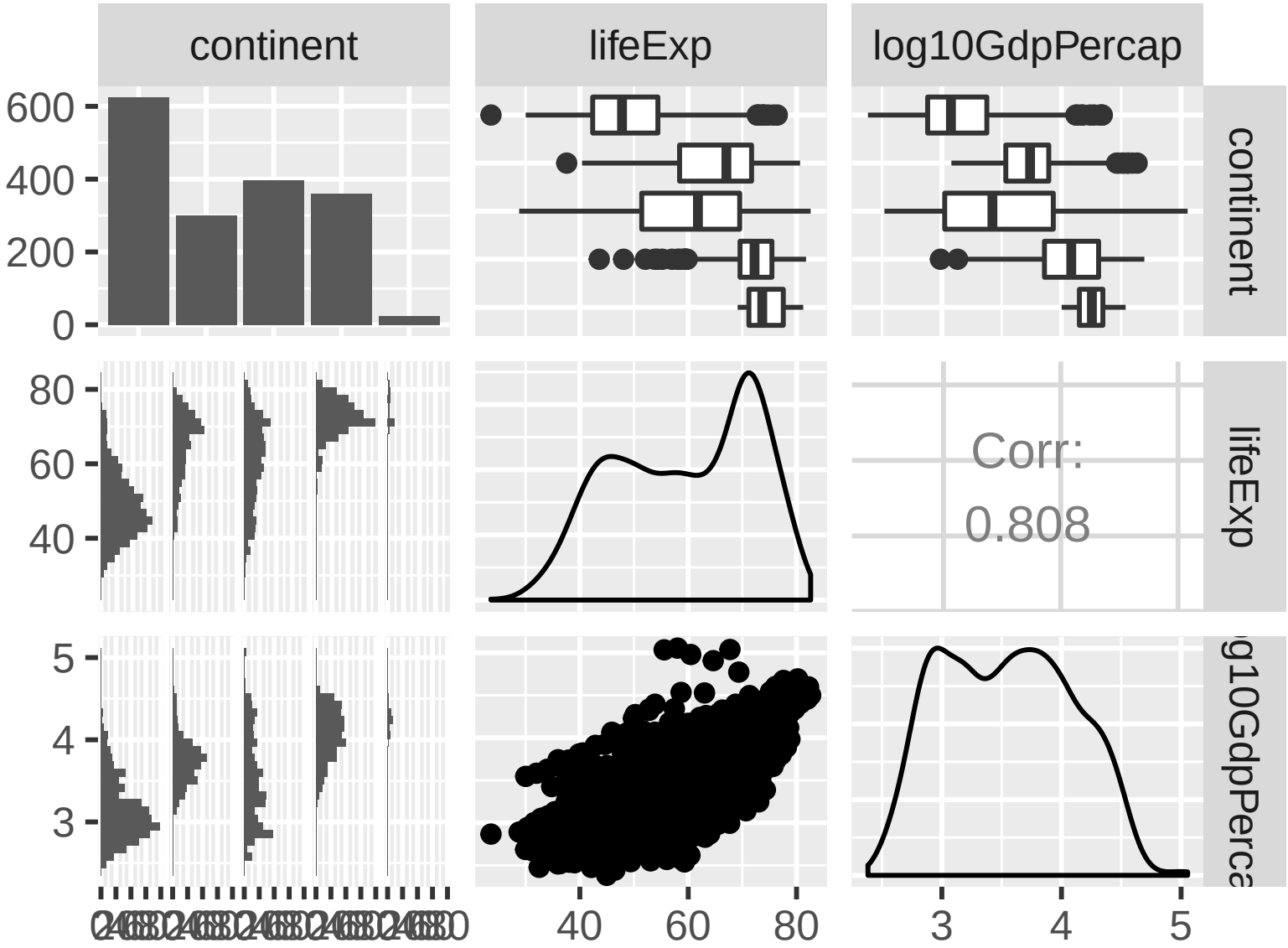


Pairwise Regression relationships

- Though pairwise relationships don't tell the whole story, they are a useful starting point.
- The `GGally` package provides the function `ggpairs()` to facilitate this.
    - Can do all possible pairs of variables, but I find this too hard to read for more than three variables.

Pairwise plots

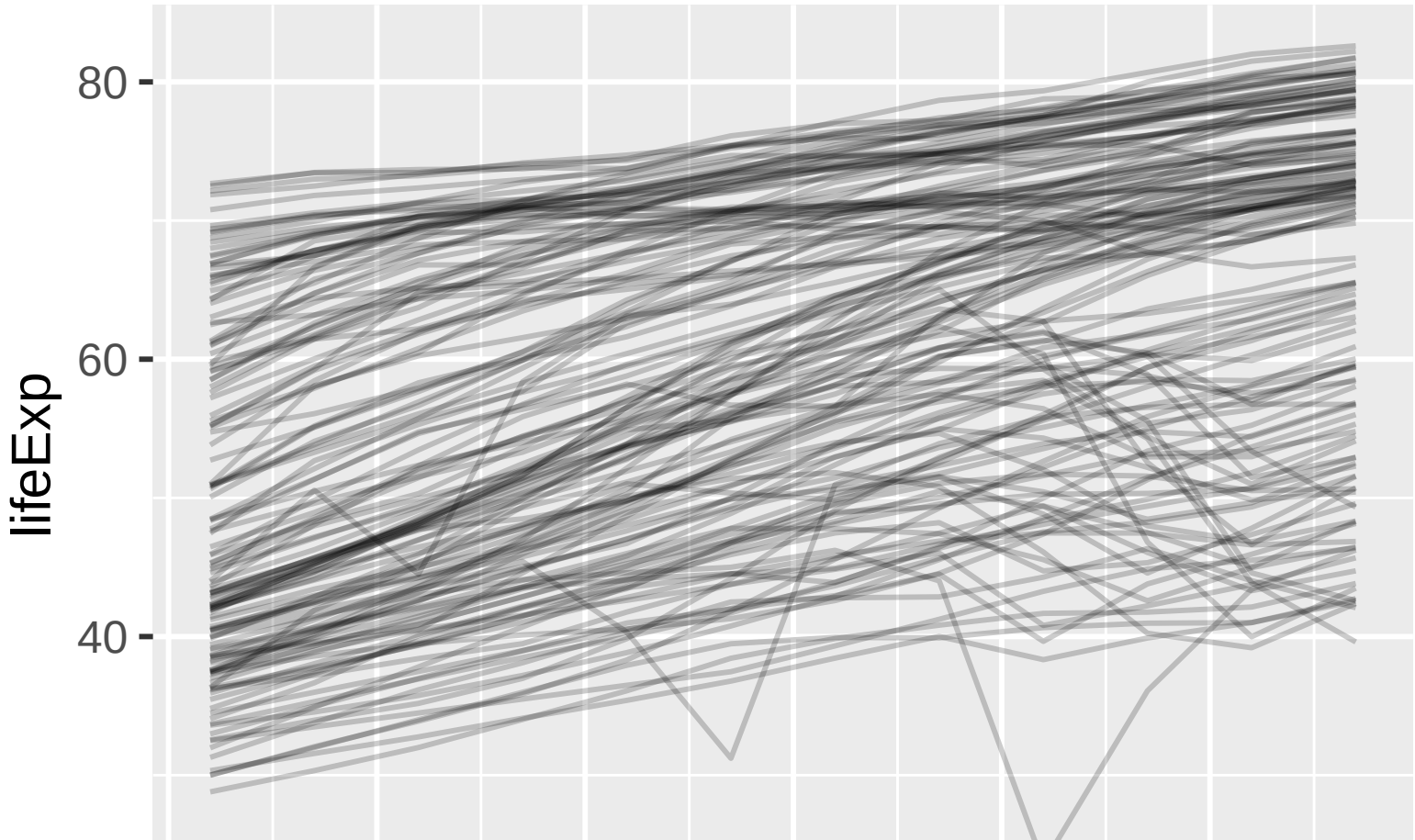
```
library(GGally)
gm_sub <- select(gapminder,continent,lifeExp,log10GdpPercap)
ggpairs(gm_sub) # Cut and paste into console to see better
```



Time trends

- Can represent time series by lines.
- There are many time series in these data – need to make each line slightly transparent to account for overplotting

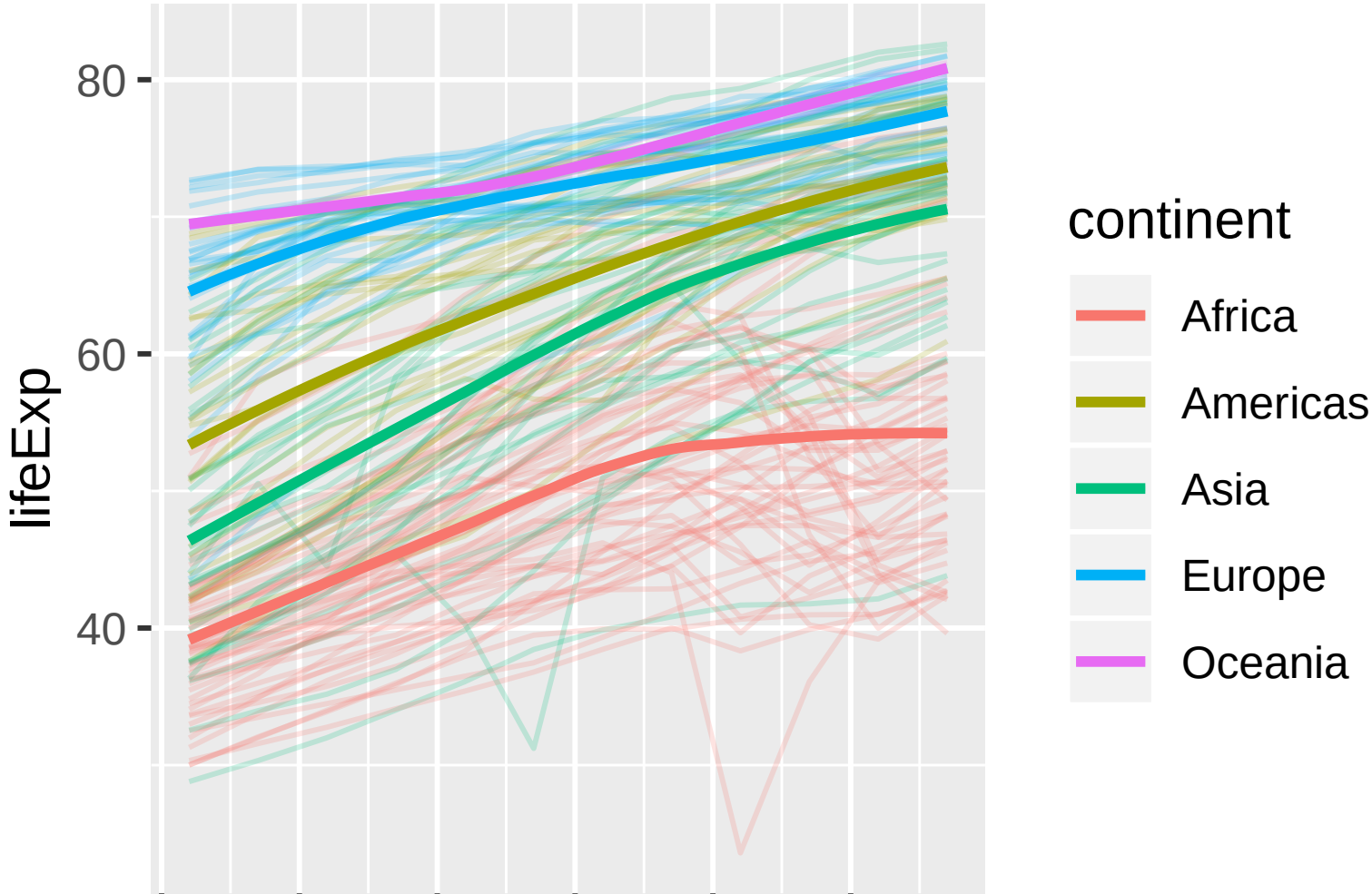
```
ggplot(gapminder,aes(x=year,y=lifeExp,group=country)) +
  geom_line(alpha=0.2)
```



Time trends, cont.

- Can add a statistical summary, like medians at each time, or a smoother.
- Can also add colours for different continents.

```
ggplot(gapminder,aes(x=year,y=lifeExp,group=country,
                     color=continent)) + geom_line(alpha=0.2) +
  geom_smooth(aes(x=year,y=lifeExp,group=continent),se=FALSE)
```



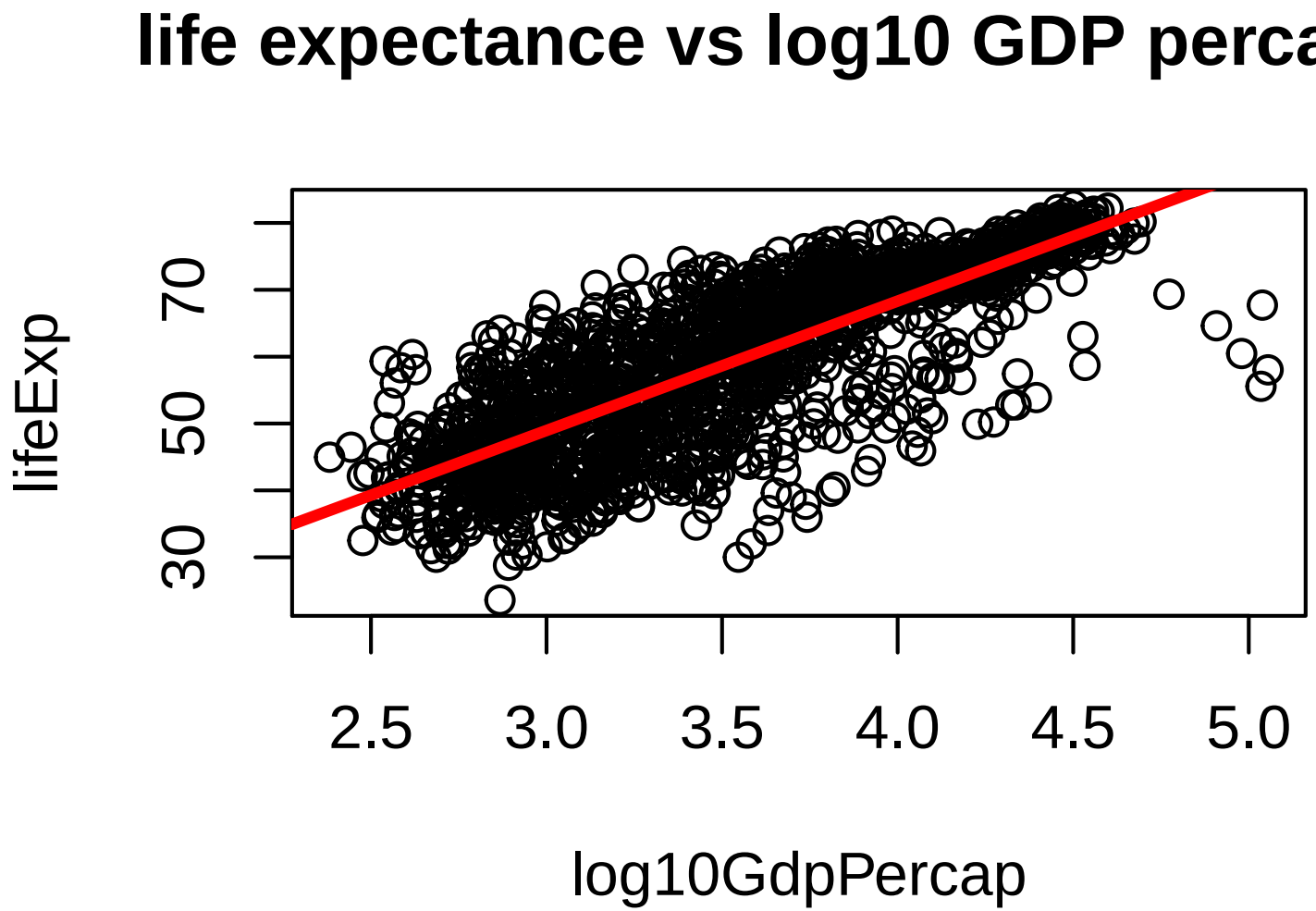
Base R graphics

Base R graphics

- Very serviceable graphics system capable of producing publication-quality graphs.
- Create graphics by calling functions that either produce complete plots or add to plots
- Like adding paint to a canvas

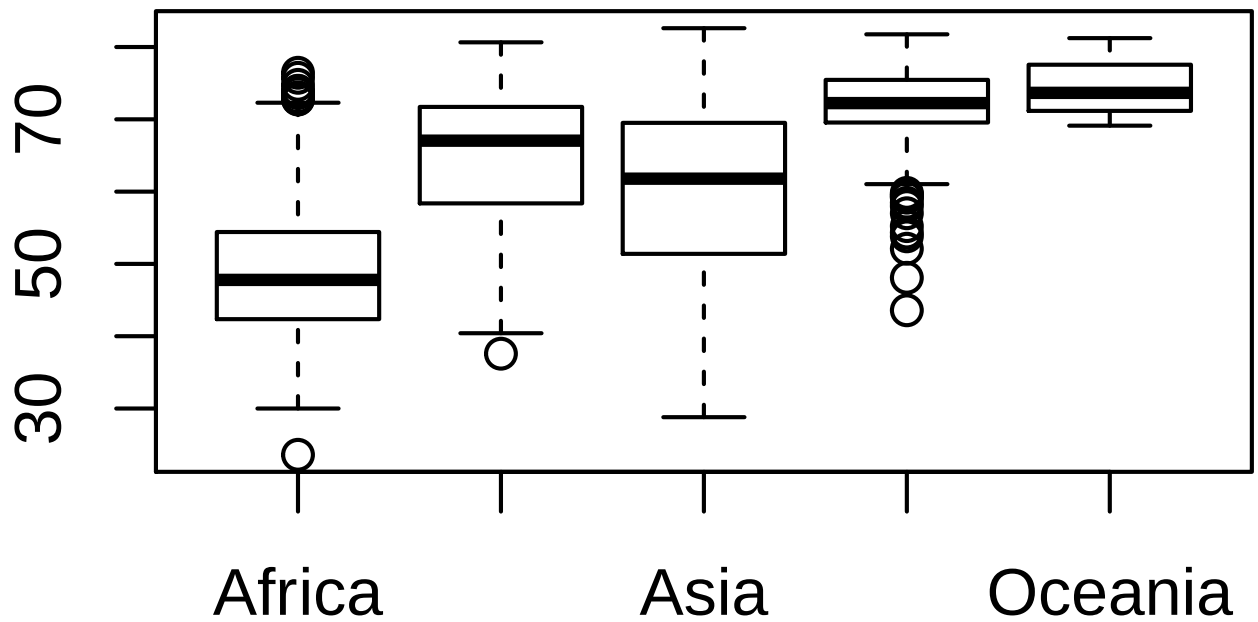
Base R examples

```
with(gapminder,plot(log10GdpPercap,lifeExp)) # or plot(lifeExp ~ log10GdpPercap)
title(main="life expectance vs log10 GDP percapita")
abline(lm(lifeExp ~ log10GdpPercap,data=gapminder),col="red",lwd=3)
```



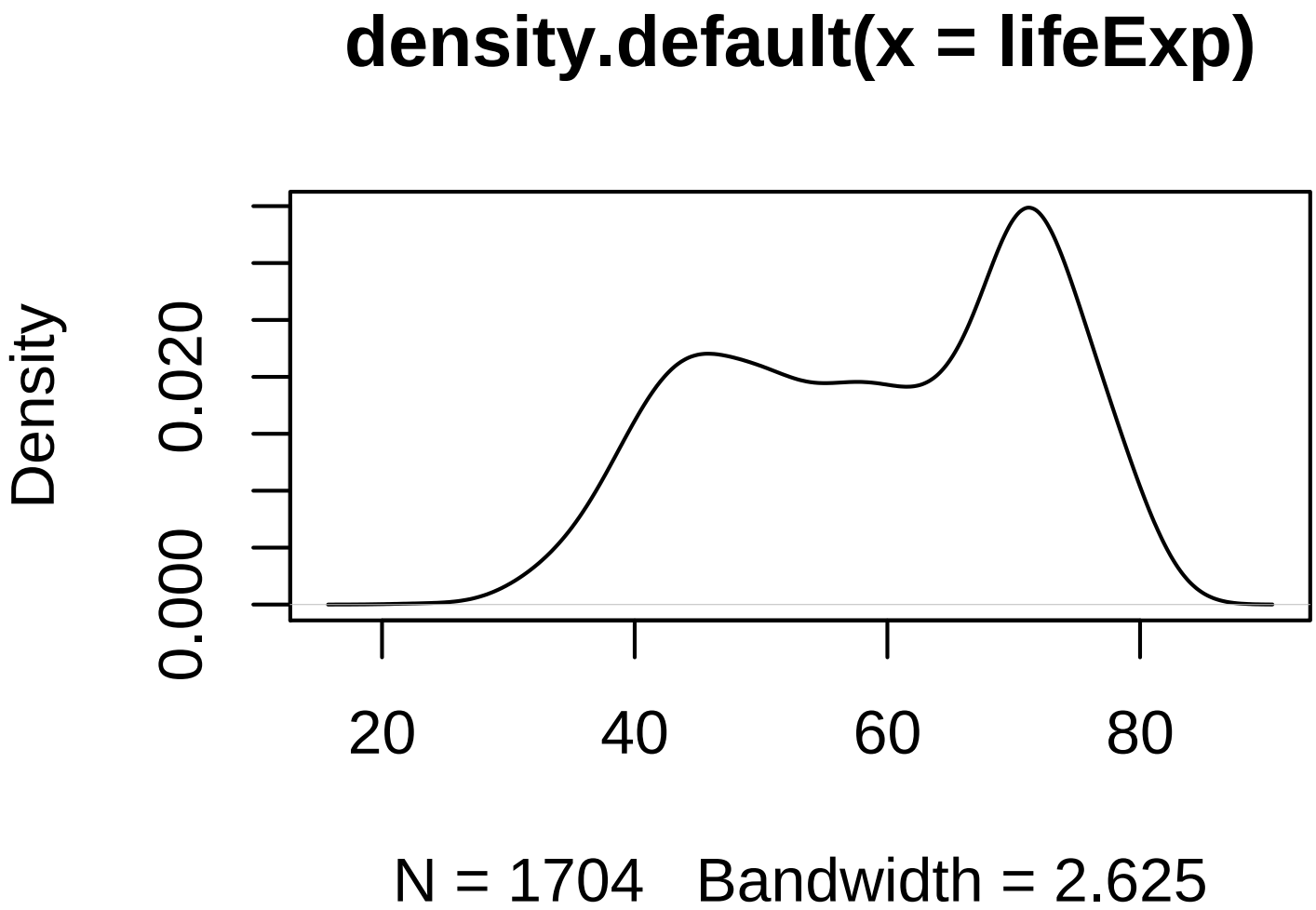
Base R examples

```
with(gapminder,boxplot(split(lifeExp,continent)))
```



Base R examples

```
with(gapminder,plot(density(lifeExp)))
```



Base R graphics: Where to learn more

- Paul Murrell's book: [https://www.stat.auckland.ac.nz/~paul/RG2e/]
- Ross Ihaka's lectures: [https://www.stat.auckland.ac.nz/~ihaka/787/lectures-r-graphics.pdf]

`grid` graphics

`grid` graphics

- `grid` graphics is a low-level graphics system that allows fine control of graphics elements
- Users can create multiple graphics regions, or "viewports", that are arranged on the graphics device or nested within one another.
- Graphical objects, or "grobs" can be created and drawn on these viewports (e.g., lines, shapes).
- Grobs can be editted (e.g., change color of lines) and re-drawn

`grid` graphics: Where to learn more

- Paul Murrell's book:
  [https://www.stat.auckland.ac.nz/~paul/RG2e/]

ggplot2 basics

ggplot2

- ggplot2 is implemented in grid graphics
- The g's stand for Grammar of Graphics.
  - Like English grammar is the way in which words are put together to form sentences, a grammar of graphics is a way to put together basic graphical elements to make a graph.
- To understand the grammar we need to define the basic elements.
  - Start with definitions (in bold), some of which are too abstract to be useful until we get into details.
- ggplots can be built in layers, comprised of **data** a **mapping**, a **geom** and optionally **stats**
- The layers are arranged and labelled on the graph by **scale**s and **coord**s.
- The data can also be broken into subsets and displayed in separate graphs by a **facet** specification.

Components of a ggplot: data and mappings

- We start with the **data** we want to visualize and a **mapping**, or aesthetic, that describes how these data map to attributes on the plot.

```
p <- ggplot(gapminder,aes(x=log10GdpPercap,y=lifeExp,color=continent))
```

- From the dataset `gapminder`, the variable `log10GdpPercap` will be mapped to y-coordinates, `lifeExp` will be mapped to the x-coordinates, and `continent` will be perceived as colours.

Components of a ggplot: geometric objects (geoms)

- Geometric objects or **geoms** are things like points and lines that we see on the plot.

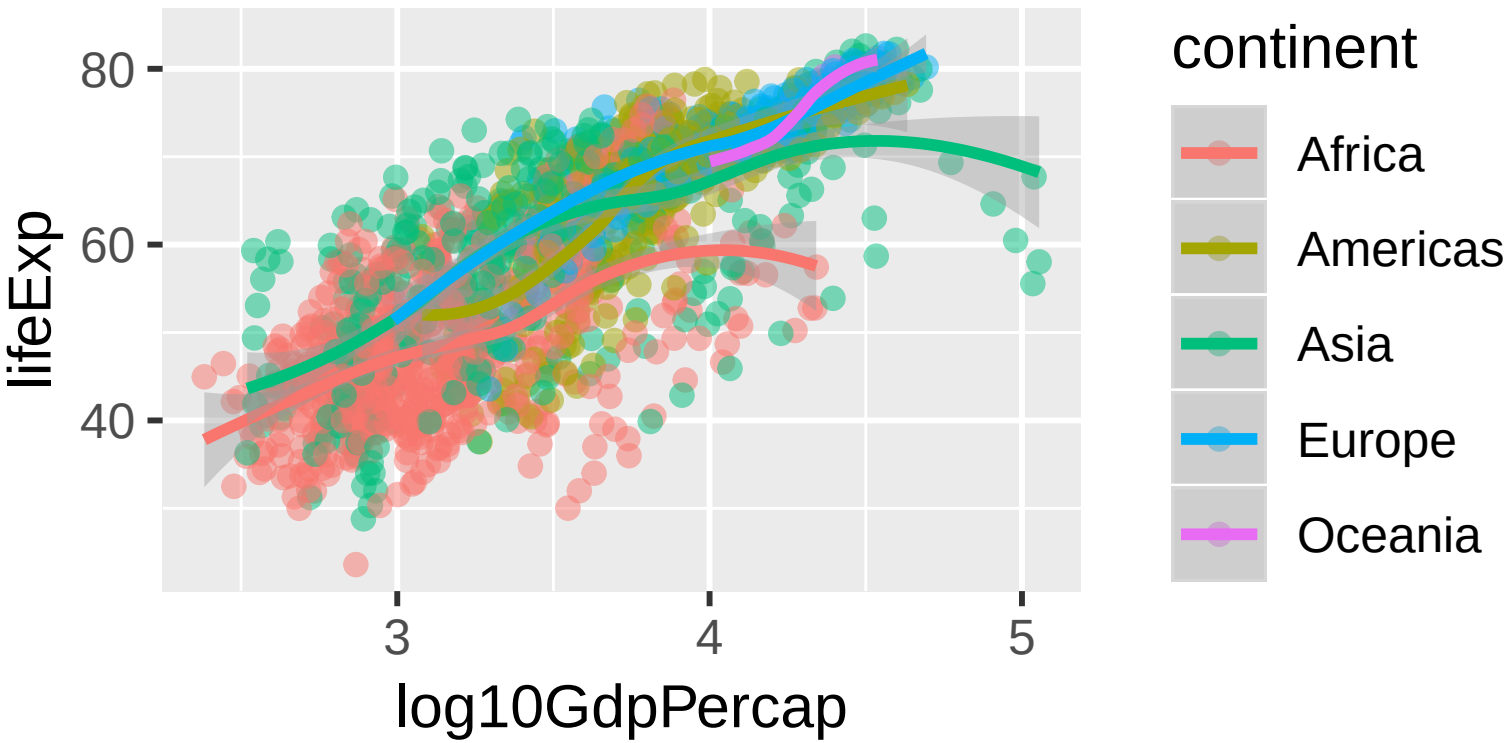
```
p2 <- p + geom_point(alpha=0.5)
```

- alpha is the transparency aesthetic, between 0 and 1, best applied directly to the geom.

Components of a ggplot: statistical transformations

- Statistical transformations or **stats** summarize the data; e.g., a scatterplot smoother

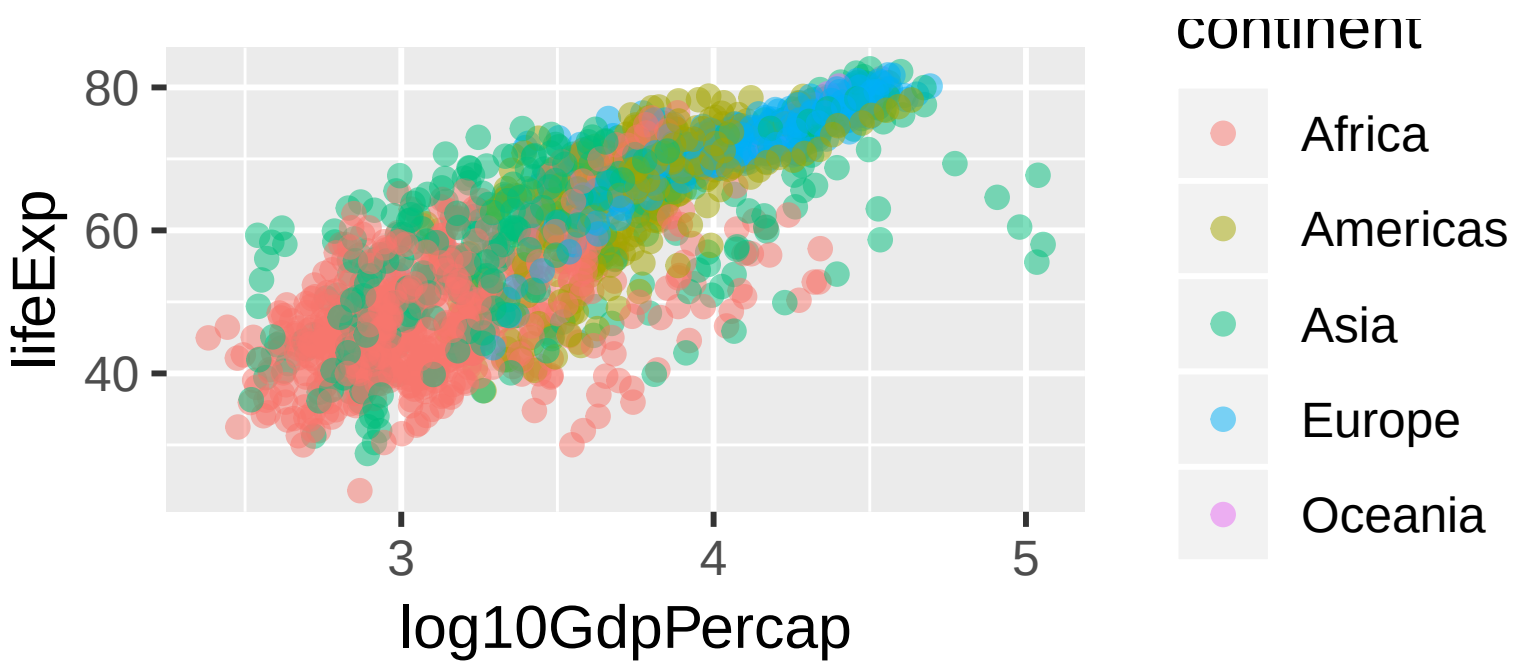
```
p2 + stat_smooth()
```



Components of a ggplot: scales

- The **scales** are mappings from the data to the graphics device
  - domain of `continent` is the five continents, range is the hexidecimal of the five colors represented on the graph
  - domain of `lifeExp` is 23.599 to 82.603, range is [0,1], which `grid` converts to a range of vertical pixels on the graph.
  - legends and axes provide the inverse mapping

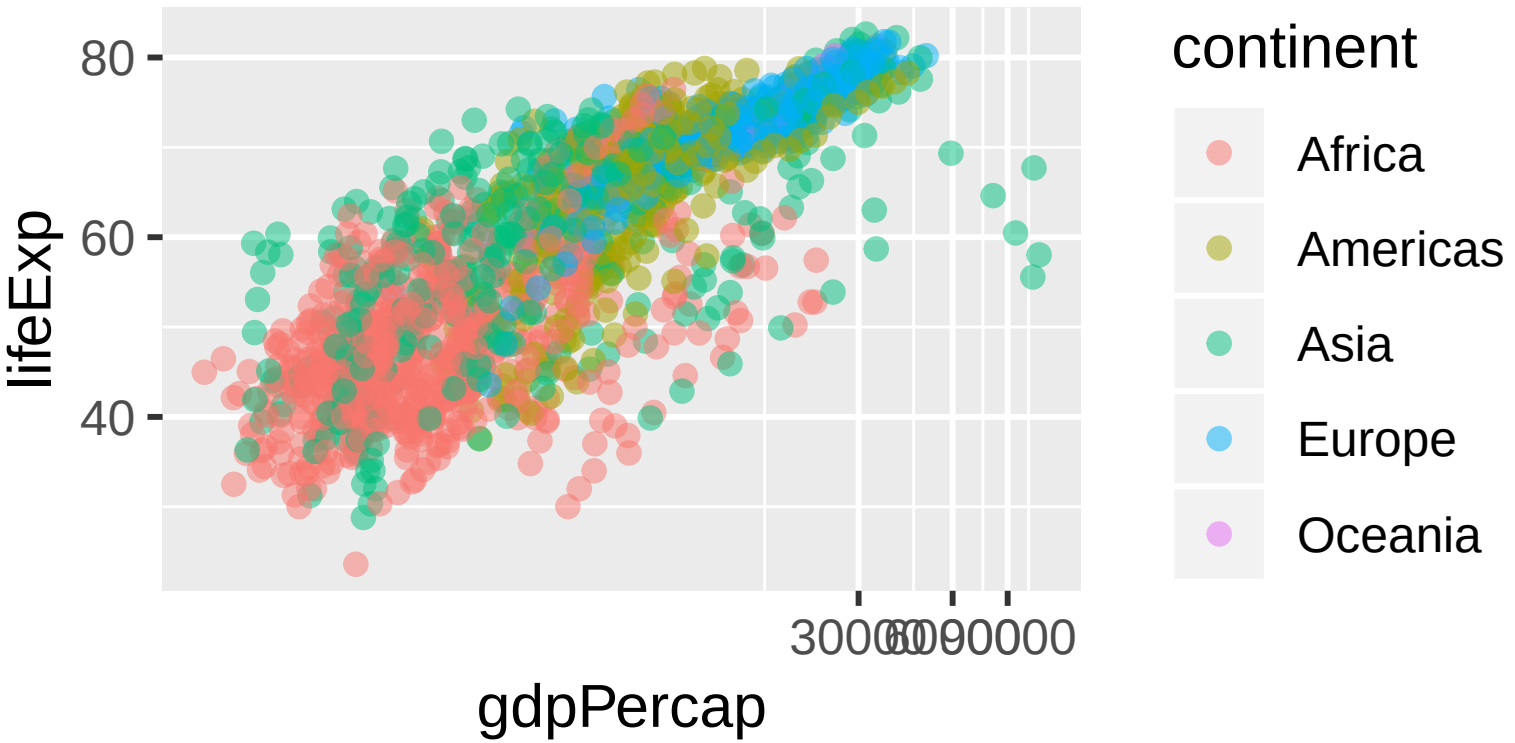
```
p2
```



Components of a ggplot: coodinate system

- The coordinate system is another layer in how the data get mapped to the graphics device.
  - Usually Cartesian, but could be, e.g., polar coordinates, or a transformation.

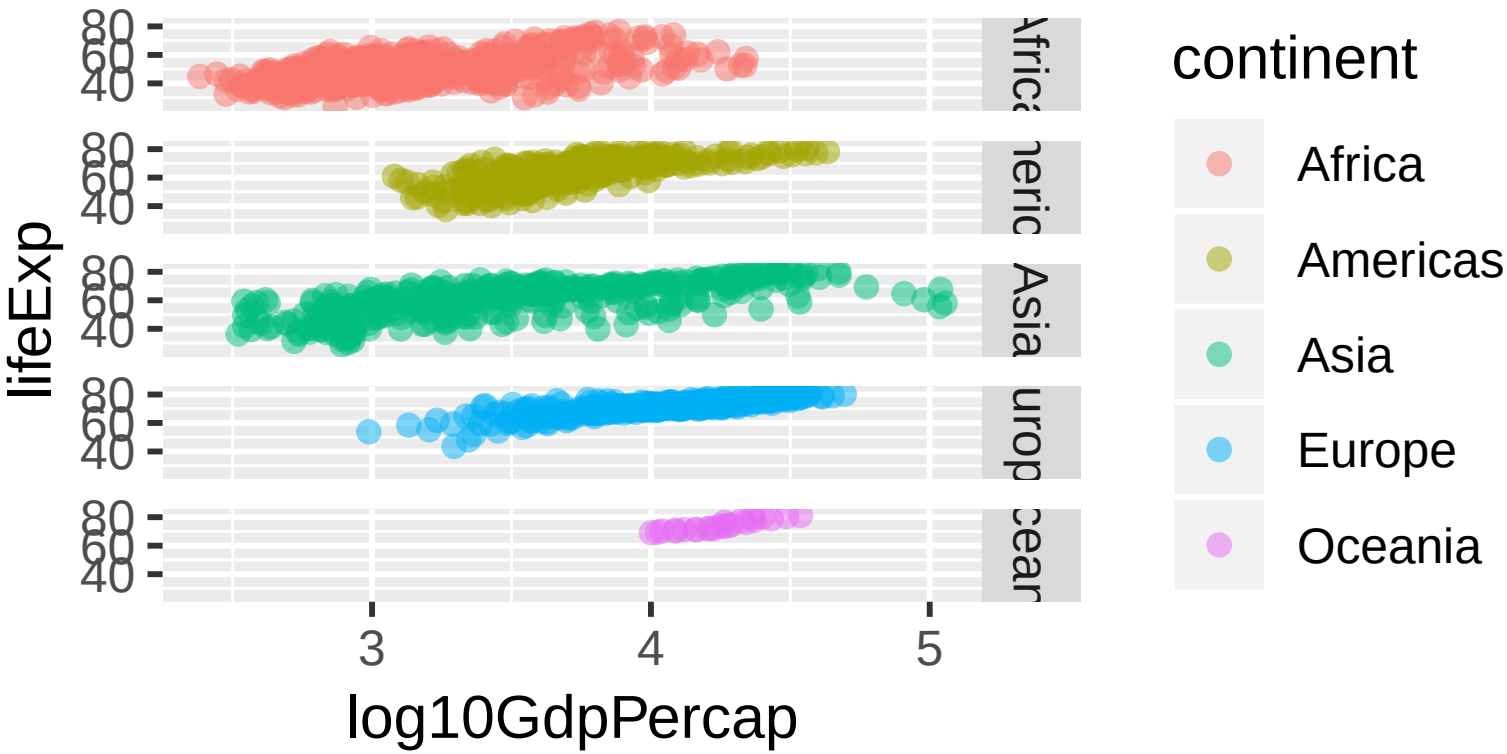
```
ggplot(gapminder,aes(x=gdpPercap,y=lifeExp,color=continent)) +
  geom_point(alpha=0.5) + coord_trans(x="log10")
```



Components of a ggplot: faceting

- How to break up the data into subsets and arrange multiple plots on the graphics device.

```
p2 +  facet_grid(continent ~ .)
```



Why so many components?

- A framework for the components of a graph.
- Gives the user the ability to change indvidual components one at a time.

More details

- Layers
  - data, aesthetic mapping, geom, statistical transformation and position adjustment (to be defined)
- Tools for working with layers
- Scales, axes and legends
- Positioning: faceting and coordinate systems

Example dataset: Diamonds

- Price and quality of about 54,000 diamonds.
- Quality measures are carat (size), cut, colour and clarity
- Also included are three measures of the dimensions of each diamond labelled x, y and z.

```
data(diamonds)
head(diamonds)
```

```
## # 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 0.23  Ideal     E     SI2      61.5    55   326  3.95  3.98  2.43
## 2 0.21  Premium   E     SI1      59.8    61   326  3.89  3.84  2.31
## 3 0.23  Good      E     VS1      56.9    65   327  4.05  4.07  2.31
## 4 0.290 Premium   I     VS2      62.4    58   334  4.2   4.23  2.63
## 5 0.31  Good      J     SI2      63.3    58   335  4.34  4.35  2.75
## 6 0.24  Very Good J     VVS2     62.8    57   336  3.94  3.96  2.48
```

Initialization

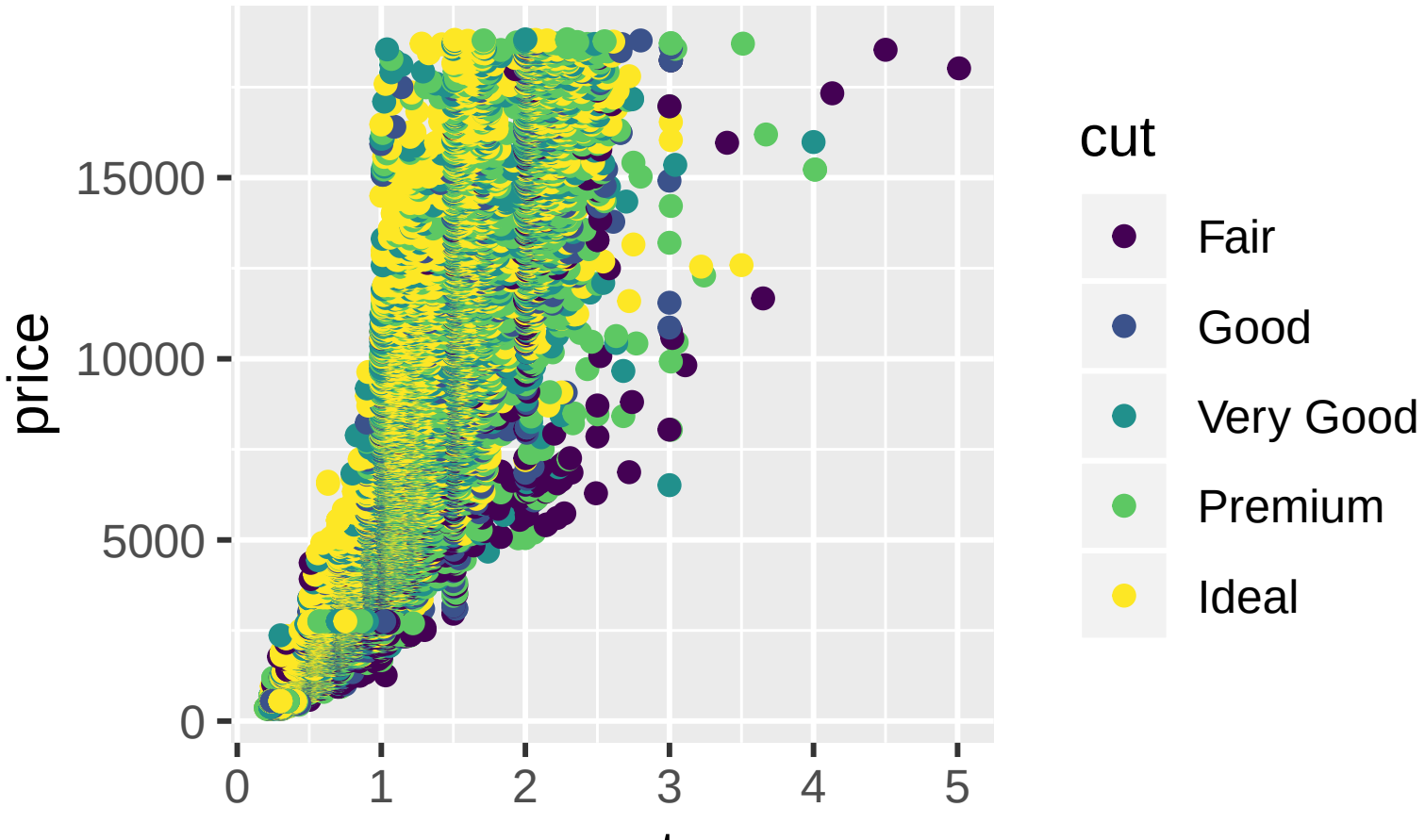
- We first initialize the plot.
- Initializing is done with `ggplot()`.
  - We usually specify the default data and aesthetic mappings for all subsequent layers, though this is not necessary.
  - Without layers, the plot is not displayed.

```
p <- ggplot(diamonds,aes(x=carat,y=price,colour=cut))
```

Adding layers

- Add with a +
- The `layer()` function can be used to specify a geom, stat and position
  - data and mapping will be inherited from initialization

```
p + layer(geom="point", stat="identity", position="identity")
```



Shortcuts for adding layers

- Shortcut functions are of the form `geom_XXX()` and `stat_XXX()`.
  - The `geom_XXX()` functions have a default stat and position
  - The `stat_XXX()` functions have a default geom and position
  - The `geom_XXX()` can over-ride the default stat and the `stat_XXX()` can over-ride the default geom though
- Call on the previous slide is equivalent to

```
p <- p + geom_point()
```

Aside: Plot objects

- Notice that plot objects can be stored as R objects:

```
summary(p)
```

```
## data: carat, cut, color, clarity, depth, table, price, x, y, z
##   [53940x10]
## mapping:  x = ~carat, y = ~price, colour = ~cut
## faceting: <ggproto object: Class FacetNull, Facet, gg>
##     compute_layout: function
##     draw_back: function
##     draw_front: function
##     draw_labels: function
##     draw_panels: function
##     finish_data: function
##     init_scales: function
##     map_data: function
##     params: list
##     setup_data: function
##     setup_params: function
##     shrink: TRUE
##     train_scales: function
##     vars: function
##     super:  <ggproto object: Class FacetNull, Facet, gg>
## -----------------------------------
## geom_point: na.rm = FALSE
## stat_identity: na.rm = FALSE
## position_identity
```