Air Toxics Data in R: Zero to Shiny

Kali Frost and Nathan Byers

October 26, 2015

Who we are

- Nathan Byers
  - Database Analyst at Indiana University (IU) School of Medicine
- Kali Frost
  - Research Associate at IU School of Public Health
- Eric Bailey (*in absentia*)
  - Web Application Developer at IU School of Medicine
- Former employees at the Indiana Department of Environmental Management
- Experienced data analysts and R programmers

Who we are

- R enthusiasts
- Follow along at
  `https://ebailey78.shinyapps.io/epaToxicsPresentation`

What this is

- R presentation using ioslides
- Source code is on GitHub
- This is entirely reproducible
- Comic credit: `https://xkcd.com/242/`

Training Outline

- What is R and RStudio
- R basics
- The Hadleyverse
  - `dplyr`
  - `tidyr`
  - `ggplot2`
- Useful packages for air toxics
  - `raqdm`
  - `rucl`
  - `openair`
- Air toxics analysis demo
- Interactive web app with `shiny`

What is R and RStudio

The R Project

- R is free and open-source software for statistical computing and graphics
- Download here
- It has been very popular in academia for more than a decade
- Statisitcal software that can do complex analyses using built-in functions, similar to SAS
- Also a programming language that is extendable (i.e. you can write your own functions/software)

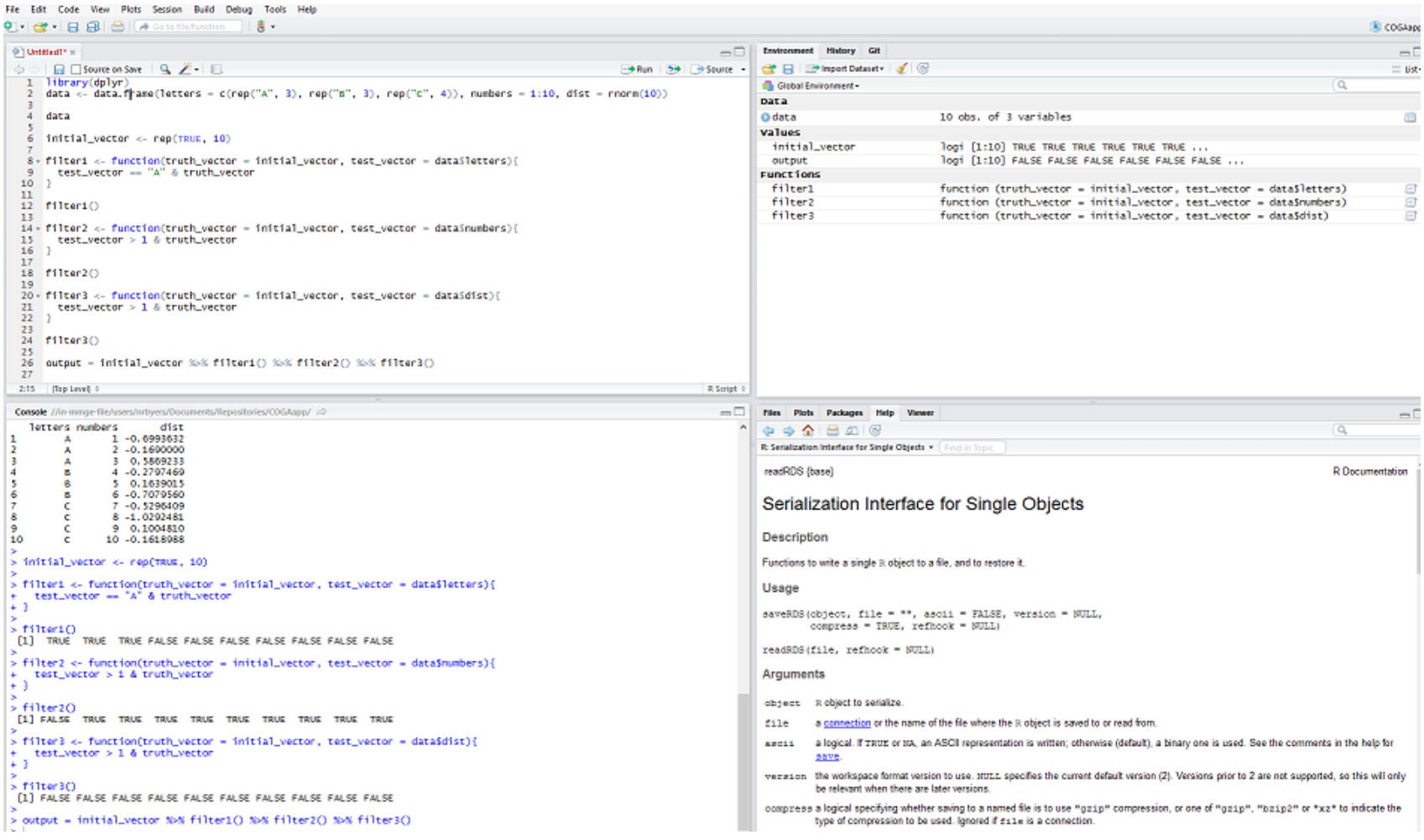
Popularity

- Originally written by statisticians for statisticians
- Now widely used in academia (not just stats departments)
- Making headway into government and industry, especially the biotech and finance sectors.
- Here is a link describing the increasing popularity of R.

RStudio

- After you download R, you may want to use an integrated development environment (IDE) like RStudio
- An IDE makes R a little more user friendly
- RStudio is free and can be downloaded at rstudio.com

RStudio

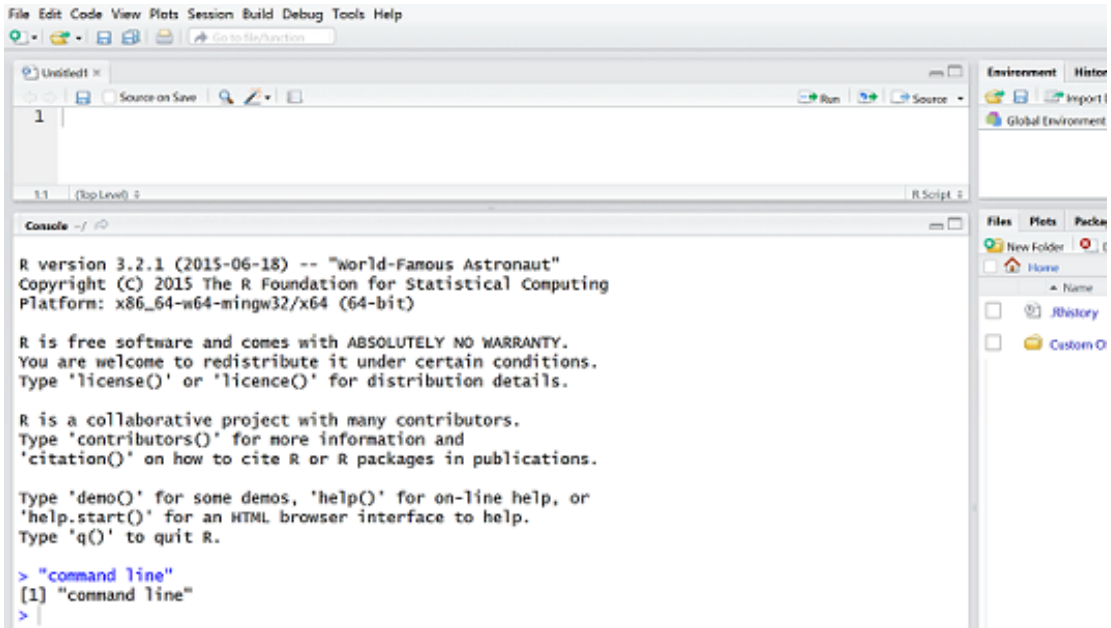

File Edit Code View Plots Session Build Debug Tools Help
Untitled1*
Source on Save
Run
Source
1 library(dplyr)
2 data <- data.frame(letters = c(rep("A", 3), rep("B", 3), rep("C", 4)), numbers = 1:10, dist = rnorm(10))
3
4 data
5
6 initial_vector <- rep(TRUE, 10)
7
8 filter1 <- function(truth_vector = initial_vector, test_vector = data$letters){
9 test_vector == "A" & truth_vector
10 }
11
12 filter1()
13
14 filter2 <- function(truth_vector = initial_vector, test_vector = data$numbers){
15 test_vector > 1 & truth_vector
16 }
17
18 filter2()
19
20 filter3 <- function(truth_vector = initial_vector, test_vector = data$dist){
21 test_vector > 1 & truth_vector
22 }
23
24 filter3()
25
26 output = initial_vector %>% filter1() %>% filter2() %>% filter3()
27
2:15 (Top Level) R Script
Environment History Git
Import Dataset
Global Environment
Data
data 10 obs. of 3 variables
Values
initial_vector logi [1:10] TRUE TRUE TRUE TRUE TRUE TRUE ...
output logi [1:10] FALSE FALSE FALSE FALSE FALSE FALSE ...
Functions
filter1 function (truth_vector = initial_vector, test_vector = data$letters)
filter2 function (truth_vector = initial_vector, test_vector = data$numbers)
filter3 function (truth_vector = initial_vector, test_vector = data$dist)
Console
letters numbers dist
1 A 1 -0.6993632
2 A 2 -0.1690000
3 A 3 0.5869233
4 B 4 -0.2797469
5 B 5 0.1639015
6 B 6 -0.7079560
7 C 7 -0.5296409
8 C 8 -1.0292481
9 C 9 0.1004810
10 C 10 -0.1618988
> initial_vector <- rep(TRUE, 10)
> filter1 <- function(truth_vector = initial_vector, test_vector = data$letters){
+ test_vector == "A" & truth_vector
+ }
> filter1()
[1] TRUE TRUE TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
> filter2 <- function(truth_vector = initial_vector, test_vector = data$numbers){
+ test_vector > 1 & truth_vector
+ }
> filter2()
[1] FALSE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
> filter3 <- function(truth_vector = initial_vector, test_vector = data$dist){
+ test_vector > 1 & truth_vector
+ }
> filter3()
[1] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
> output = initial_vector %>% filter1() %>% filter2() %>% filter3()
Files Plots Packages Help Viewer
R: Serialization Interface for Single Objects
readRDS {base} R Documentation
Serialization Interface for Single Objects
Description
Functions to write a single R object to a file, and to restore it.
Usage
saveRDS(object, file = "", ascii = FALSE, version = NULL,
compress = TRUE, refhook = NULL)
readRDS(file, refhook = NULL)
Arguments
object R object to serialize.
file a connection or the name of the file where the R object is saved to or read from.
ascii a logical. If TRUE or NA, an ASCII representation is written; otherwise (default), a binary one is used. See the comments in the help for save.
version the workspace format version to use. NULL specifies the current default version (2). Versions prior to 2 are not supported, so this will only be relevant when there are later versions.
compress a logical specifying whether saving to a named file is to use "gzip" compression, or one of "gzip", "bzip2" or "xz" to indicate the type of compression to be used. Ignored if file is a connection.

Training Outline

- What is R and RStudio
- R basics
- The Hadleyverse
  - dplyr
  - tidyr
  - ggplot2
- Useful packages for air toxics
  - raqdm
  - rucl
  - openair
- Air toxics analysis demo
- Interactive web app with shiny

R Basics - Command line

- R is a language and an environment
- You type in the "command line" and hit enter to do something, in contrast to pointing and clicking to do something



R Basics - Command line

- In this presentation, command line code will be shown in blocks with gray background shading
- The output will be shown in a separate block below the command line input with a lighter shadow and ## at the beginning of each line

```
"command line"
```

```
## [1] "command line"
```

```
1 + 1
```

```
## [1] 2
```

R Basics - Math

As we demonstrated in the previous slide, you can use R as a simple calculator

```
3 - 1
```

```
## [1] 2
```

```
2 * 2
```

```
## [1] 4
```

```
10 / 5
```

```
## [1] 2
```

```
log(10)
```

```
## [1] 2.302585
```

R Basics - Variables

We can store numbers and text in variables

```
x <- 1
x
```

```
## [1] 1
```

```
x <- 10
x
```

```
## [1] 10
```

```
y <- 2
x * y
```

```
## [1] 20
```

R Basics - Variables

```
pollutant <- "benzene"
pollutant
```

```
## [1] "benzene"
```

```
pollutant <- "toluene"
pollutant
```

```
## [1] "toluene"
```

R Basics - Vectors

- A series of numbers or text values and be stored together in a vector
- The container for a vector is c( )

```
c(1, 2, 3)
```

```
## [1] 1 2 3
```

```
x <- c(5, 6, 7)
x
```

```
## [1] 5 6 7
```

```
z <- c("mercury", "cadmium")
z
```

```
## [1] "mercury" "cadmium"
```

R Basics - Functions

- Variables and vectors contain data
- Functions do stuff to data
- You recongnize a function by parentheses ( )

```
x <- c(1, 2, 3, 3, 4, 5, 5, 6, 7, 7, 7)
mean(x)
```

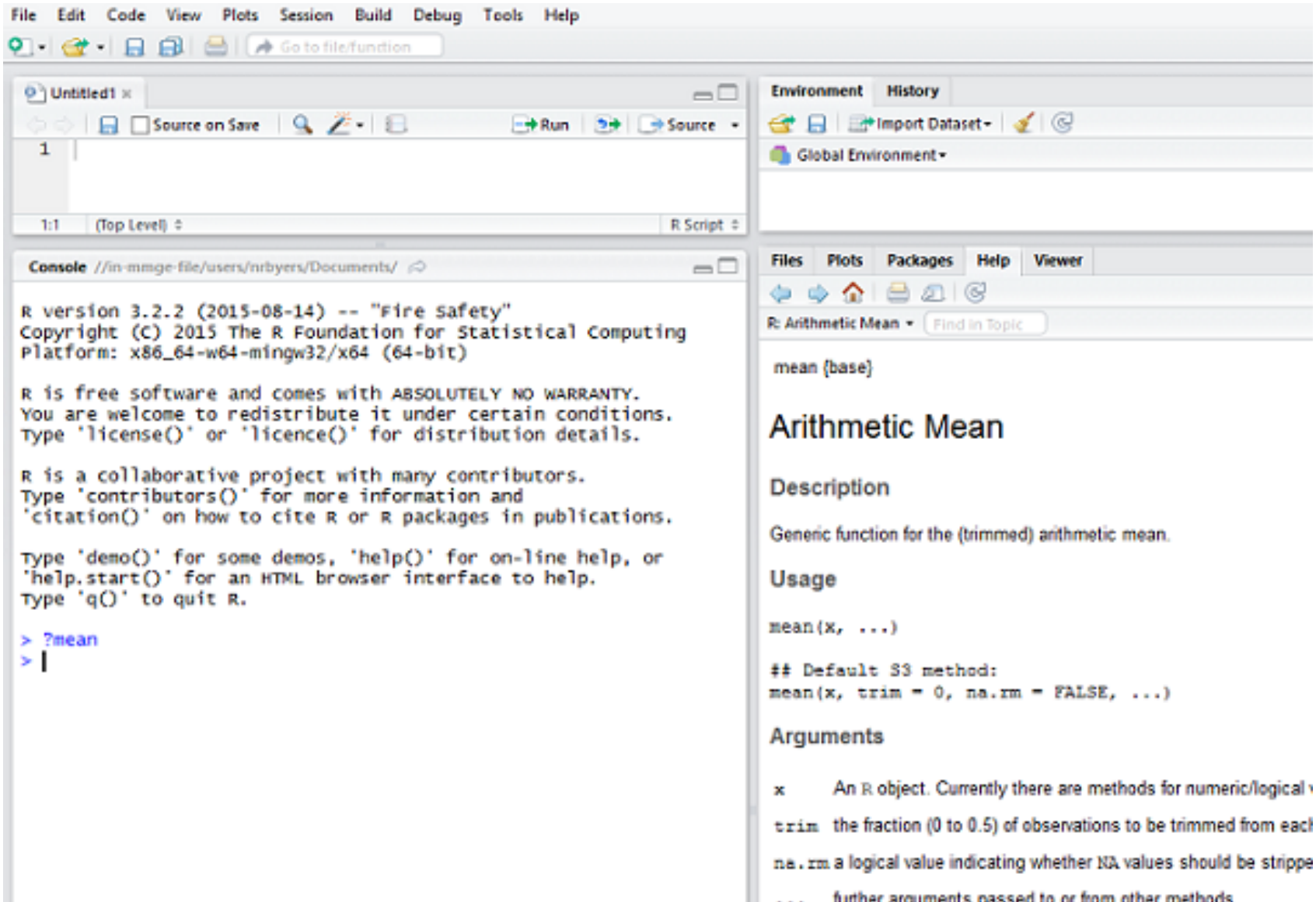
```
## [1] 4.545455
```

```
median(x)
```

```
## [1] 5
```

R Basics - Functions

- To find out how to use a function, type ? then the function name
- Below is an image of what you see in RStudio if you type `?mean` and hit return



R Basics - Data Frames

- A data frame is a collection of vectors with the same length
- Basically a spreadsheet

```
pollutant <- c("benzene", "acrolein")
value <- c(.7, .8)
unit <- c("ug/m^3", "ug/m^3")
df <- cbind(pollutant, value, unit)
df
```

```
##       pollutant  value unit
## [1,] "benzene"  "0.7" "ug/m^3"
## [2,] "acrolein" "0.8" "ug/m^3"
```

R Basics - Data Objects and Functions

- Those are the basic type of objects you'll need to be familiar with to understand this training/demonstration
- Vectors and data frames store numbers and text (a variable with a single value is actually just a vector of length 1)
- Functions do things to vectors and data frames then return an output

R Basics - Installing/loading packages

- R comes with functions immediately available
- Some functions come with R, but they are only available after loading a package using `library()`

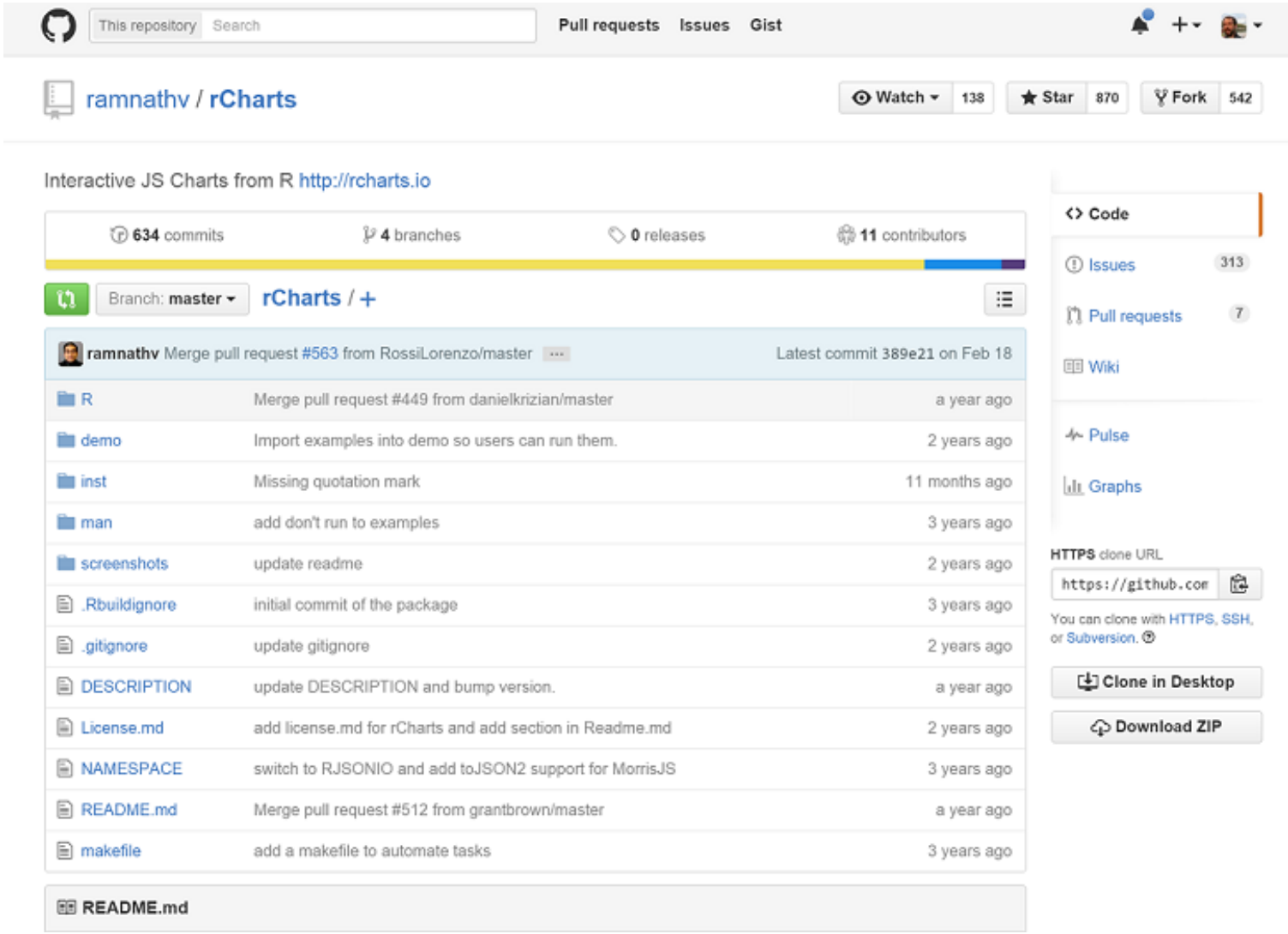
```
library(lattice)
```

- Some packages do not come with an R download
- Packages that are on CRAN can be downloaded and installed using `install.packages()`

```
install.packages("devtools")
```

R Basics - Installing from GitHub

- You may want to use a package that isn't on CRAN
- Many R developers put their packages on GitHub



R Basics - Installing from GitHub

- To install a package from GitHub, load the `devtools` package

```
library(devtools)
```

- Then use the `install_github()` function by specifying the user name and the repository

```
install_github("ramnathv/rCharts")
```

R Basics - Resources

- Many great resources for learning R
- Beginners material
  - Quick R
  - UCLA
  - DataCamp
  - Code School
- Intermediate/advanced material
  - Cookbook for R
  - Coursera
  - Advanced R

Training Outline

- What is R and RStudio
- R basics
- The Hadleyverse
  - `dplyr`
  - `tidyr`
  - `ggplot2`
- Useful packages for air toxics
  - raqdm
  - rucl
  - openair
- Air toxics analysis demo
- Interactive web app with shiny

The Hadleyverse

- The Hadleyverse is a collection of packages written by Hadley Wickham
- These packages make R much easier to use
- We will introduce three useful packages for data manipulation (`dplyr`), reshaping data (`tidyr`), and data visualization (`ggplot2`)
- Image credit

Data manipulation with `dplyr`

`dplyr` - Overview

- A very handy data manipulation package
- Very fast (much of it is written in C++)
- Can work with tables from databases
- Main functions are `filter()`, `summarize()`, and `mutate()`
- These main functions take a data frame as input and return a data frame as output

dplyr - Data

Below is a *made up* data frame that will be used to easily visualize `dplyr` operations

```
tox <- read.table(header=T, text='
  monitor  parameter        day   hour  value  screen
        A    benzene   20140601  08:00   0.72     1.3
        A    benzene   20140601  09:00   0.84     1.3
        A    benzene   20140602  08:00   1.35     1.3
        A    benzene   20140602  09:00   0.94     1.3
        B    benzene   20140601  08:00   0.61     1.3
        B    benzene   20140601  09:00   0.70     1.3
        B    benzene   20140602  08:00   0.99     1.3
        B    benzene   20140602  09:00   1.70     1.3
        A    toluene   20140601  08:00   6.10     300
        A    toluene   20140601  09:00   2.51     300
                      ')
```

dplyr - Filtering

- The first argument of `filter()` is a data frame, `filter(tox, ...)`
- The data frame can then be filters using logical expressions
- Here we filter the `tox` data frame so that we just get values from monitor A

```
library(dplyr)
filter(tox, monitor == "A")
```

```
##   monitor parameter      day  hour value screen
## 1       A   benzene 20140601 08:00  0.72    1.3
## 2       A   benzene 20140601 09:00  0.84    1.3
## 3       A   benzene 20140602 08:00  1.35    1.3
## 4       A   benzene 20140602 09:00  0.94    1.3
## 5       A   toluene 20140601 08:00  6.10  300.0
## 6       A   toluene 20140601 09:00  2.51  300.0
```

dplyr - Filtering

- You can enter more than one logical expression separated by a comma

```
filter(tox, monitor == "B", value > screen)
```

```
##   monitor parameter      day  hour value screen
## 1       B   benzene 20140602 09:00   1.7    1.3
```

- This is equivalent to using the & operator

```
filter(tox, monitor == "B" & value > screen)
```

```
##   monitor parameter      day  hour value screen
## 1       B   benzene 20140602 09:00   1.7    1.3
```

dplyr - Summarize

- The first argument of `summarize()` is also a data frame
- However, the input data frame requires grouping information
- For example, if we wanted to summarize the `tox` data frame by returning daily averages for each pollutant, we need to group the data frame by `monitor`, `parameter`, and `day`

```
head(tox)
```

```
##   monitor parameter      day  hour value screen
## 1       A   benzene 20140601 08:00  0.72    1.3
## 2       A   benzene 20140601 09:00  0.84    1.3
## 3       A   benzene 20140602 08:00  1.35    1.3
## 4       A   benzene 20140602 09:00  0.94    1.3
## 5       B   benzene 20140601 08:00  0.61    1.3
## 6       B   benzene 20140601 09:00  0.70    1.3
```

dplyr - Summarize

- We add grouping information by using the `group_by()` function

```
tox_daily <- group_by(tox, monitor, parameter, day)
```

- Now we feed this data frame to the summary function, `summarize(tox_daily, ...)`
- To get daily averages, we also supply a function that will return the mean, and we name it `daily_mean` (obviously not a true daily mean, with only a few hours...)

```
summarize(tox_daily, daily_mean = mean(value))
```

dplyr - Summarize

```
## Source: local data frame [5 x 4]
## Groups: monitor, parameter [?]
##
##   monitor parameter      day daily_mean
##    (fctr)    (fctr)    (int)      (dbl)
## 1       A   benzene 20140601      0.780
## 2       A   benzene 20140602      1.145
## 3       A   toluene 20140601      4.305
## 4       B   benzene 20140601      0.655
## 5       B   benzene 20140602      1.345
```

dplyr - Add Columns

- You can add new columns to a data frame by using the `mutate()` function
- The output will have the same number of rows
- The first argument is the input data frame and the subsequent arguments must be functions that return a single value for each row (i.e. *not* a summary function)

```
mutate(tox, above_screen = value > screen)
```

dplyr - Add Columns

```
mutate(tox, above_screen = value > screen)
```

```
##    monitor parameter      day  hour value screen above_screen
## 1        A   benzene 20140601 08:00  0.72    1.3         FALSE
## 2        A   benzene 20140601 09:00  0.84    1.3         FALSE
## 3        A   benzene 20140602 08:00  1.35    1.3          TRUE
## 4        A   benzene 20140602 09:00  0.94    1.3         FALSE
## 5        B   benzene 20140601 08:00  0.61    1.3         FALSE
## 6        B   benzene 20140601 09:00  0.70    1.3         FALSE
## 7        B   benzene 20140602 08:00  0.99    1.3         FALSE
## 8        B   benzene 20140602 09:00  1.70    1.3          TRUE
## 9        A   toluene 20140601 08:00  6.10  300.0         FALSE
## 10       A   toluene 20140601 09:00  2.51  300.0         FALSE
```

dplyr - Add Columns

Here we add more than one column at a time

```
mutate(tox, above_screen = value > screen,
       screen_diff = value - screen)
```

```
##    monitor parameter      day  hour value screen above_screen
## 1        A   benzene 20140601 08:00  0.72    1.3         FALSE
## 2        A   benzene 20140601 09:00  0.84    1.3         FALSE
## 3        A   benzene 20140602 08:00  1.35    1.3          TRUE
## 4        A   benzene 20140602 09:00  0.94    1.3         FALSE
## 5        B   benzene 20140601 08:00  0.61    1.3         FALSE
## 6        B   benzene 20140601 09:00  0.70    1.3         FALSE
## 7        B   benzene 20140602 08:00  0.99    1.3         FALSE
## 8        B   benzene 20140602 09:00  1.70    1.3          TRUE
## 9        A   toluene 20140601 08:00  6.10  300.0         FALSE
## 10       A   toluene 20140601 09:00  2.51  300.0         FALSE
```

Reshape data with `tidyr`

`tidyr` - Overview

- `tidyr` is a very simple but very useful package
- Just does two things
  - reshapes wide to long
  - reshapes long to wide

tidyr - Long to Wide

- The tox data frame is in a long format
- You can recognize a long format if there is only one column with values

```
head(tox)
```

```
##   monitor parameter      day  hour value screen
## 1       A   benzene 20140601 08:00  0.72    1.3
## 2       A   benzene 20140601 09:00  0.84    1.3
## 3       A   benzene 20140602 08:00  1.35    1.3
## 4       A   benzene 20140602 09:00  0.94    1.3
## 5       B   benzene 20140601 08:00  0.61    1.3
## 6       B   benzene 20140601 09:00  0.70    1.3
```

tidyr - Long to Wide

- The `spread()` function takes a long data frame and spreads it out into a wide data frame
- The first argument is the long data frame
- The second argument is the column name of the key
- The third argument is the column name of the values

```
library(tidyr)
tox_wide <- spread(tox, key = parameter, value = value)
```

tidyr - Long to Wide

```
tox_wide
```

```
##    monitor       day  hour screen benzene toluene
## 1        A 20140601 08:00    1.3    0.72      NA
## 2        A 20140601 08:00  300.0      NA    6.10
## 3        A 20140601 09:00    1.3    0.84      NA
## 4        A 20140601 09:00  300.0      NA    2.51
## 5        A 20140602 08:00    1.3    1.35      NA
## 6        A 20140602 09:00    1.3    0.94      NA
## 7        B 20140601 08:00    1.3    0.61      NA
## 8        B 20140601 09:00    1.3    0.70      NA
## 9        B 20140602 08:00    1.3    0.99      NA
## 10       B 20140602 09:00    1.3    1.70      NA
```

tidyr - Long to Wide

We could also spread the data frame by monitor

```
spread(tox, key = monitor, value = value)
```

```
##   parameter      day  hour screen     A     B
## 1   benzene 20140601 08:00    1.3 0.72 0.61
## 2   benzene 20140601 09:00    1.3 0.84 0.70
## 3   benzene 20140602 08:00    1.3 1.35 0.99
## 4   benzene 20140602 09:00    1.3 0.94 1.70
## 5   toluene 20140601 08:00  300.0 6.10   NA
## 6   toluene 20140601 09:00  300.0 2.51   NA
```

`tidyr` - Wide to Long

- The `gather()` function takes a wide data frame and gathers the columns into a long data frame
- The first argument is the wide data frame
- The second argument is the name of the key that will be created
- The third argument is the name of the value column that will be created
- The remaining arguments are the names of the columns to be gathered

tidyr - Wide to Long

```
head(tox_wide)
```

```
##   monitor      day  hour screen benzene toluene
## 1       A 20140601 08:00    1.3    0.72      NA
## 2       A 20140601 08:00  300.0      NA    6.10
## 3       A 20140601 09:00    1.3    0.84      NA
## 4       A 20140601 09:00  300.0      NA    2.51
## 5       A 20140602 08:00    1.3    1.35      NA
## 6       A 20140602 09:00    1.3    0.94      NA
```

```
tox_long <- gather(tox_wide, key = pollutant,
                   value = sample_measurement,
                   benzene, toluene)
```

tidyr - Wide to Long

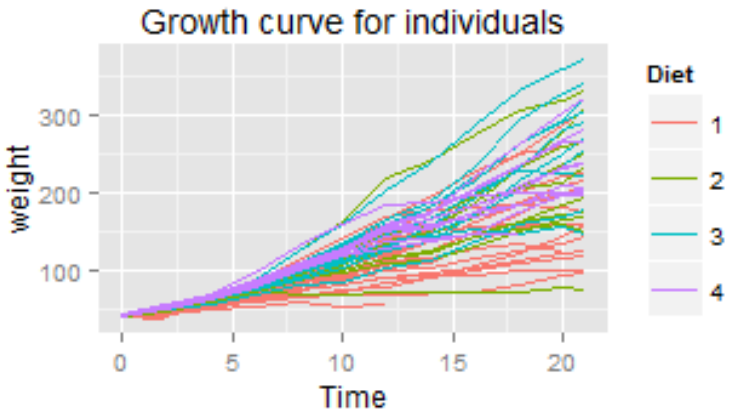
```
tox_long
```

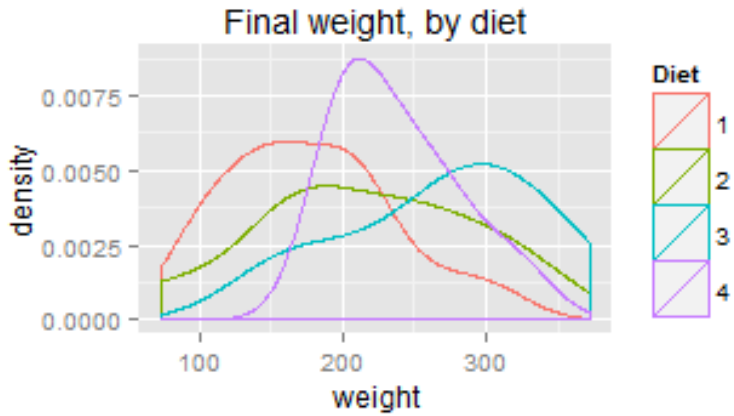
```
##    monitor       day  hour screen pollutant sample_measurement
## 1        A 20140601 08:00    1.3   benzene                0.72
## 2        A 20140601 08:00  300.0   benzene                  NA
## 3        A 20140601 09:00    1.3   benzene                0.84
## 4        A 20140601 09:00  300.0   benzene                  NA
## 5        A 20140602 08:00    1.3   benzene                1.35
## 6        A 20140602 09:00    1.3   benzene                0.94
## 7        B 20140601 08:00    1.3   benzene                0.61
## 8        B 20140601 09:00    1.3   benzene                0.70
## 9        B 20140602 08:00    1.3   benzene                0.99
## 10       B 20140602 09:00    1.3   benzene                1.70
## 11       A 20140601 08:00    1.3   toluene                  NA
## 12       A 20140601 08:00  300.0   toluene                6.10
## 13       A 20140601 09:00    1.3   toluene                  NA
## 14       A 20140601 09:00  300.0   toluene                2.51
## 15       A 20140602 08:00    1.3   toluene                  NA
## 16       A 20140602 09:00    1.3   toluene                  NA
## 17       B 20140601 08:00    1.3   toluene                  NA
```

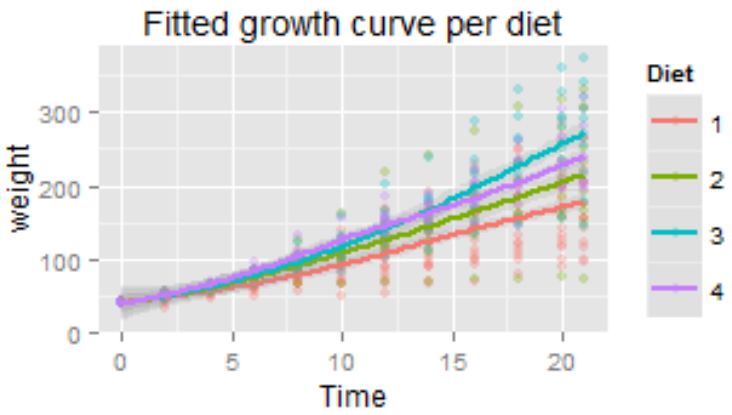
Visualize data with `ggplot2`

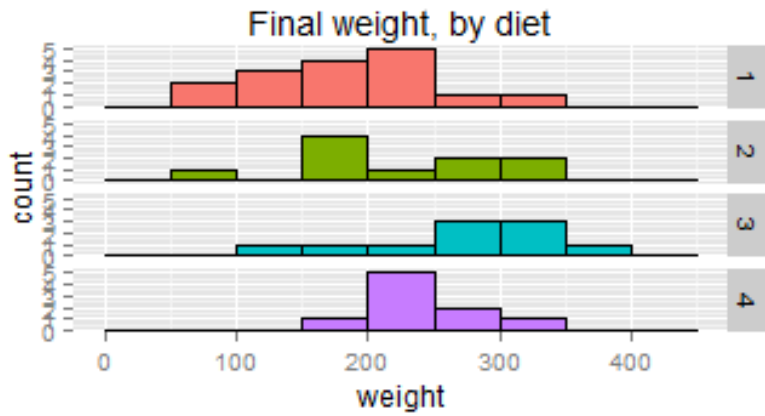
ggplot2 - Overview

- Base R does have graphing functions for common plots, such as scatter plots, line graphs, box plots, and histograms
- ggplot2 makes it easier to create multi-panel/complex plots









ggplot2 - Example Data

For demonstration we'll use the following randomly generated data

```
rtox <- data.frame(
  date = rep(seq(as.Date("2014-01-01"), by = 6, length = 60), 2),
  monitor = rep(c("A", "B"), each = 60),
  benzene = rgamma(120, shape = 1.5, scale = 3),
  formaldehyde = rgamma(120, shape = 1, scale = 2),
  acrolein = rgamma(120, shape = 1.5, scale = 2.5),
  p_dichlorobenzene = rgamma(120, shape = 1, scale = 3)
)
head(rtox, 3)
```

```
##         date monitor  benzene formaldehyde acrolein p_dichlor
## 1 2014-01-01       A 4.798135    0.9994482 3.647809
## 2 2014-01-07       A 3.360651    0.0396585 3.043189
## 3 2014-01-13       A 3.341292    3.3611858 2.503075
```

ggplot2 - Example Data

```
rtox_long <- gather(rtox, parameter, value = sample,
                    benzene:p_dichlorobenzene)
head(rtox_long)
```

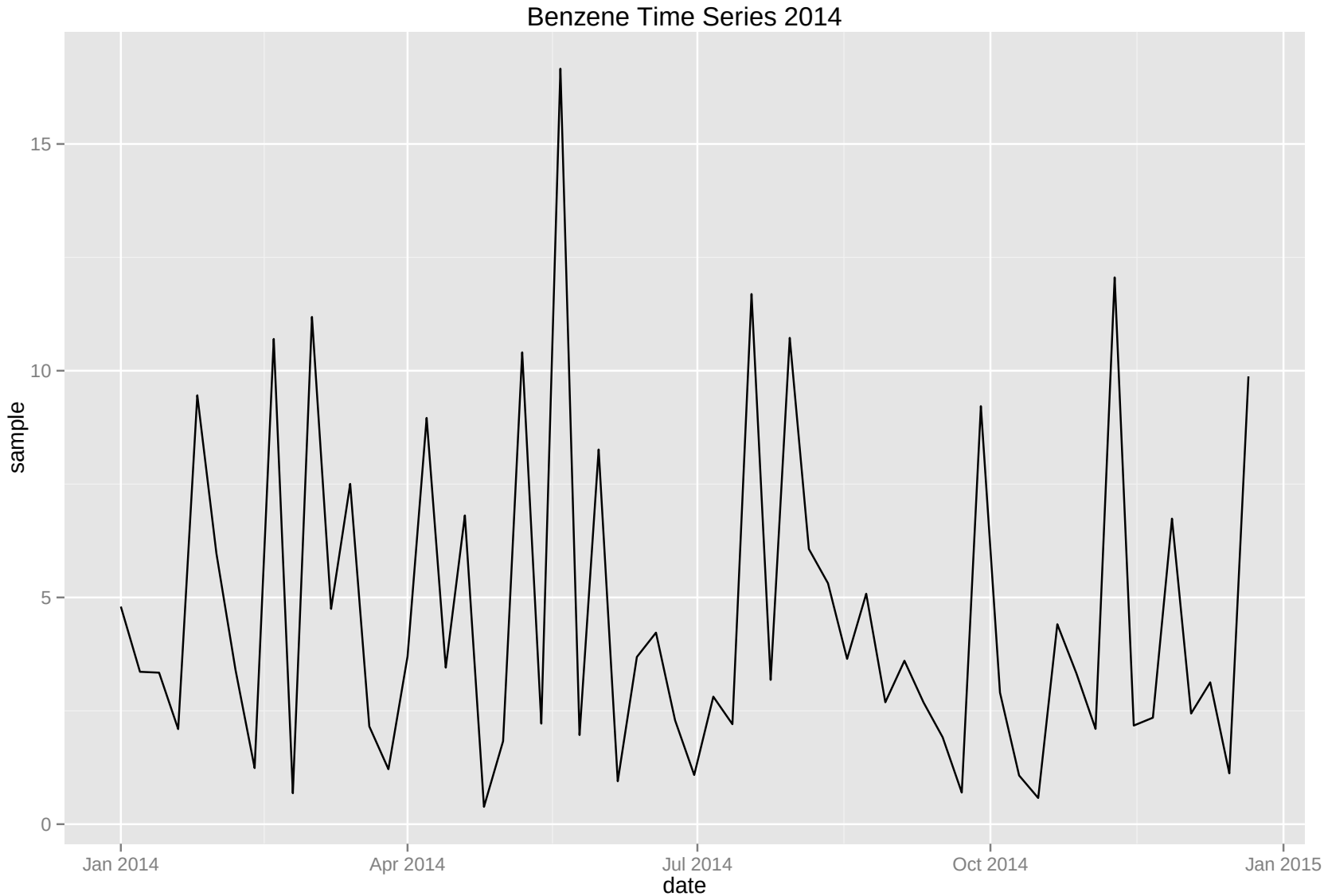
```
##         date monitor parameter   sample
## 1 2014-01-01       A   benzene 4.798135
## 2 2014-01-07       A   benzene 3.360651
## 3 2014-01-13       A   benzene 3.341292
## 4 2014-01-19       A   benzene 2.097056
## 5 2014-01-25       A   benzene 9.457852
## 6 2014-01-31       A   benzene 5.969694
```

ggplot2 - Time Series

- Here is code to make a time series plot of benzene at site A
- The `aes()` parameter is where we specify the x and y axes
- `geom_line()` makes it a line graph

```
library(ggplot2)

benzene_A <- filter(rtox_long, parameter == "benzene",
                    monitor == "A")

ggplot(benzene_A, aes(x=date, y=sample)) + geom_line() +
    ggtitle("Benzene Time Series 2014")
```

ggplot2 - Time Series

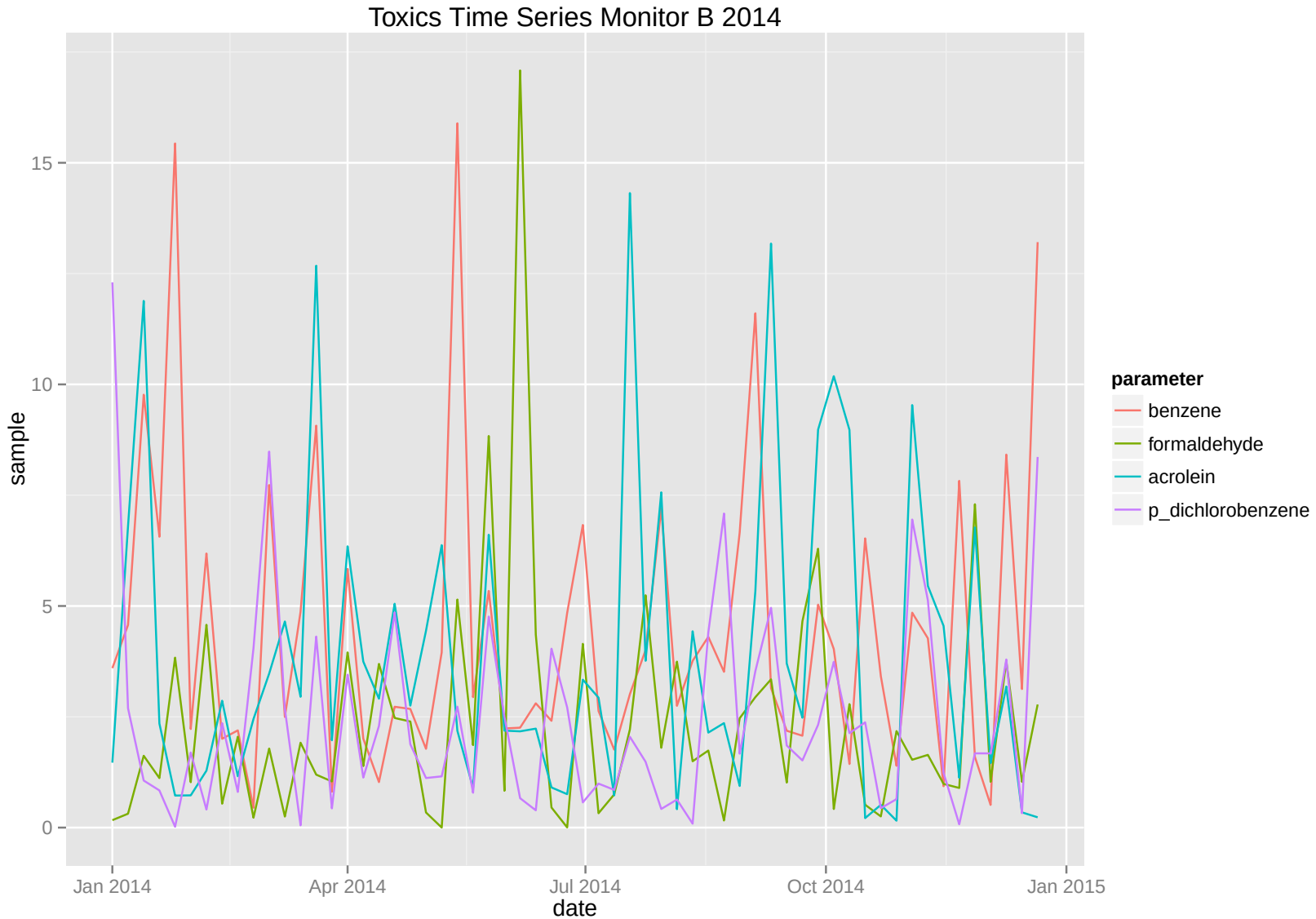


ggplot2 - Time Series

Here we make a time series plot of all pollutants at monitor B

```
site_B <- filter(rtox_long, monitor == "B")

ggplot(site_B, aes(x=date, y=sample, color=parameter)) +
    geom_line() +
    ggtitle("Toxics Time Series Monitor B 2014")
```

ggplot2 - Time Series

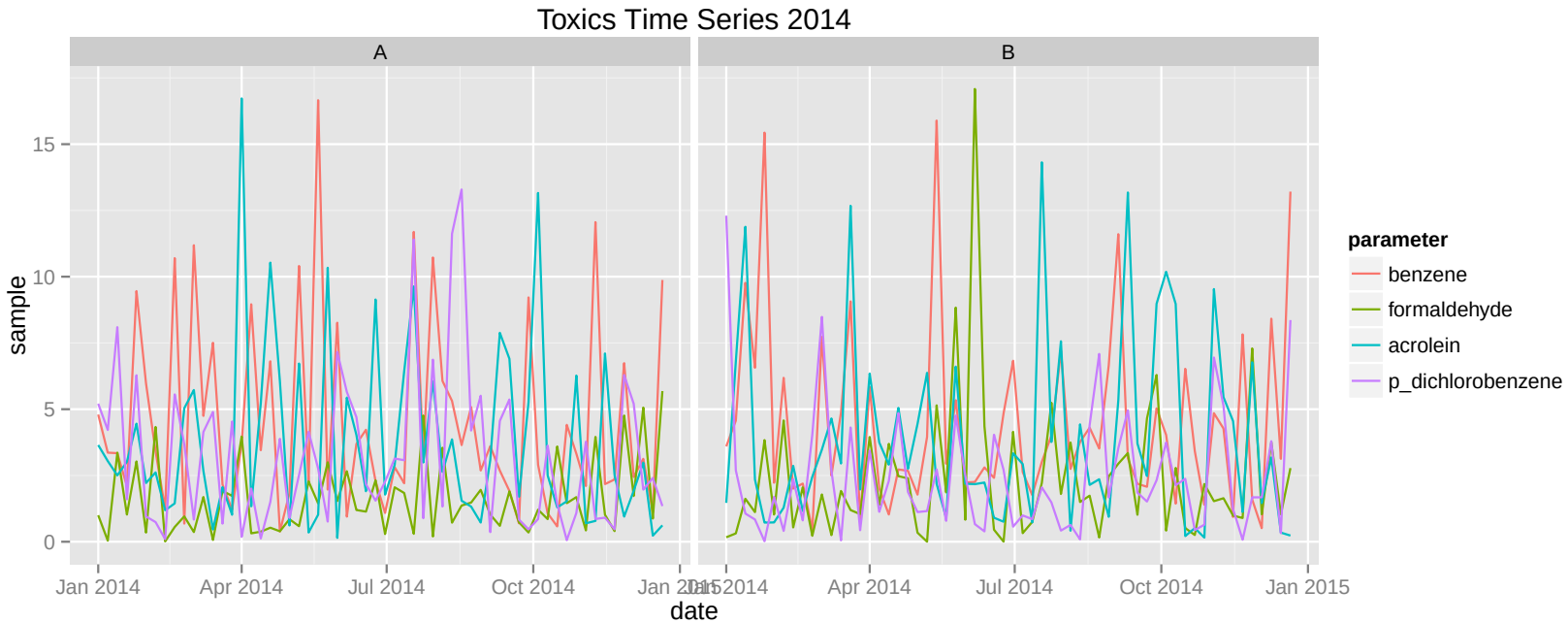


ggplot2 - Time Series

Here we plot all toxics data for both monitors

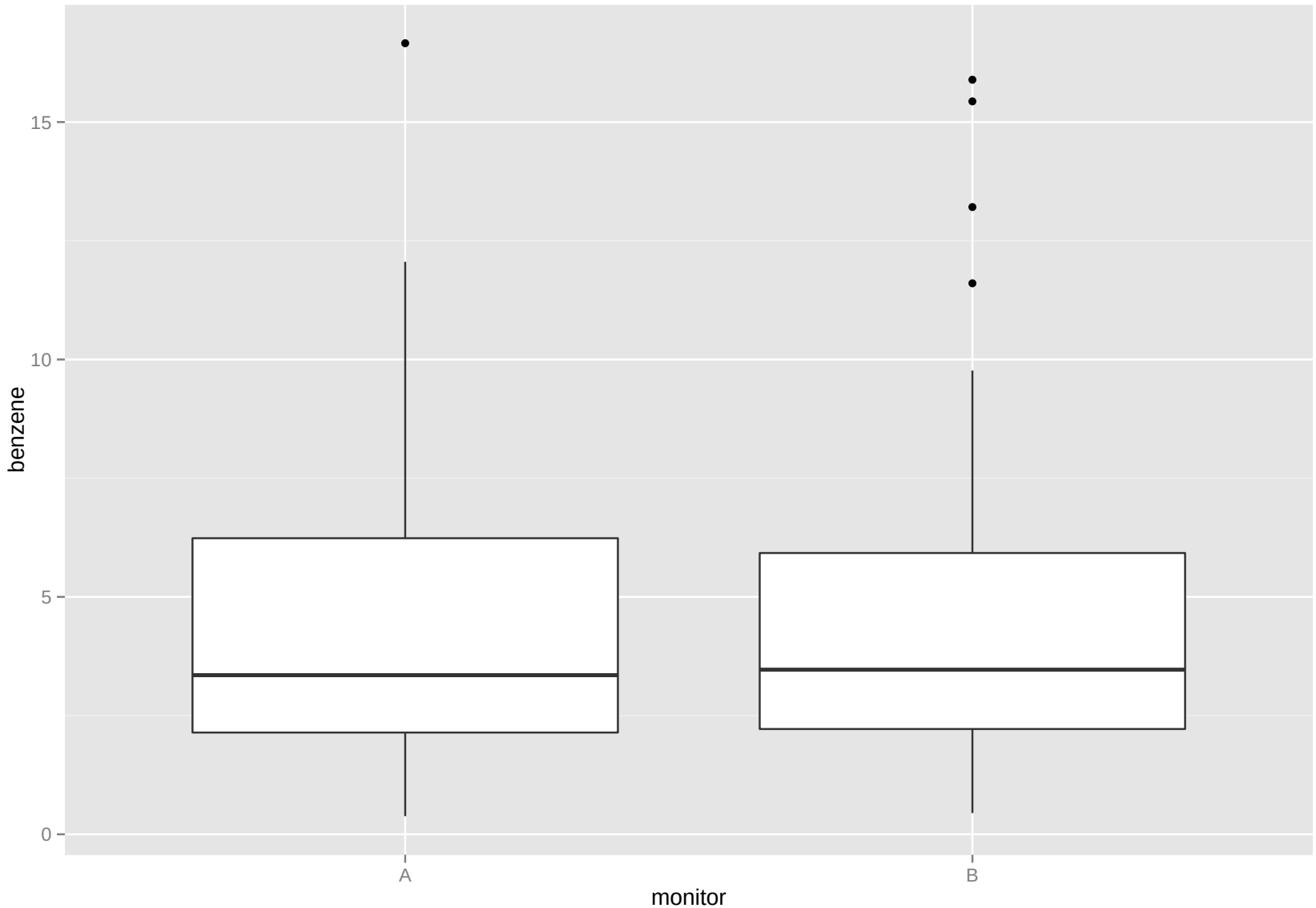
```
ggplot(rtox_long, aes(x=date, y=sample, color=parameter)) +
    geom_line() + facet_grid( ~ monitor) +
    ggtitle("Toxics Time Series 2014")
```

ggplot2 - Time Series



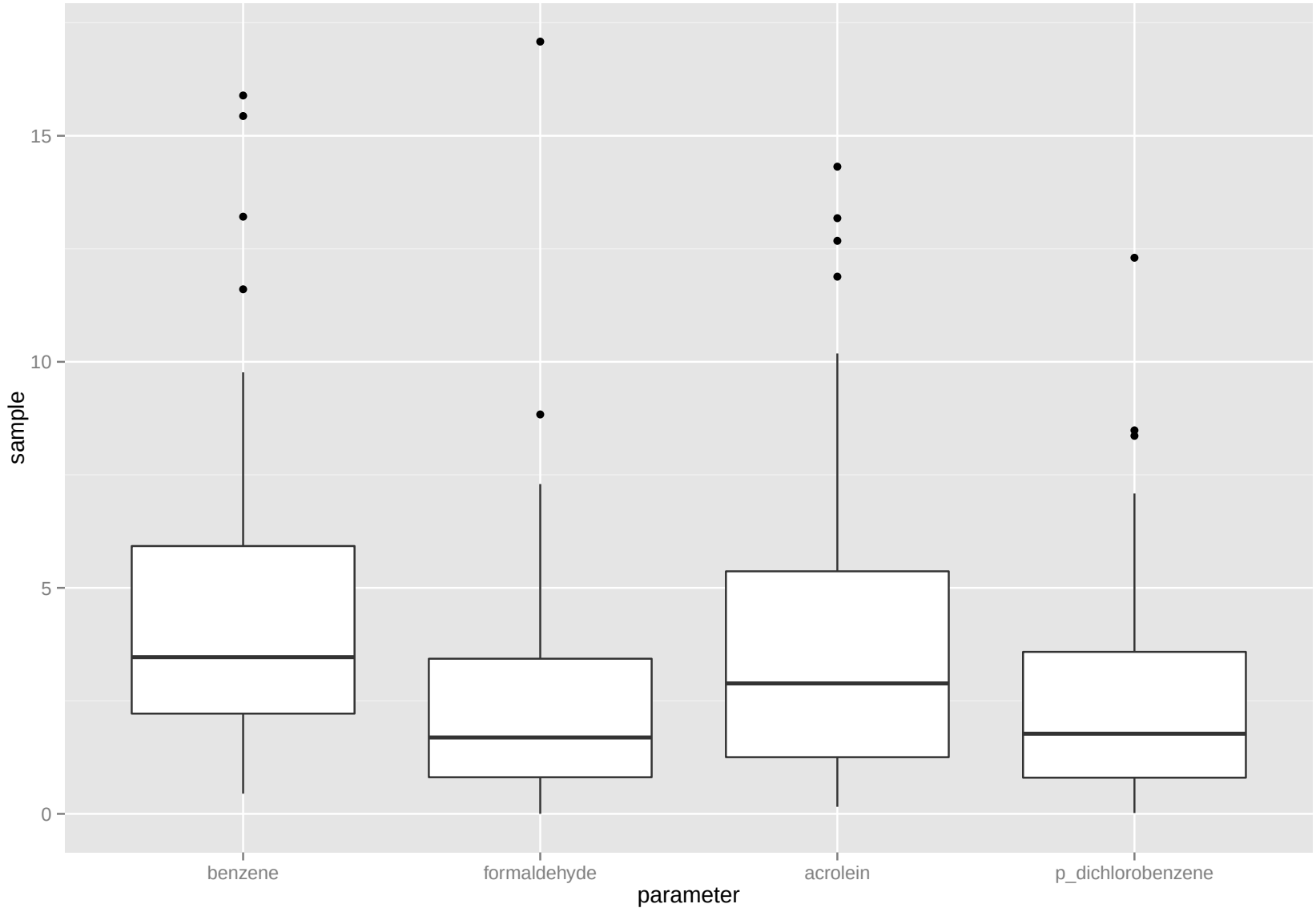
ggplot2 - Boxplots

```
ggplot(rtox, aes(x=monitor, y=benzene)) + geom_boxplot()
```



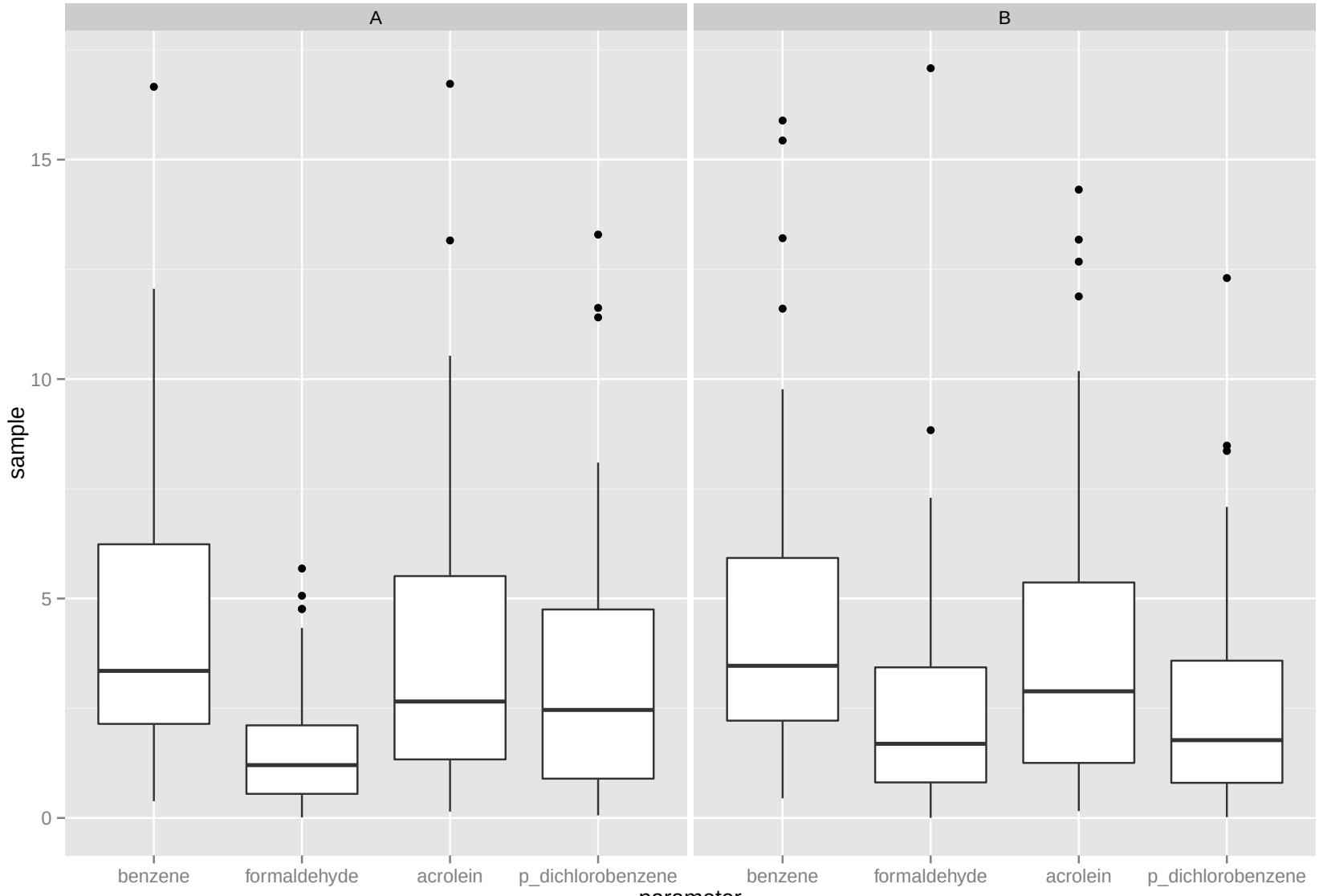
ggplot2 - Boxplots

```
ggplot(site_B, aes(x=parameter, y=sample)) + geom_boxplot()
```



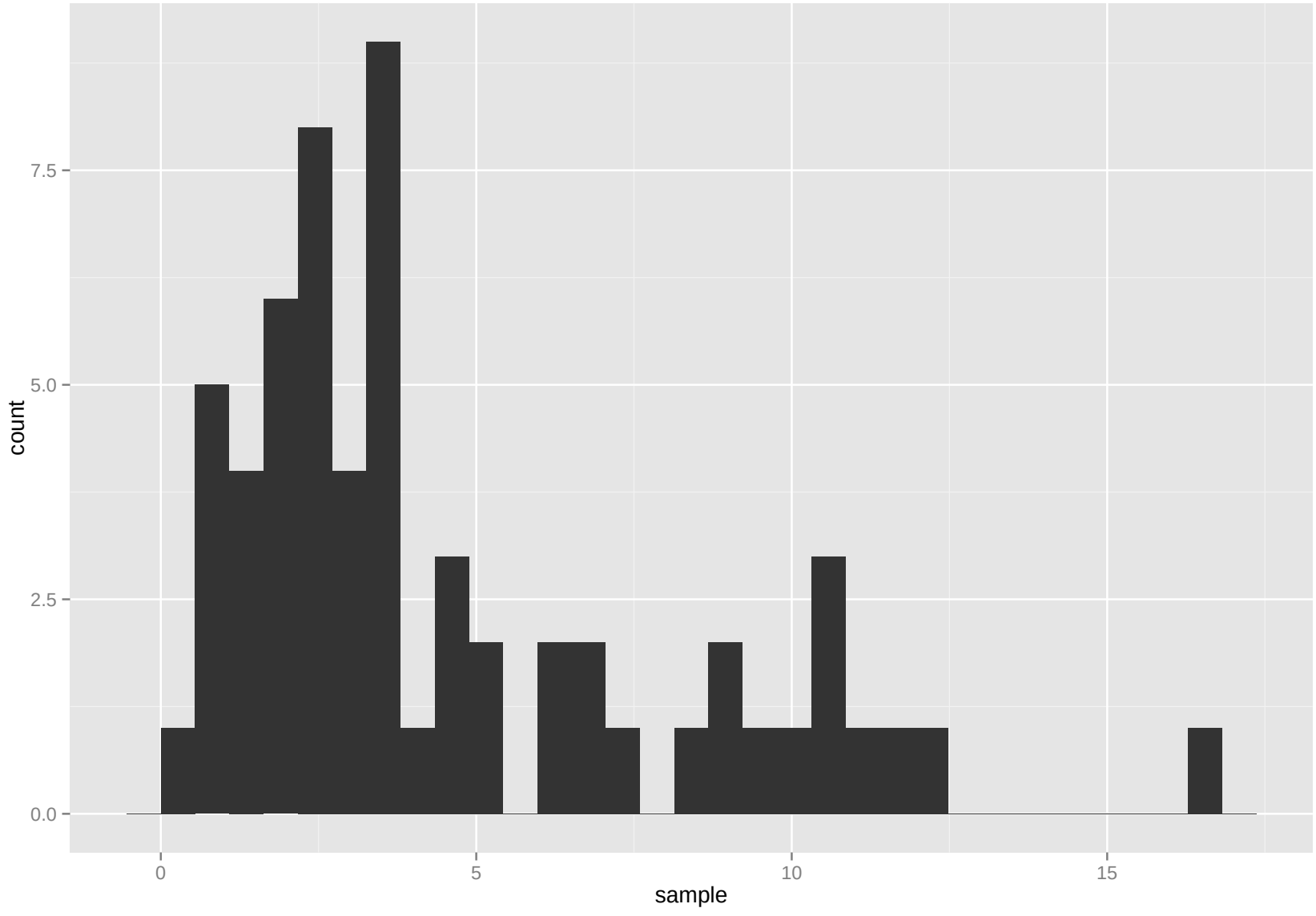
ggplot2 - Boxplots

```
ggplot(rtox_long, aes(x=parameter, y=sample)) +
  geom_boxplot() + facet_grid( ~ monitor)
```



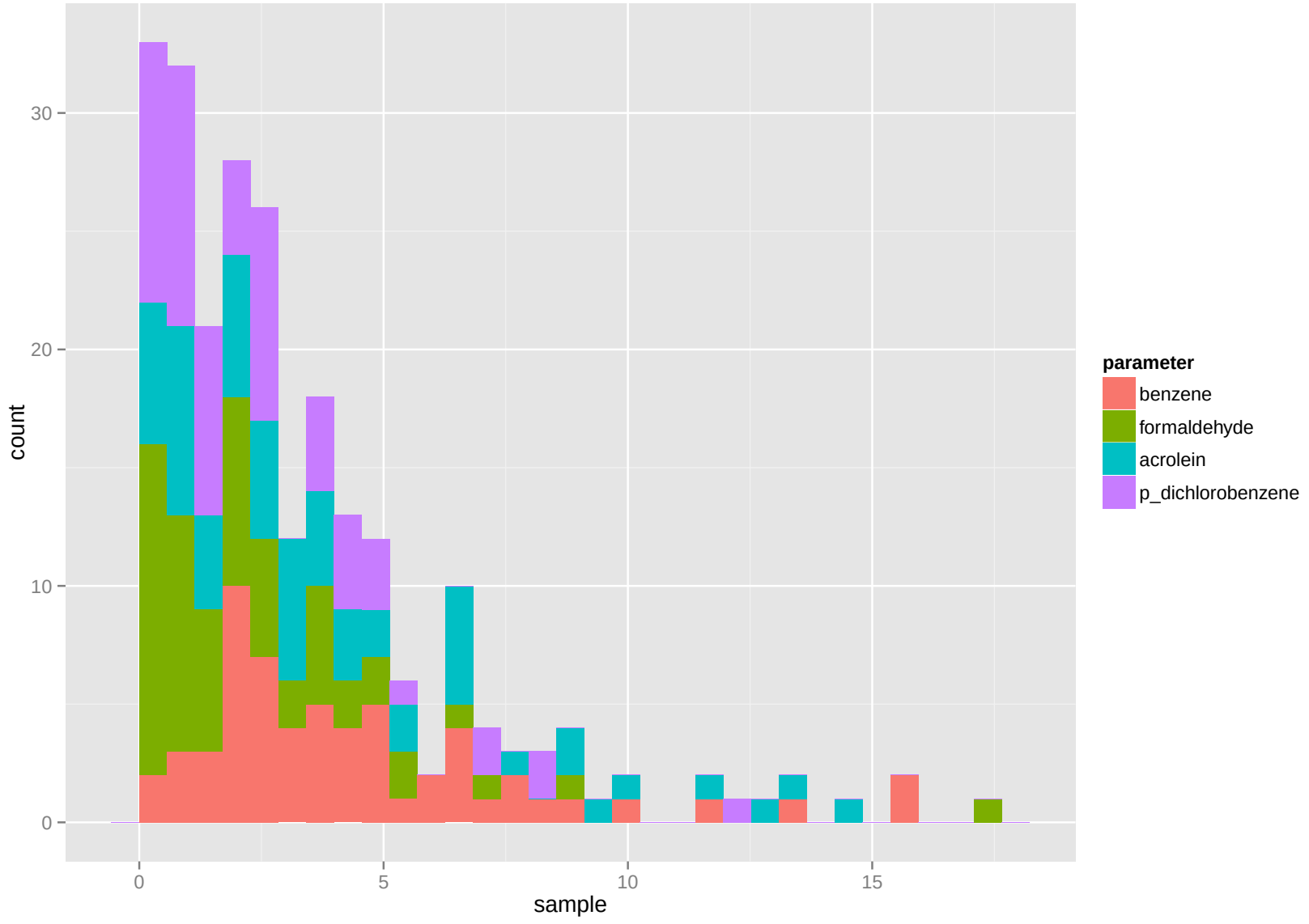
ggplot2 - Histograms

```
ggplot(benzene_A, aes(x=sample)) + geom_histogram()
```



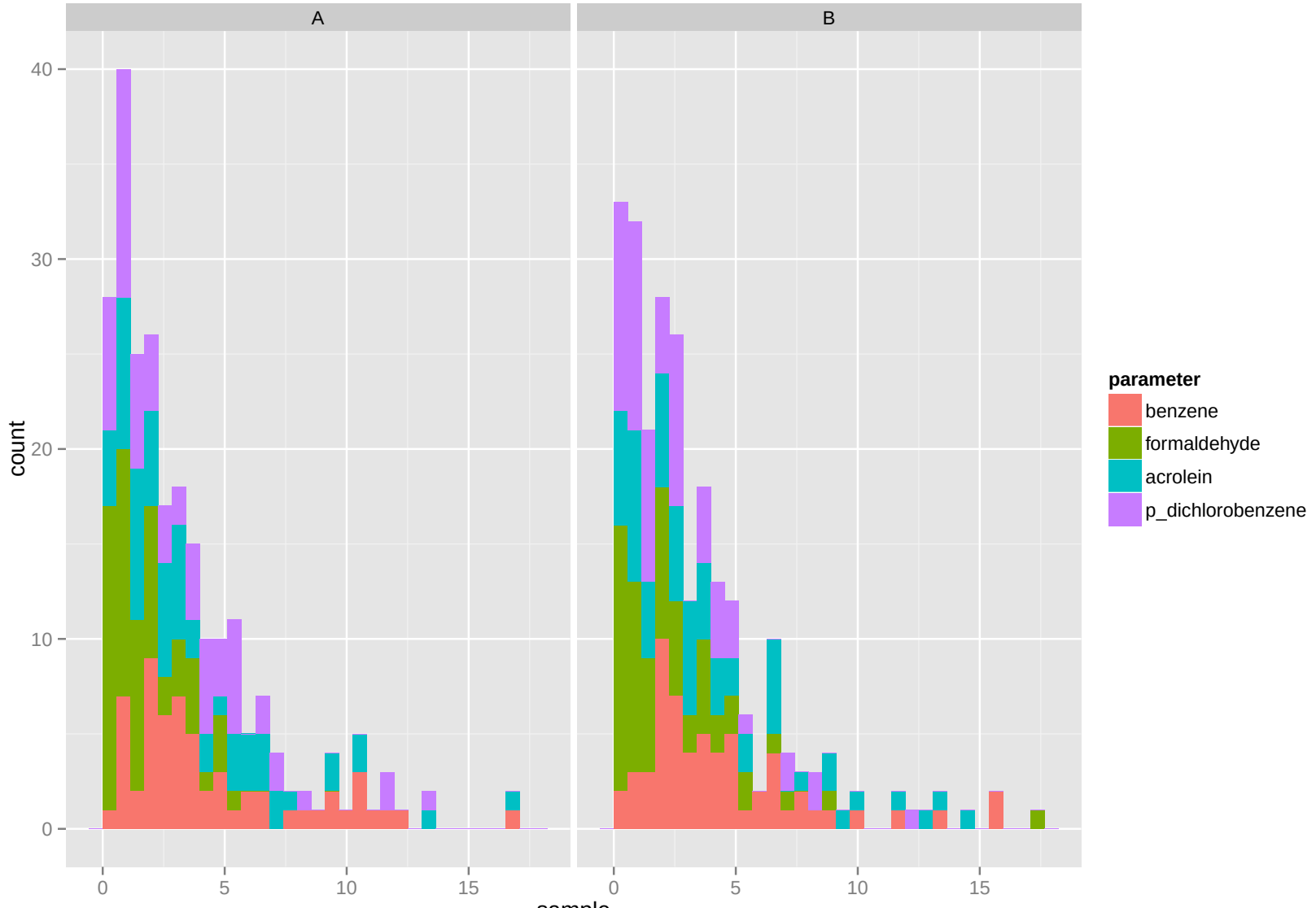
ggplot2 - Histograms

```
ggplot(site_B, aes(x=sample, fill=parameter)) + geom_histogram()
```



ggplot2 - Histograms

```
ggplot(rtox_long, aes(x=sample, fill=parameter)) +
  geom_histogram() + facet_grid(~ monitor)
```



Training Outline

- What is R and RStudio
- R basics
- The Hadleyverse
  - dplyr
  - tidyr
  - ggplot2
- Useful packages for air toxics
  - `raqdm`
  - `rucl`
  - `openair`
- Air toxics analysis demo
- Interactive web app with shiny

Air Toxics related R Packages

raqdm - Overview

- Provides convenient access to US EPA's AQS Data Mart in R
- Makes use of the API discussed at `http://www3.epa.gov/airdata/toc.html`
- Additional details and sourcecode on github (`https://github.com/ebailey78/raqdm`)
- Still under development - Comments and Suggestions Welcome (`eb11307@gmail.com`)

raqdm - Features

- Query AQS Data Mart from the R console or through a convienient GUI
- Save your most common parameter options so you don't have to enter them repeatedly
- Access to all options available in EPA's web interface
- Import requested data directly into an R data.frame for further analysis
- Can do both synchronous and asynchronous data pulls from the AQS Data Mart

raqdm - Installation

- To install raqdm you will need the devtools package available on CRAN:

```
install.packages("devtools")
```

- With devtools installed, install raqdm with the install_github function:

```
library(devtools)
install_github("ebailey78/raqdm")
library(raqdm)
```

raqdm - Setup

- You will need a username and password from EPA to access the data
- Request username and password from EPA by emailing aqsdatamart@epa.gov
- Once you have user credentials you can save them in raqdm with the setAQDMuser function

```
setAQDMuser("me@mystate.gov", "my_password", save = TRUE)
```

- You can set other default parameters with the setAQDMdefaults function

```
setAQDMdefaults(state = "18", bdate = "20140101",
                edate = "20141231")
```

- Setting save = TRUE will cause defaults to be saved across R sessions

raqdm - Requesting Data

- We've set defaults for Indiana (18), and bdate(20140101) and edate(20141231) in the previous slide
- Now we can request 2014 benzene data from Indiana with

```
benz_req <- getAQDMdata(param = "45201", synchronous = FALSE)
# Request benzene
```

- Or we can request all available met data with

```
met_req <- getAQDMdata(pc = "MET", synchronous = FALSE)
```

raqdm - Retrieving Data

- Once the requests are processed on the server, we read in the data.

```
benz <- getAQDMrequest(benz_req)
met <- getAQDMrequest(met_req)
```

Exposure Estimates with `rucl`

`rucl` Overview

- `rucl` is an R package that assists in calculating Upper Confidence Limits of the Mean (UCLs) in R
- Based heavily on U.S. EPA's ProUCL software version 4.1. (`http://www2.epa.gov/land-research/proucl-software`)
- Needs additional development and testing before official release
- Not well documented yet

`rucl` Features

- Test for normal, lognormal, or gamma distributions
- Handles censored and uncensored datasets
- Can calculate over 30 different UCLs
- Will recommend UCLs based on data characteristics (experimental)

rucl Installation

- To install rucl you will need the devtools package available on CRAN:

```
install.packages("devtools")
```

- With devtools installed, install raqdm with the install_github function:

```
library(devtools)
install_github("ebailey78/rucl")
library(rucl)
```

rucl Usage

- The primary function in rucl is ucl()
- The only required argument is a numeric vector that represents concentrations

```
  # Create a random dataset with 50 values
# from a gamma distribution
  x <- rgamma(50, 5, 2)
  head(x)
```

```
## [1] 4.786941 1.325178 2.257445 3.193702 2.860478 4.403182
```

```
  # Return the recommended UCL
  ucl(x)
```

```
##   n.tucl   n.modt
## 2.832101 2.832155
```

rucl Usage

- You can also request specific UCL calculations

```
# Calculate the modified-t-based UCL for normal distributions
ucl(x, "n.modt")
```

```
##   n.modt
## 2.832155
```

rucl Usage

- Arguments can also be used to change the confidence level and number of bootstrap iterations

```
ucl(x, confidence = 0.95, N = 10000)
```

```
##   n.tucl   n.modt
## 2.832101 2.832155
```

```
ucl(x, confidence = 0.9, N = 10000)
```

```
##   n.tucl   n.modt
## 2.774649 2.774703
```

rucl Usage

- `type = detailed` will create a `rucl` object that contains a great deal of information about the dataset

```
ucl(x, type = "detailed")
```

rucl Usage

```
  Summary for uncensored dataset 'x'
--------------------------------------------------------------------------------
    Confidence Coefficient: 95%
Bootstrap Operations(N): 2000

--------------------------------------------------------------------------------
  Summary Statistics
--------------------------------------------------------------------------------
                   Sample Size: 50     |      Minimum Value of Log Data: -0.916
                 Minimum Value: 0.4    |      Maximum Value of Log Data: 2.01
                 Maximum Value: 7.46   |                Mean of Log Data: 0.15
               Arithmetic Mean: 1.73   | Standard Deviation of Log Data: 0.879
                Geometric Mean: 1.16   |              MLE of Gamma Shape: 1.32
                        Median: 1.05   |              MLE of Gamma Scale: 1.31
            Standard Deviation: 1.77   |               MLE of Gamma Rate: 0.761
                Standard Error: 0.25   |               MLE of Gamma Mean: 1.73
      Coefficient of Variance: 1.02    |                MLE of Gamma SSD: 1.51
                      Skewness: 2.03   |

--------------------------------------------------------------------------------
  Distribution Testing
--------------------------------------------------------------------------------
    Normal: FALSE           Lognormal: TRUE           Gamma: FALSE

    Recommendation: Lognormal

--------------------------------------------------------------------------------
  Upper Confidence Limits of the Mean (UCLs)
--------------------------------------------------------------------------------
                     Student's t UCL: 2.15
Adjusted Central Limit Theorem UCL: 2.22
           Modified Student's t UCL: 2.15
                       Land's H UCL: 2.25   ****
            95% Chebyshev UCL (MVUE): 2.74
          97.5% Chebyshev UCL (MVUE): 3.19
            99% Chebyshev UCL (MVUE): 4.08
               Approximate Gamma UCL: 2.15
                  Adjusted Gamma UCL: 2.16
           Central Limit Theorem UCL: 2.15
              Standard Bootstrap UCL: 2.13
                     Bootstrap t UCL: 2.28
                Hall's Bootstrap UCL: 2.24
   Simple Percentile Bootstrap UCL: 2.15
           BCA Percentile Bootstrap: 2.2
      95% Chebyshev UCL (mean, sd): 2.83
     97.5% Chebyshev UCL (mean, sd): 3.3
      99% Chebyshev UCL (mean, sd): 4.23
```

rucl Censored Data

- rucl can handle censored datasets using Kaplan-Meier
- Requires a second vector with TRUE/FALSE indicating whether the corresponding reading is a detect (TRUE) or nondetect (FALSE)
- For non-detects, assumes reported reading is detection limit

```
# Create a lognormal dataset with 50 readings censored at 0.4
x <- rlnorm(50)
d <- x > 0.4
x[!d] <- 0.4

ucl(x, d = d)
```

rucl Censored Data

```
## o.km.cheb95
##    2.842027
```

Data visualization with `openair`

The openair project

- The `openair` package was created by Dr. David Carslaw at King's College London.
- The goals of the openair project are to create tools in R that use the wealth of air pollution data that is publicly available to make it easy to carry out sophisticated analyses quickly and in a reproducible way.
- Allow the user to quickly summarize and visualize air pollution data through the use of wind and pollution roses, trend analyses, and other helpful tools.
- Comprehensive user manual can be found here: (`http://www.openair-project.org/downloads/openairmanual.aspx`)

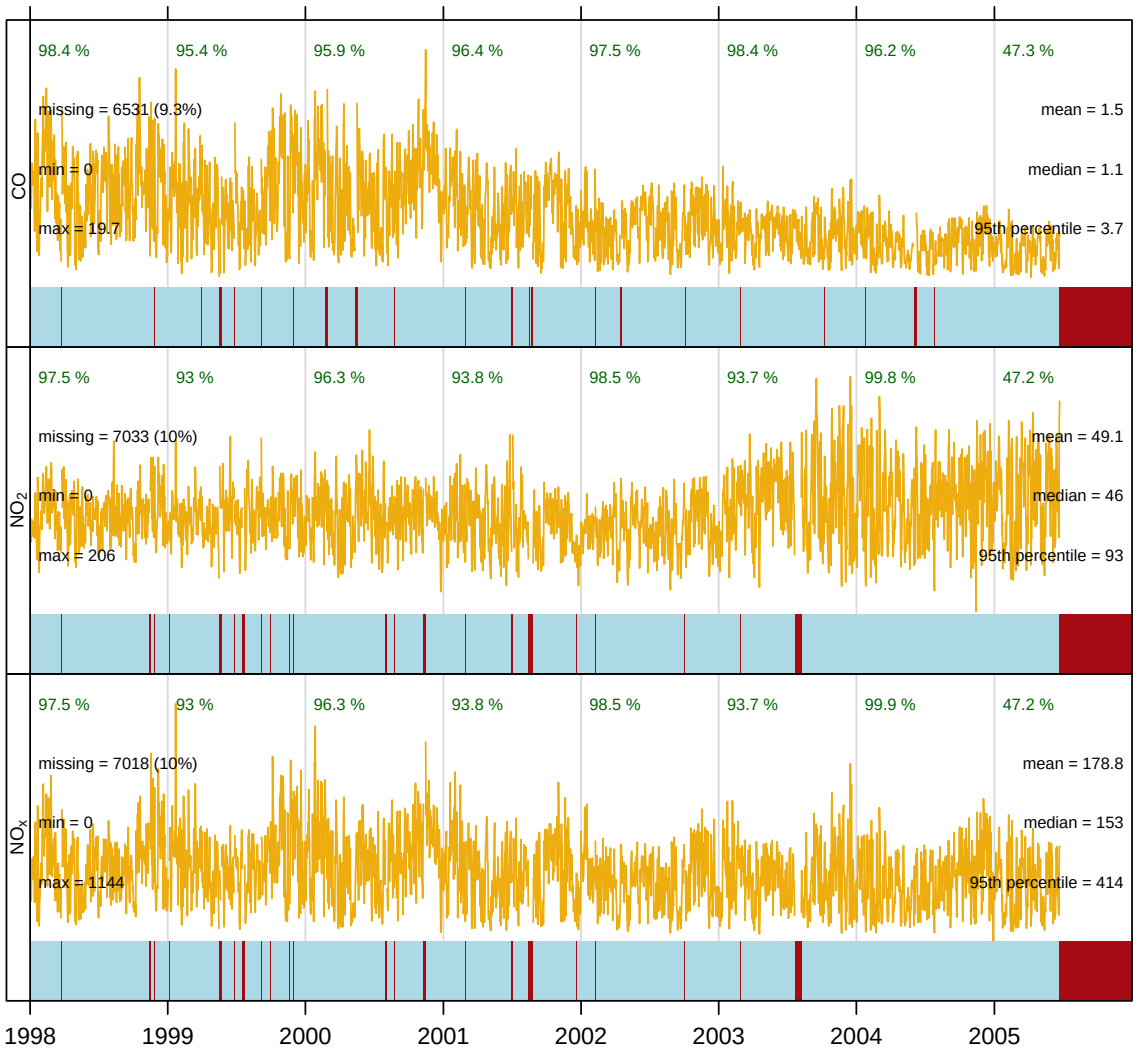
Summary plot

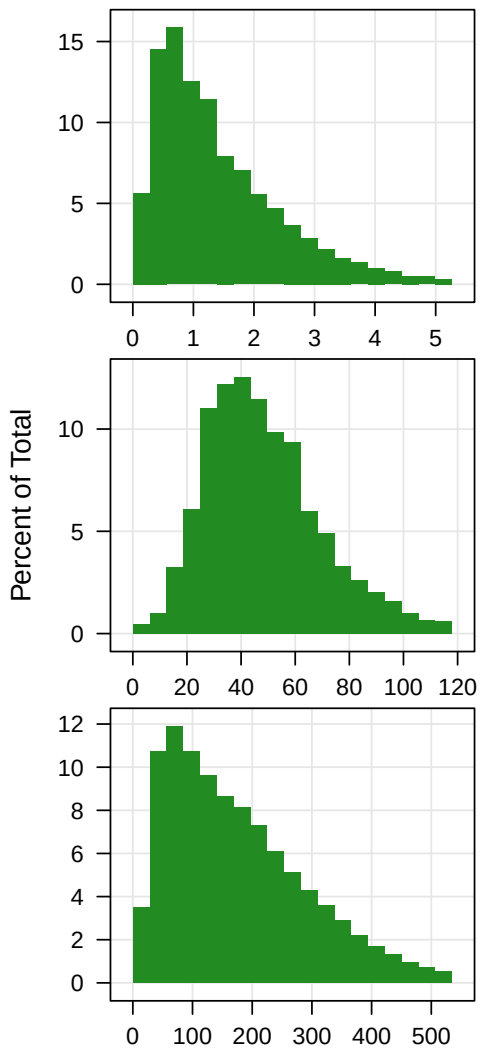
- The first thing we want to do after importing our data is a quick summary plot.
- Creates time-series plots and makes it easy to see chunks of missing data.
- The summary plot also displays basic summary stats such as mean, median and the 95th percentile.
- A histogram helps the user view the distributions of each of their parameters.
- You can call this plot using the following code:

```
library(openair)
summaryPlot(mydata)
```

Summary Plot

```
##      date1      date2        nox        no2         co
##  "POSIXt" "POSIXct" "integer" "integer" "numeric"
```



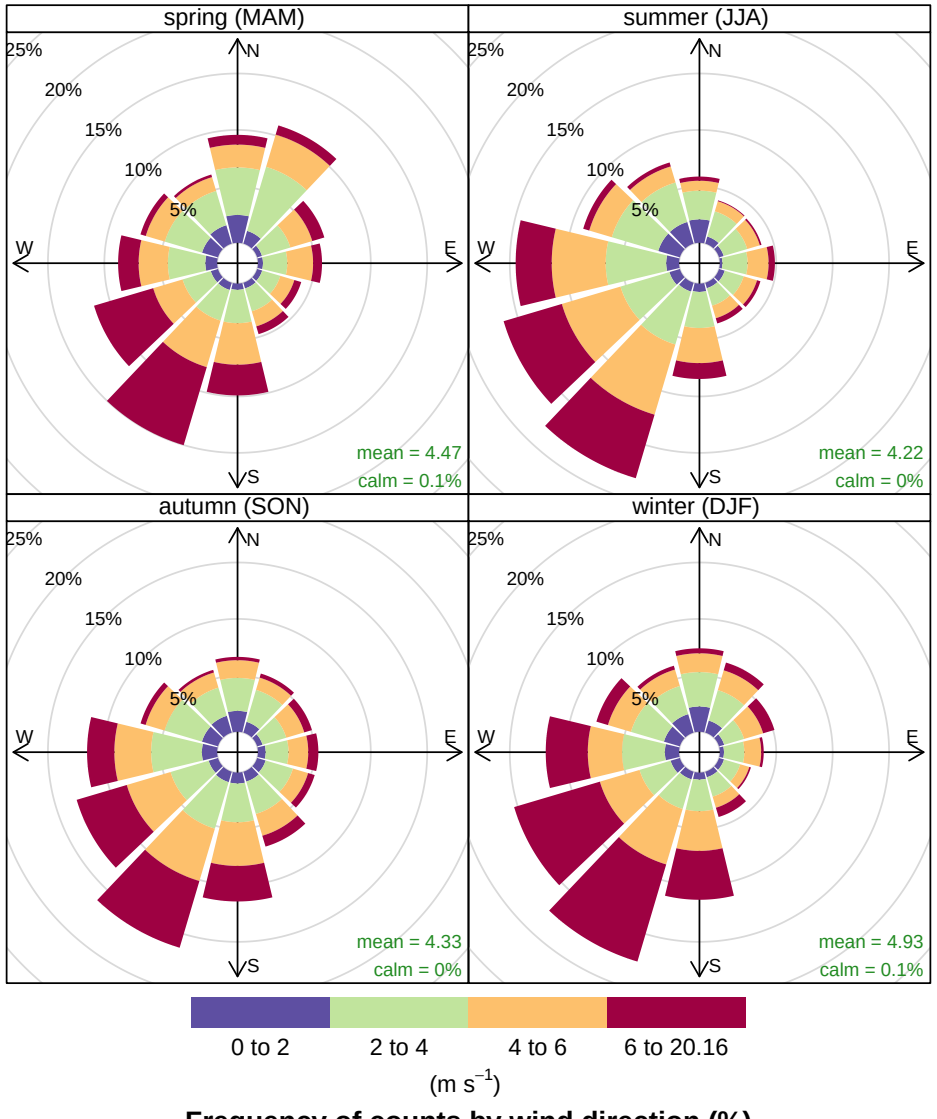


Windrose

- The windrose plot allows easy visualization of wind speed and wind direction data.
- Could be especially useful for a modeler or analyst who wants to look at many years or different seasons of wind data at a monitor.

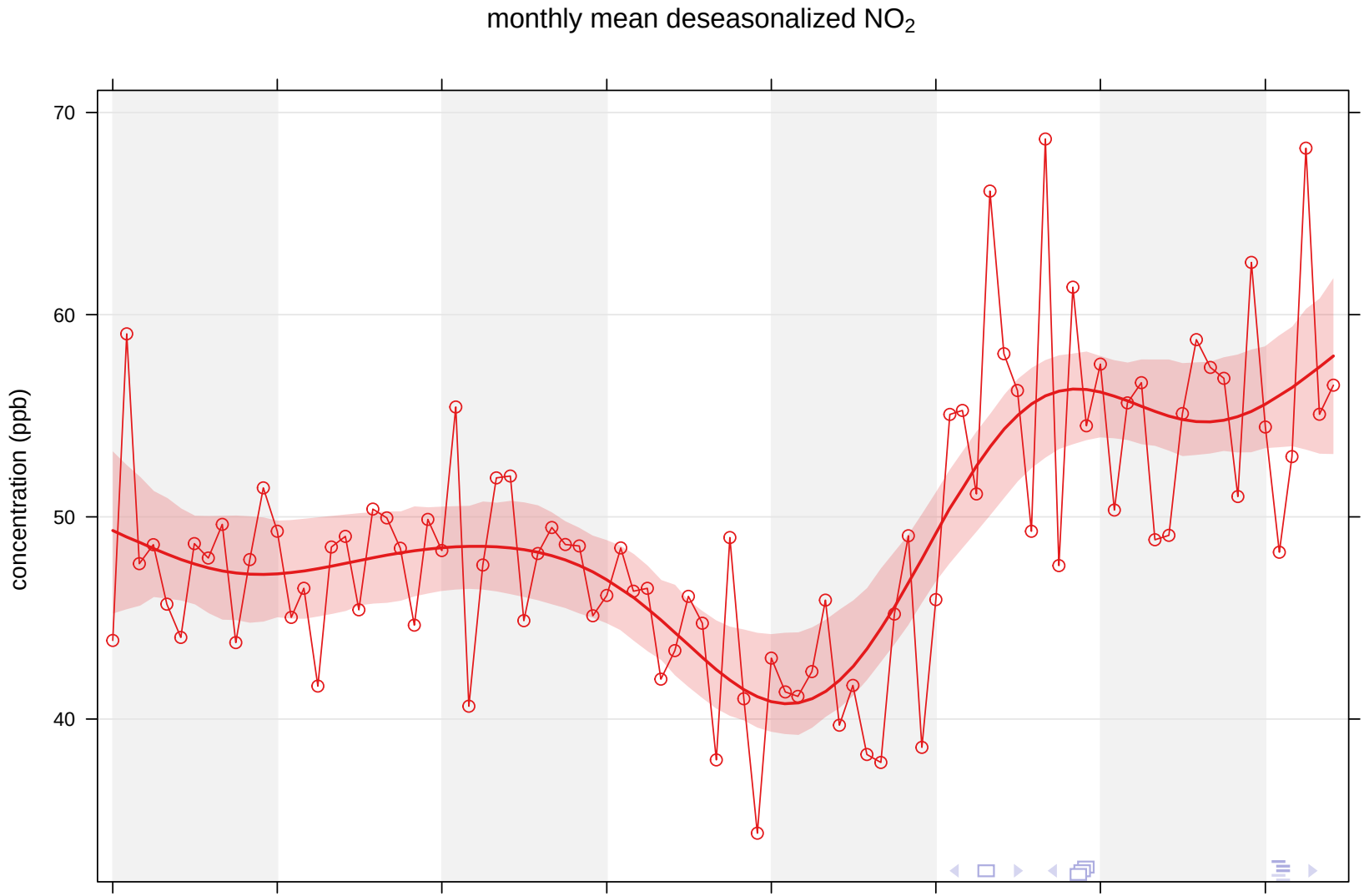
Windrose

```
windRose(mydata, type="season", paddle=F)
```



Trend Plots

```
smoothTrend(mydata, pollutant = "no2", deseason = TRUE,
  simulate =TRUE, ylab = "concentration (ppb)",
  main = "monthly mean deseasonalized no2")
```



Training Outline

- What is R and RStudio
- R basics
- The Hadleyverse
  - dplyr
  - tidyr
  - ggplot2
- Useful packages for air toxics
  - raqdm
  - rucl
  - openair
- Air toxics analysis demo
- Interactive web app with shiny

Getting the data

- Use `raqdm` to retrieve 2014 core HAPs data for the Gary IITRI monitor in Lake County, Indiana
- Below is another example of an asynchronous AQDM data pull

```
haps_request <- getAQDMdata(state = "18", county = "089",
                            site = "0022", pc = "CORE_HAPS",
                            format = "DMCSV", dur = "7",
                            bdate = "20140101", edate = "20141231")

haps <- getAQDMrequest(haps_request)
```

Summarizing data with dplyr

- Group the data using dplyr's group_by function to group the data by parameter

```
haps <- group_by(haps, AQS.Parameter.Desc)
```

- Then summarize the data in a table

```
haps_summary <- summarize(haps, n = n(),
                  max = max(Sample.Measurement),
                  median = median(Sample.Measurement),
                  mean = signif(mean(Sample.Measurement), 2),
                  st.dev = signif(sd(Sample.Measurement), 2),
                  ucl = signif(max(ucl(Sample.Measurement)), 2))
# from rucl package

# Remove pollutants with no detectable readings
haps_summary <- haps_summary[haps_summary$max != 0, ]
```

Summarizing data with dplyr

```
head(haps_summary, n=8)
```

```
## Source: local data frame [8 x 7]
##
##      AQS.Parameter.Desc     n   max median    mean st.dev
##                   (fctr) (int) (dbl)  (dbl)   (dbl)  (dbl)  (d
## 1          1,3-Butadiene    55 0.300  0.000 0.06400 0.1000 0.0
## 2           Acetaldehyde    68 2.400  1.200 1.30000 0.4100 1.4
## 3 Acrolein - Unverified    55 2.900  1.300 1.40000 0.5800 1.6
## 4      Arsenic PM2.5 LC    57 0.011  0.001 0.00110 0.0018 0.0
## 5                Benzene   110 9.400  0.900 1.80000 2.1000 2.7
## 6      Cadmium PM2.5 LC    57 0.009  0.000 0.00061 0.0017 0.0
## 7  Carbon tetrachloride    55 0.100  0.100 0.09600 0.0190 0.1
## 8     Chromium PM2.5 LC    57 0.013  0.000 0.00110 0.0020 0.0
```

A closer look at benzene

- Use `raqdm` to retrieve 2013-2014 24-hour benzene data for all of Indiana

```
benzene_request <- getAQDMdata(state = "18", param = "45201",
                               format = "DMCSV", dur = "7",
                               bdate = "20130101", edate = "20141231")

benzene <- getAQDMrequest(benzene_request)
```

Prepare the data

```
# Convert from ppbc to ppbv
benzene$Sample.Measurement <- benzene$Sample.Measurement / 6
# Convert from ppbv to ug/m3
benzene$Sample.Measurement <-
  benzene$Sample.Measurement  * 78.11 / 24.45

# Combine the State.Code, County.Code, and Site.Num,
# and POC fields into a single Site.ID field
  benzene$Site.ID <- sprintf("%02i-%03i-%04i-%i",
                             benzene$State.Code,
                             benzene$County.Code,
                             benzene$Site.Num,
                             benzene$POC)

  benzene <- group_by(benzene, Site.ID)
```

Summarize the data

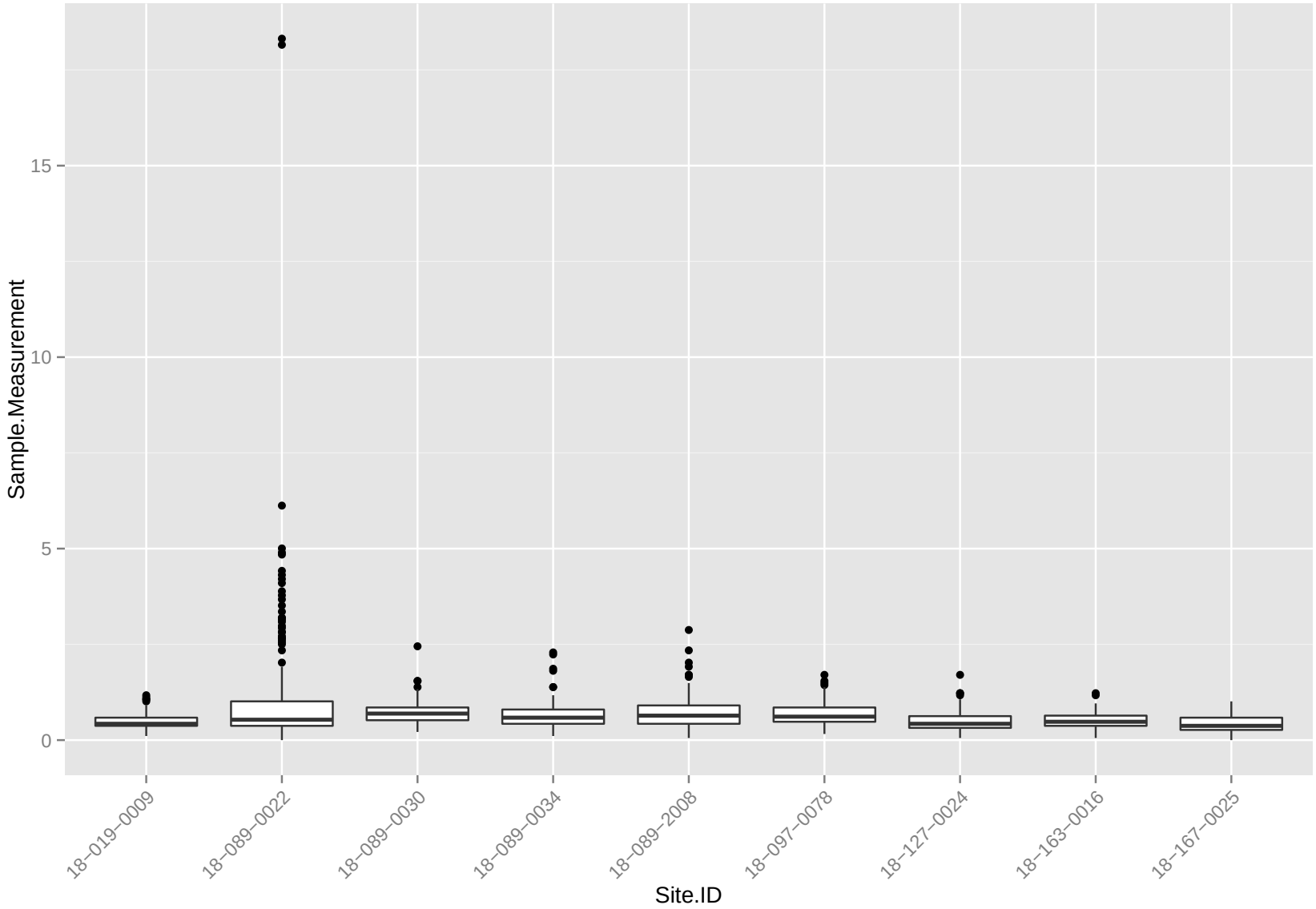
```
  summarize(benzene,
            n = n(), max = max(Sample.Measurement),
            ucl = ucl(Sample.Measurement)[1],
            risk = ucl * 7.8e-6)
```

```
## Source: local data frame [10 x 5]
##
##          Site.ID     n       max       ucl          risk
##            (chr) (int)     (dbl)     (dbl)         (dbl)
## 1  18-019-0009-1   116  1.171384 0.4699129 3.665321e-06
## 2  18-089-0022-2   110 18.156449 1.8441180 1.438412e-05
## 3  18-089-0022-7   109 18.316183 2.0649492 1.610660e-05
## 4  18-089-0030-1   116  2.449257 0.7675006 5.986505e-06
## 5  18-089-0034-1   118  2.289523 0.7240966 5.647954e-06
## 6  18-089-2008-1   122  2.875215 0.8292063 6.467809e-06
## 7  18-097-0078-1   112  1.703831 0.7329372 5.716910e-06
## 8  18-127-0024-1   118  1.703831 0.6072662 4.736676e-06
## 9  18-163-0016-1   113  1.224628 0.5358455 4.179595e-06
## 10 18-167-0025-1    56  1.011650 0.5643314 4.401785e-06
```

Boxplots

```
# Create a boxplot of the benzene data
# grouped by the new Site.ID field
ggplot(benzene, aes(Site.ID, Sample.Measurement)) +
    geom_boxplot()
```

Boxplots

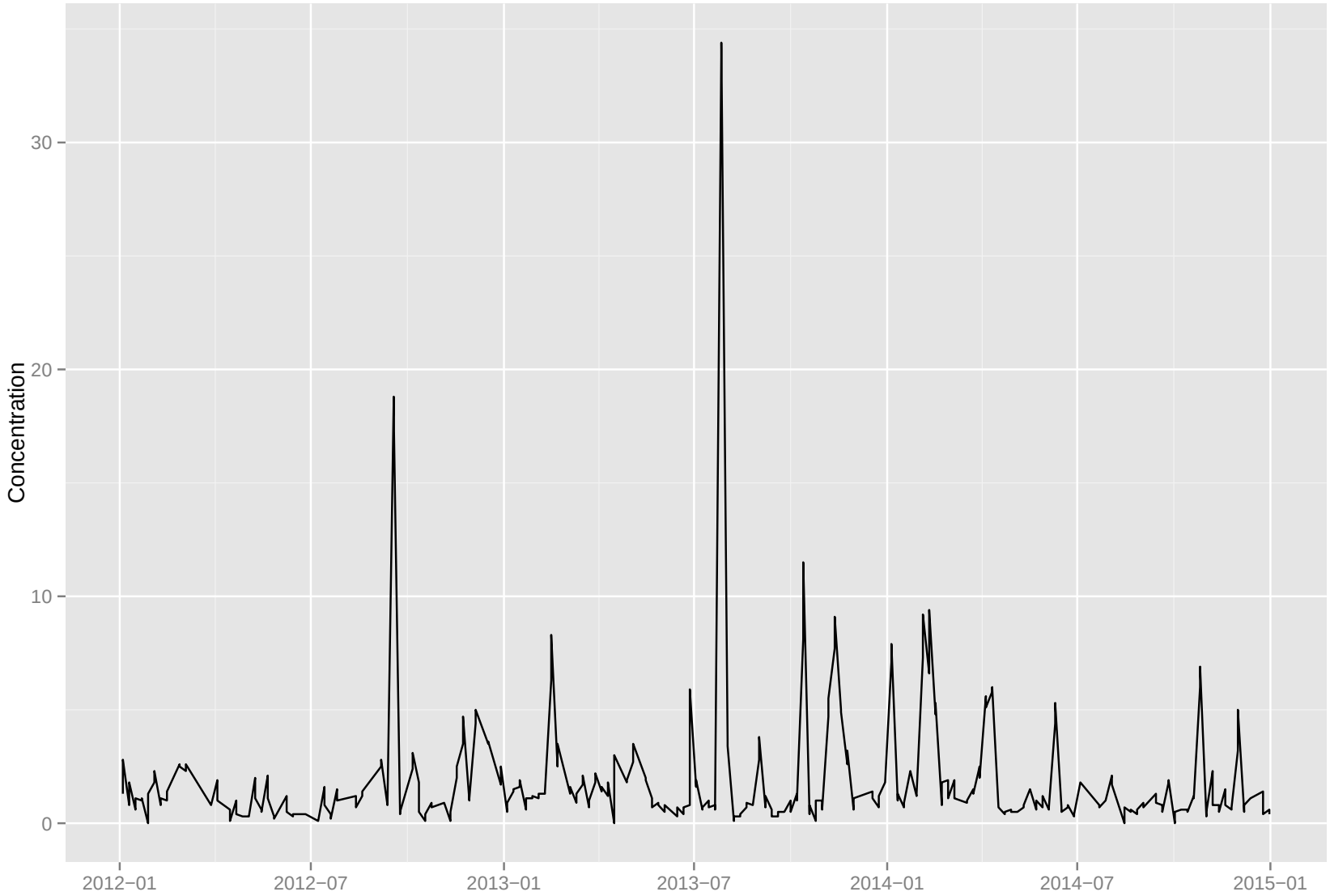

Sample.Measurement
15
10
5
0
18−019−0009
18−089−0022
18−089−0030
18−089−0034
18−089−2008
18−097−0078
18−127−0024
18−163−0016
18−167−0025
Site.ID

Line Graphs

- Lets look at benzene data at the Gary IITRI monitor over a longer time period

```
gi_benz_req <- getAQDMdata(state = "18", county = "089",
                   site = "0022", param = "45201",
                   format = "DMCSV", dur = "7",
                  bdate = "20120101", edate = "20141231")

benz <- getAQDMrequest(gi_benz_req)

ggplot(benz, aes(as.Date(Date.Local), Sample.Measurement)) +
  geom_line() + scale_x_date() + xlab("") +
  ylab("Concentration")
```

Line Graphs


Concentration
30
20
10
0
2012−01
2012−07
2013−01
2013−07
2014−01
2014−07
2015−01

Plotting Gary Benzene data with `openair`

Retrieving AQS data

- Before we can use `openair` we will review how to grab data with `raqdm` and reshape it with `tidyr`. This will get the data into a format that `openair` requires.
- We will use `raqdm` to retrieve Photochemical Assessment Monitoring Station (PAMS) data from the Gary IITRI monitor.

```
library(raqdm)
```

Synchronous query

- We will query the PAMS data from the Gary IITRI site using the following request:

```
pams <- getAQDMdata(user = "me@email.com", pw = "abc123",
            state = "18", county = "089", site = "0022",
            pc = "PAMS", param="", format = "DMCSV",
            bdate = "20140601", edate = "20140602",
            frmonly = "n", synchronous = TRUE)
```

Asynchronous query

- This previous query was only for a couple of days. If we want to query for the entire year for a whole class of parameters, then an asynchronous retrieval is the way to go.

```
pams <- getAQDMdata(user = "me@email.com", pw = "abc123",
            state = "18", county = "089", site = "0022",
            pc = "PAMS", param="", format = "DMCSV",
            bdate = "20140101", edate = "20141231",
            frmonly = "n", synchronous = FALSE)
```

```
pams <- getAQDMrequest(pams)
```

Tidying the data for openair

- As we said before we will need to use `tidyr` to reshape the data into a format that `openair` likes. `openair` requires data in a 'wide' format with all of the variables in their own column like this:

```
library(openair)
head(mydata, n=2)
```

```
##                  date   ws  wd nox no2 o3 pm10    so2     co
## 1 1998-01-01 00:00:00 0.60 280 285  39  1   29 4.7225 3.3725
## 2 1998-01-01 01:00:00 2.16 230  NA  NA NA   37     NA     NA
```

Use dplyr to filter the data

- This returns a huge dataset (513,072 rows) which includes all the VOCs, NOx and meteorological parameters for the Gary IITRI site for 2014.
- Now let's use dplyr to filter it down to just a few of the parameters that we will need for our analysis in openair (i.e. benzene, toluene, wind speed, and wind direction).

```
library(dplyr)
IITRI <- filter(pams, Parameter.Code =='61104'|
                      Parameter.Code=='61103'|
                      Parameter.Code =='45202'|
                      Parameter.Code =='45201', POC == 1)
```

Select columns of interest

- Then we will select only the columns of interest to us using the `select()` function from `dplyr`. For this analysis, we only need Date (`Date.GMT`), Hour(`X24.Hour.GMT`), Parameter(`AQS.Parameter.Desc`), and Sample Measurement(`Sample.Measurement`).

```
IITRI_sub <- select(IITRI_sub, Date.GMT,  X24.Hour.GMT,
                    AQS.Parameter.Desc, Sample.Measurement)
```

Format data

This leaves us with:

```
##     Date.GMT X24.Hour.GMT          AQS.Parameter.Desc Sample.M
## 1 2014-01-02        01:00 Wind Direction - Resultant
## 2 2014-01-03        01:00 Wind Direction - Resultant
## 3 2014-01-04        01:00 Wind Direction - Resultant
## 4 2014-01-05        01:00 Wind Direction - Resultant
## 5 2014-01-06        01:00 Wind Direction - Resultant
## 6 2014-01-07        01:00 Wind Direction - Resultant
```

Long to Wide Format

- Now that we have selected our columns of interest, lets use `tidyr` to spread out our 'long' data and make it 'wide'

```
library(tidyr)
gary_oa <- spread(IITRI_sub, key = AQS.Parameter.Desc,
                  value = Sample.Measurement)

# Convert from ppbc to ppbv
gary_oa$Benzene <- gary_oa$Benzene / 6
gary_oa$Toluene <- gary_oa$Toluene / 7
head(gary_oa, n=1)
```

```
##     Date.GMT X24.Hour.GMT Benzene Toluene Wind Direction - Re
## 1 2014-01-01        06:00      NA      NA
##   Wind Speed - Resultant
## 1                    8.1
```

- Then we will write it to a csv file for easy import into openair

```
write.csv(gary_oa,
          file = file.path(tempdir(), "Gary_openair.csv"),
          row.names=F)
```

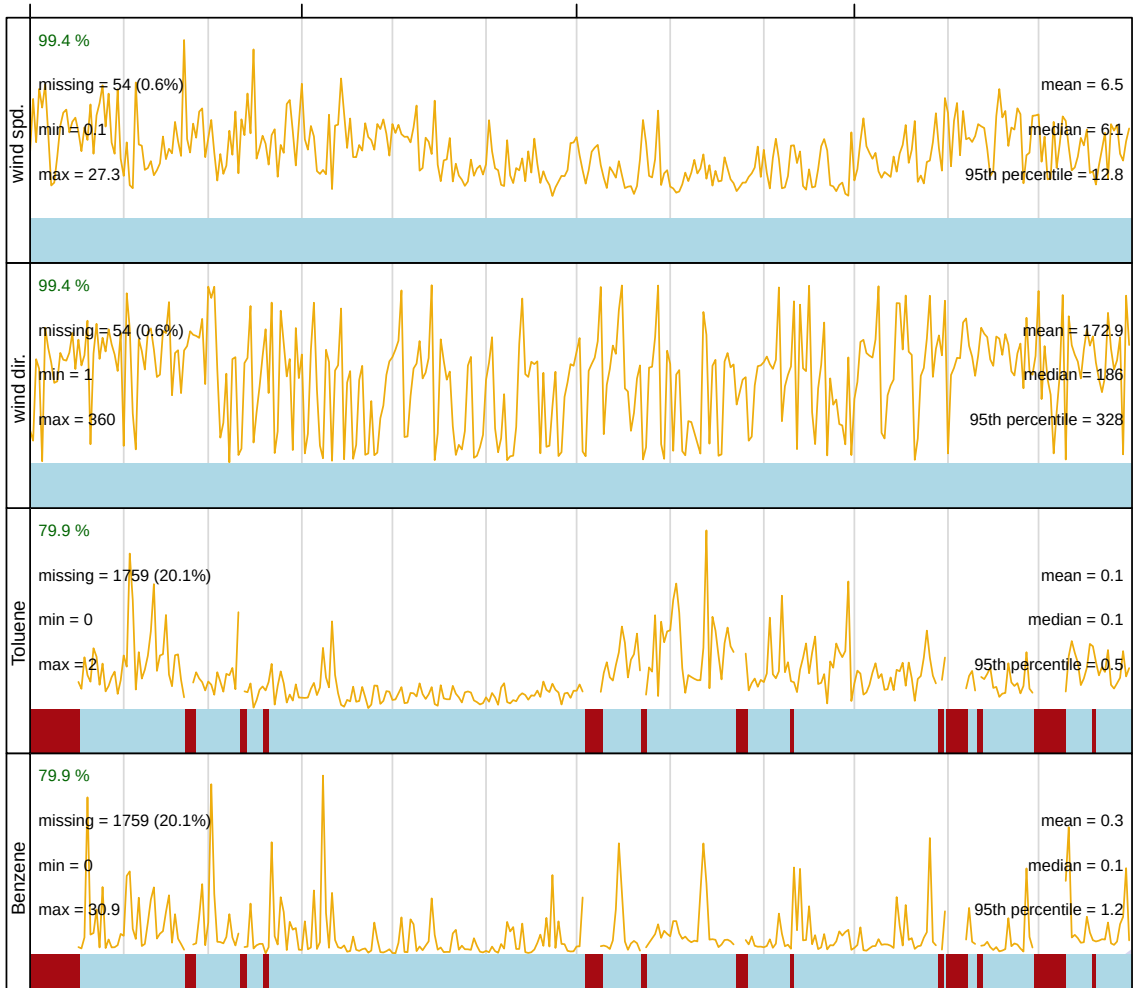
Importing into openair

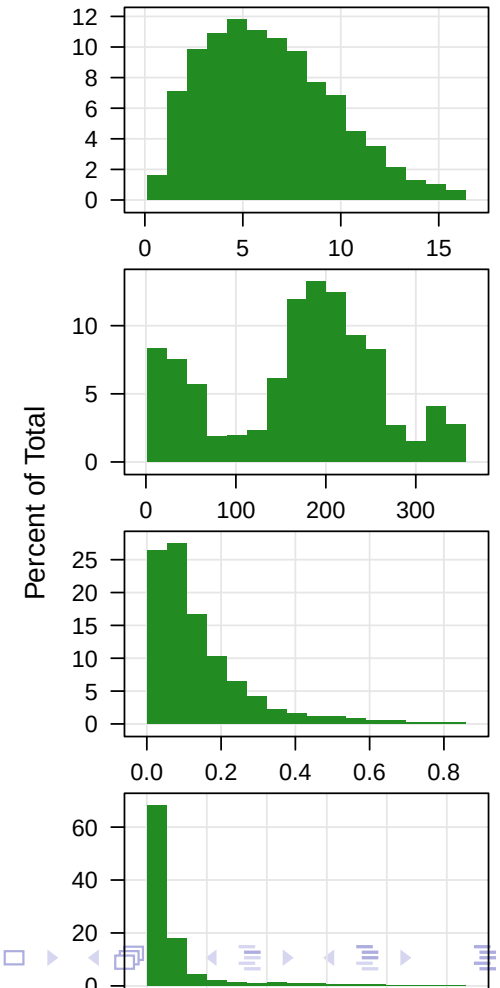
- Now our data is ready to use in openair
- We will use the `import()` function in openair to bring in our csv file.
- The `import` funtion is helpful because it takes care of all of the final date formatting for openair plots
- Once the data is imported into openair we can do a `summaryPlot` to quickly view the data

```
library(openair)
gary <- import(file = file.path(tempdir(), "Gary_openair.csv"),
               sep=",", date="Date.GMT", time="X24.Hour.GMT",
               date.format="%Y-%m-%d", time.format="%H:%M",
               ws="Wind Speed - Resultant",
               wd="Wind Direction - Resultant")

summaryPlot(selectByDate(gary, year=2014))
```

Summary Plot

```
##         date1         date2 X24.Hour.GMT      Benzene       Tolu
##     "POSIXct"     "POSIXt"     "factor"    "numeric"    "numer
##            wd            ws
##     "numeric"     "numeric"
```



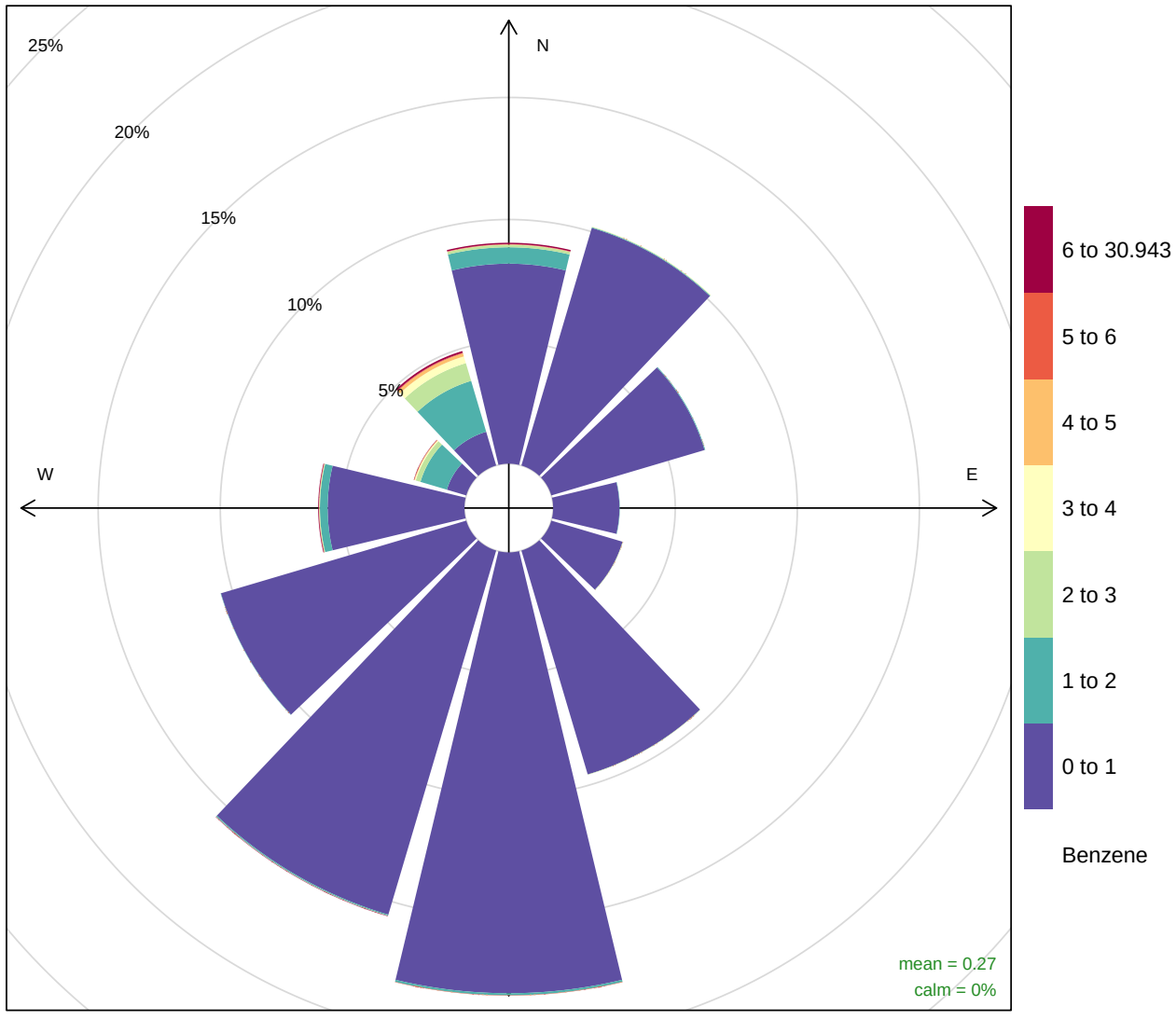


Pollution Rose

- A pollution rose plot is useful for describing the proportion of contaminant that comes from each wind direction.

Pollution Rose

```
pollutionRose(gary, pollutant= "Benzene")
```

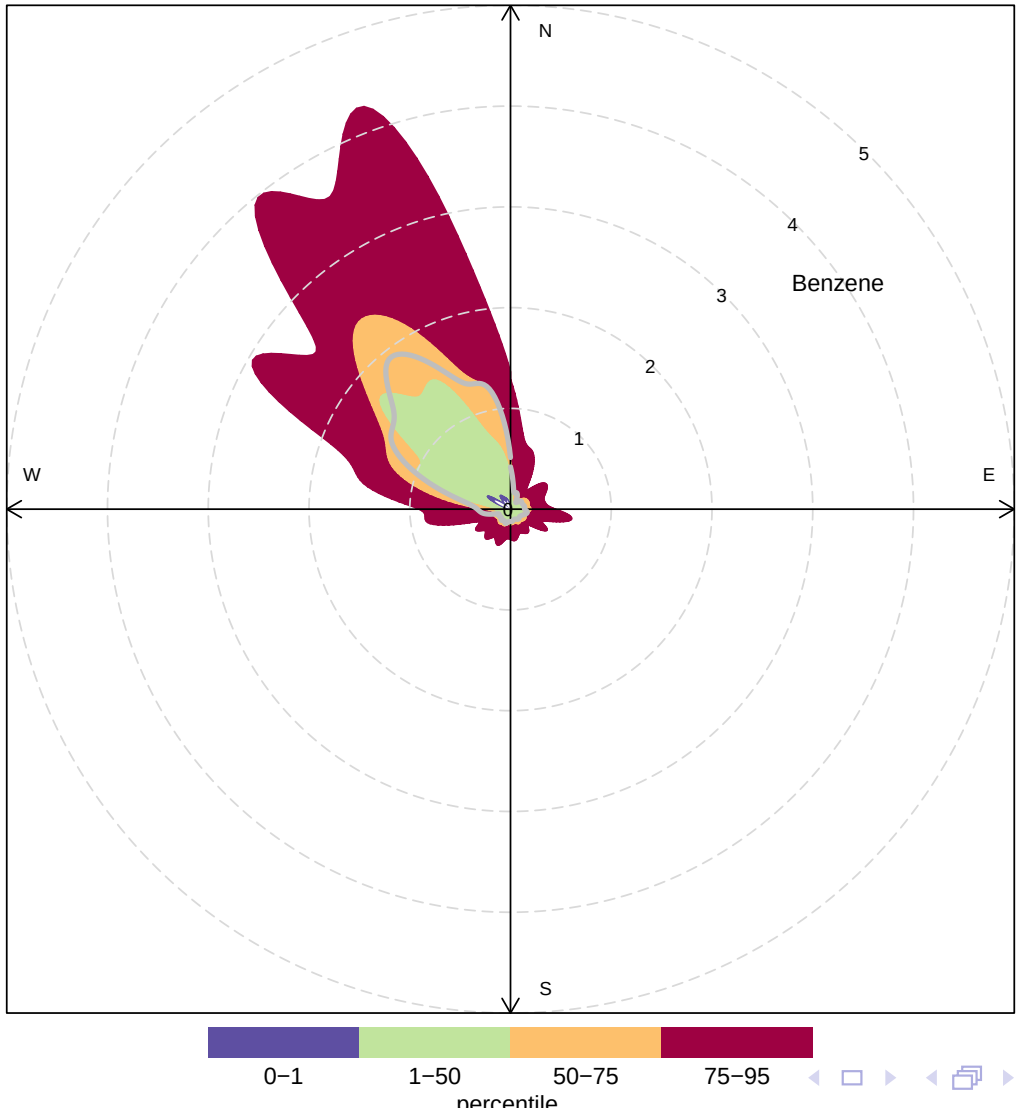


Percentile Rose

- A percentile rose plot can help you see the distribution of concentrations by wind direction

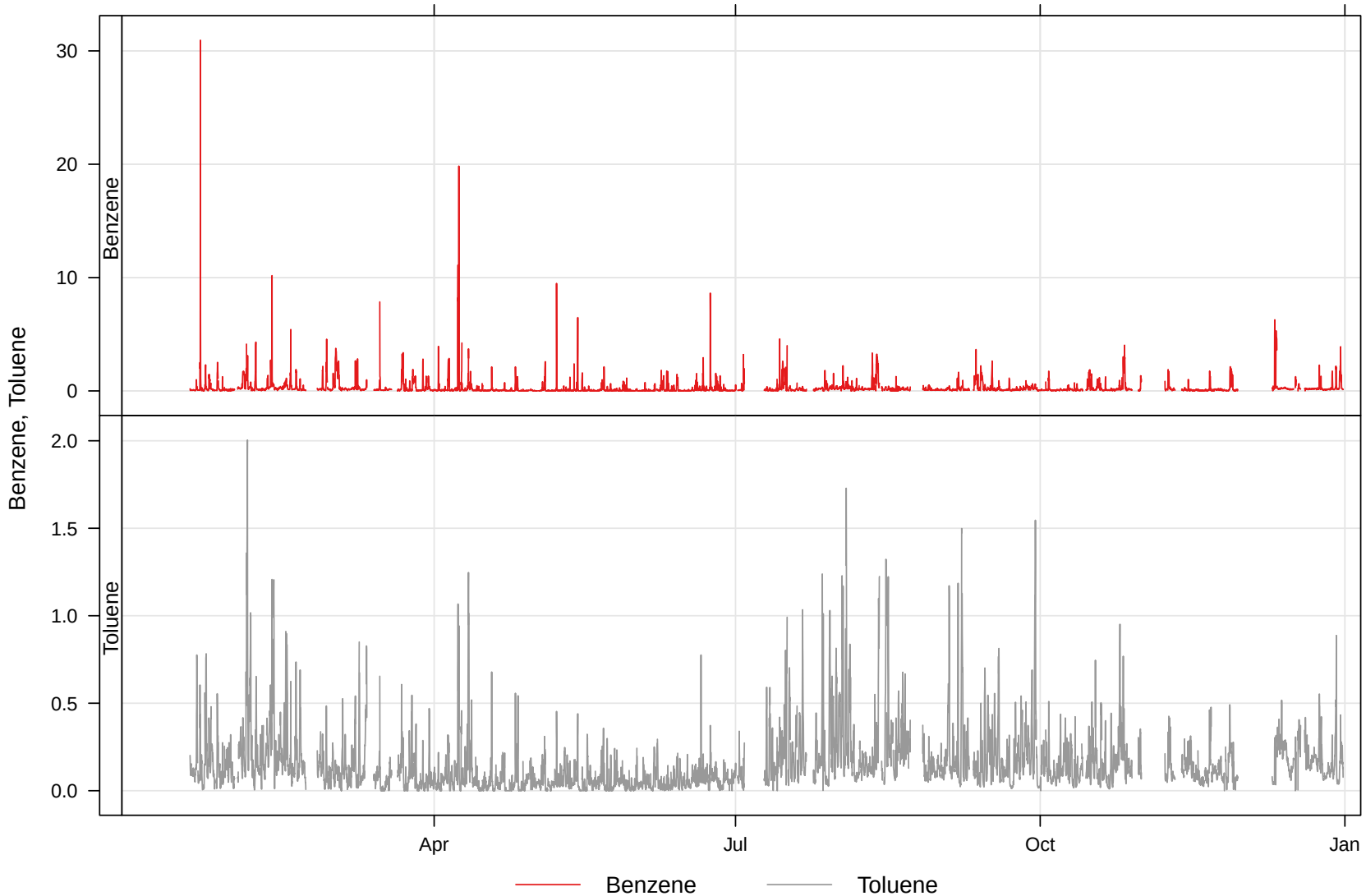
Percentile Rose

```
percentileRose(gary, pollutant="Benzene",
               percentile = c(0,1,50,75,95), smooth=TRUE)
```



Time-series plots

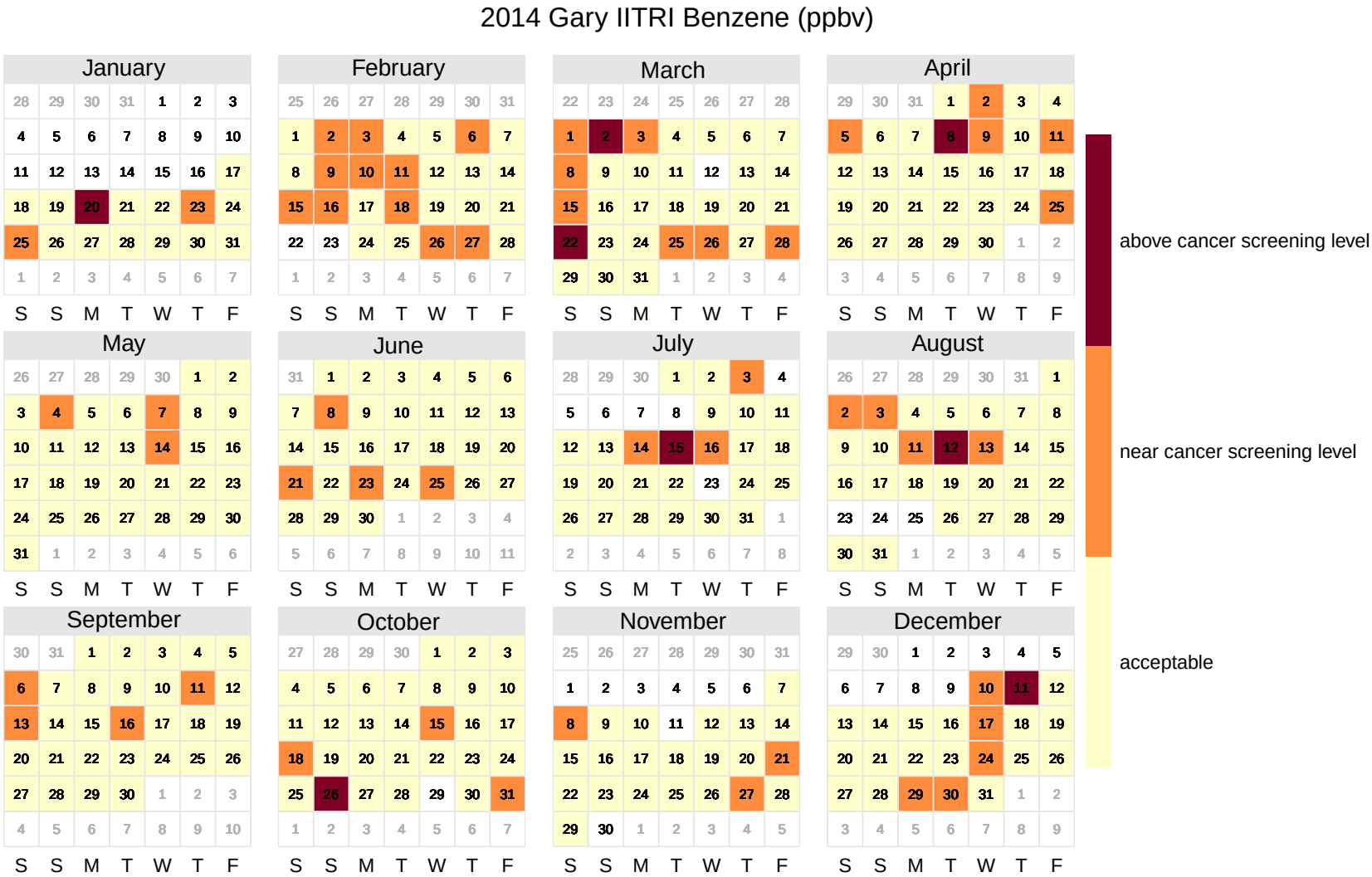
```
timePlot(gary, pollutant=c("Benzene", "Toluene"))
```



Calendar Plots

```
calendarPlot(gary, pollutant = "Benzene", year=2014,
             statistic="mean",
             labels=c("acceptable","near cancer screening level"
                      "above  cancer screening level"),
             breaks=c(0,0.4,1.4,200),
             main = "2014 Gary IITRI Benzene (ppbv)")
```

Calendar Plots

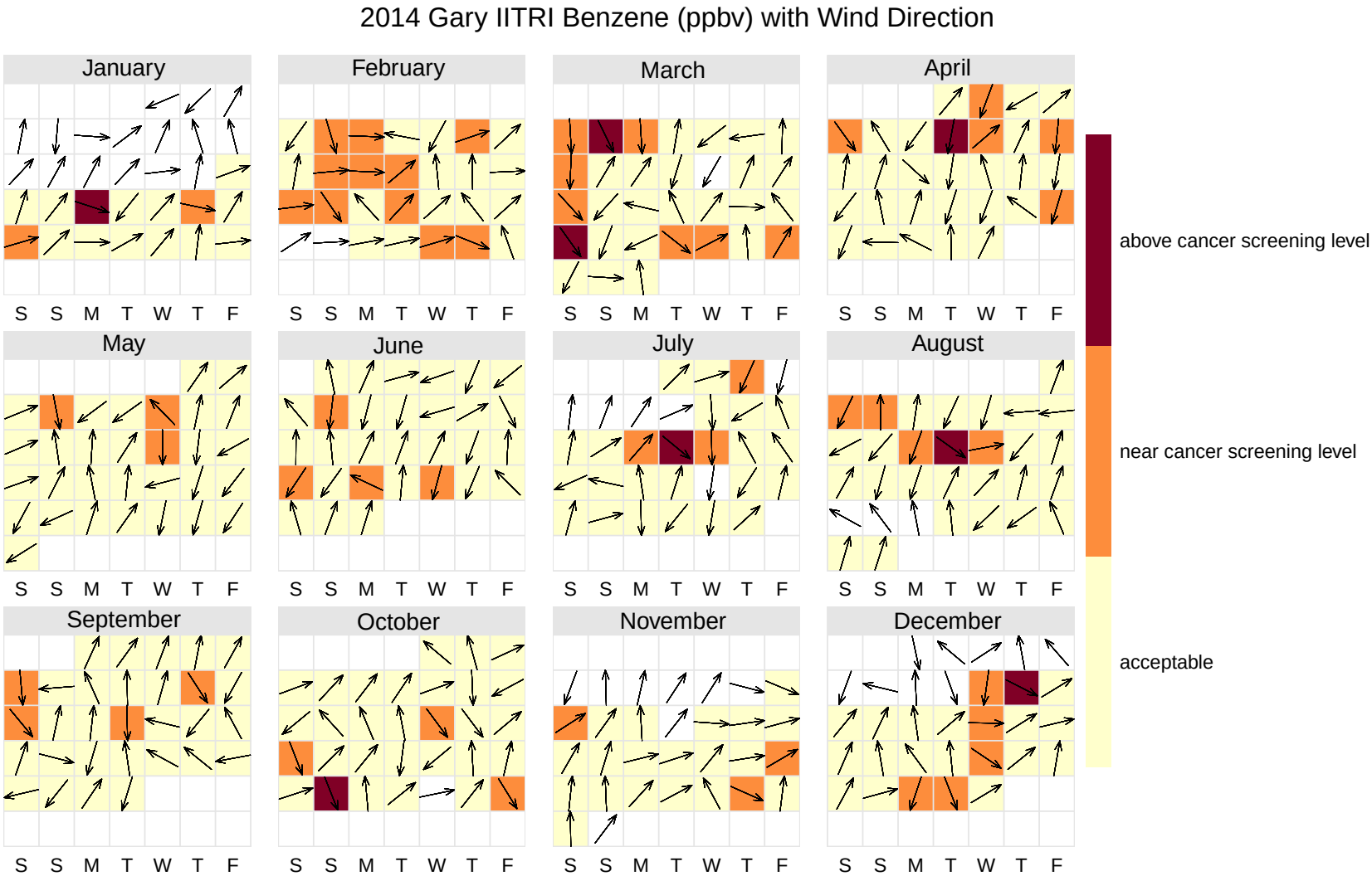


Calendar Plots

- You can use the `annotate()` function within `calendarPlot` to plot the wind direction (`annotate="wd"`) or the concentrations (`annotate = "value"`) on the calendar

```
calendarPlot(gary, pollutant = "Benzene", year=2014,
             annotate="wd", statistic="mean",
             labels=c("acceptable","near cancer screening level"
                      "above cancer screening level"),
             breaks=c(0,0.4,1.4,200),
             main = "2014 Gary IITRI Benzene (ppbv)
             with Wind Direction")
```

Calendar Plots



Training Outline

- What is R and RStudio
- R basics
- The Hadleyverse
  - dplyr
  - tidyr
  - ggplot2
- Useful packages for air toxics
  - raqdm
  - rucl
  - openair
- Air toxics analysis demo
- Interactive web app with `shiny`

Shiny - Overview

- `shiny` is a package developed by RStudio
- Makes it easy to create web applications using the R language
- Not necessary to know HTML, CSS, JavaScript
- But you can customize your apps using those web languages
- The simplest way to create an app is to make two "R Script" files
  - `ui.R` is a file that will determine what the user interface will look like
  - `server.R` is a file that will do the data manipulation and create the output for the app

ui.R

```
library(shiny)
shinyUI(fluidPage(
  titlePanel("Hello Shiny!"),
  sidebarLayout(
    sidebarPanel(
      sliderInput("bins",
                  "Number of bins:",
                  min = 1,
                  max = 50,
                  value = 30)
    ),
    mainPanel(
      plotOutput("distPlot")
    )
  )
))
```

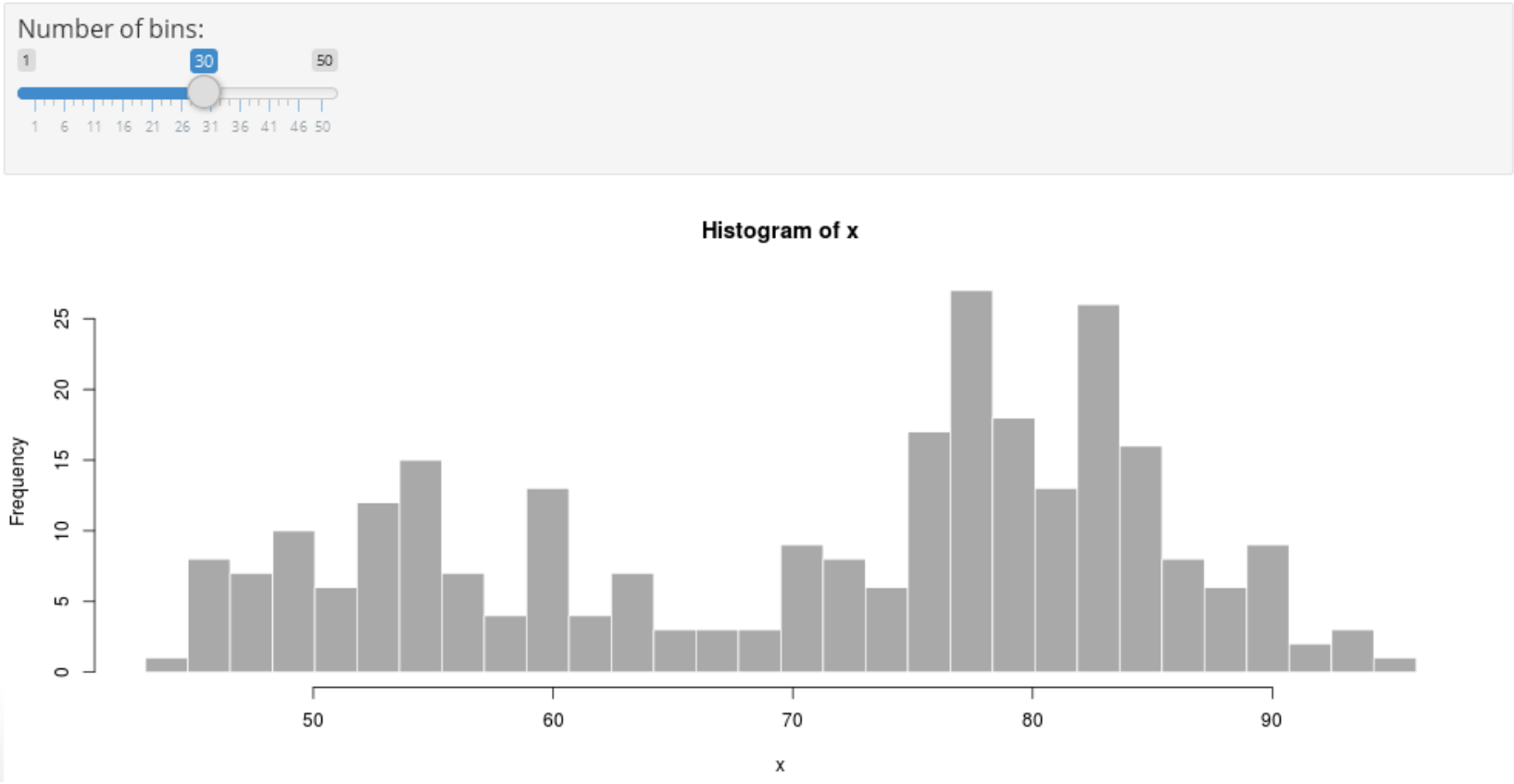
server.R

```
library(shiny)
shinyServer(function(input, output) {
  output$distPlot <- renderPlot({
    x    <- faithful[, 2]  # Old Faithful Geyser data
    bins <- seq(min(x), max(x), length.out = input$bins + 1)
    hist(x, breaks = bins, col = 'darkgray', border = 'white')
  })

})
```

Shiny - `runApp()`

- Save the `ui.R` and `server.R` files in your working directory
- Also save your data in your working directory
- Use `runApp()` to bring up your application in a web browser

Shiny app


Number of bins:
1
30
50
1 6 11 16 21 26 31 36 41 46 50
Histogram of x
Frequency
0
5
10
15
20
25
50
60
70
80
90
x

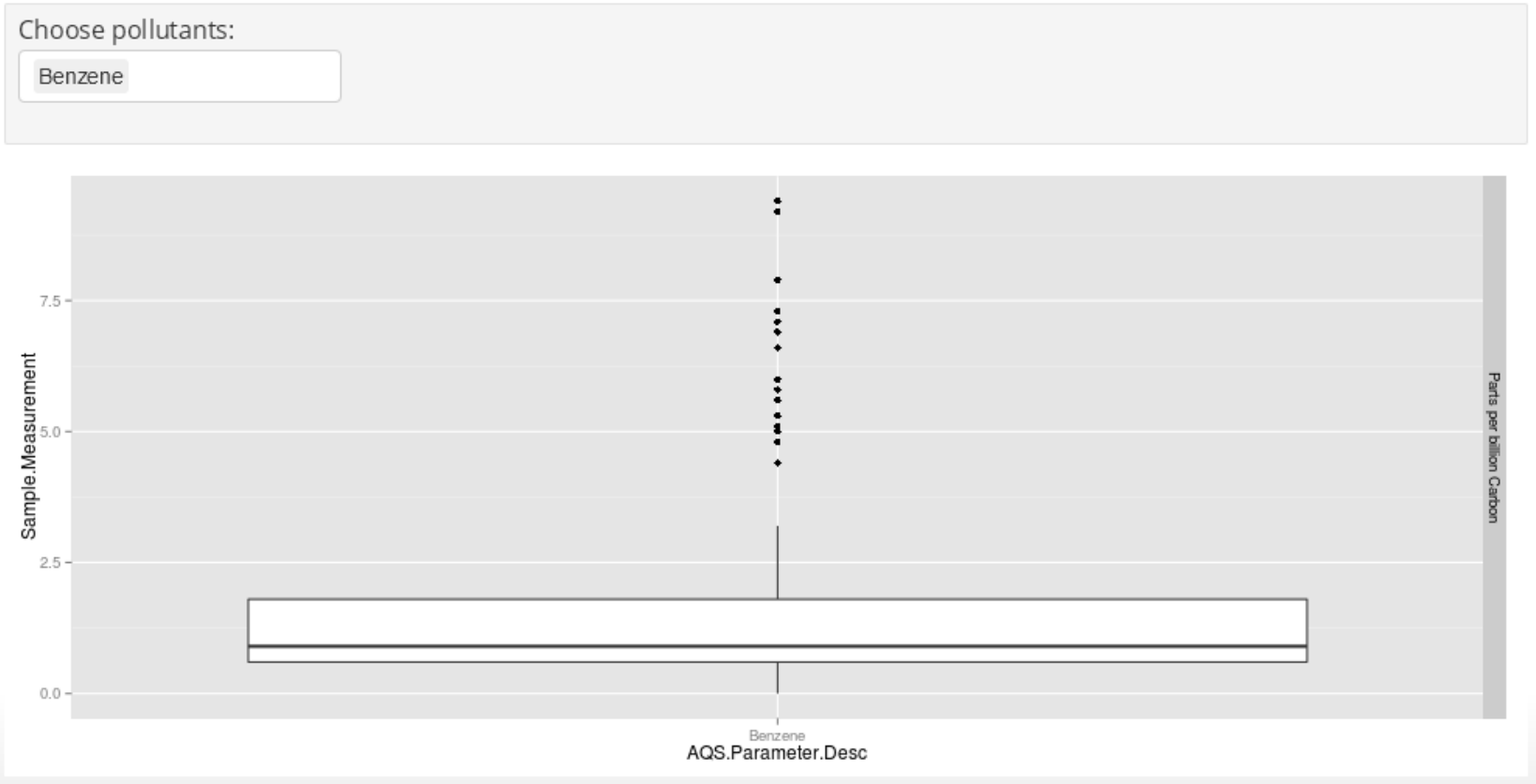
ui.R

```
library(shiny)

load("haps.rda")
pollutants <- unique(as.character(haps$AQS.Parameter.Desc))

shinyUI(fluidPage(
  titlePanel("Gary IITRI HAPS 2014"),
  sidebarLayout(
    sidebarPanel(
      selectInput("pollutants", "Choose pollutants:",
                  choices = pollutants,
                  selected = "Benzene", multiple = TRUE)
    ),
    mainPanel(
      plotOutput("ggplot")
    )
  )
))
```

server.R

```
library(shiny)
library(dplyr)
library(ggplot2)

load("haps.rda")

shinyServer(function(input, output) {

  output$ggplot <- renderPlot({

    haps <- filter(haps,
                   AQS.Parameter.Desc %in% input$pollutants)

    ggplot(haps, aes(x=AQS.Parameter.Desc, y=Sample.Measurement))
    + geom_boxplot() + facet_grid(Unit.of.Measure ~ .,
      scales = "free")
  })

})
```

Shiny app


Choose pollutants:
Benzene
7.5
5.0
2.5
0.0
Sample.Measurement
Parts per billion Carbon
Benzene
AQS.Parameter.Desc

Contact Information

- Nathan Byers, natebyers@gmail.com
- Kali Frost, kdfrost14@gmail.com
- Eric Bailey, eb11307@gmail.com