

Exploratory Data Analysis Course Notes

Xing Su

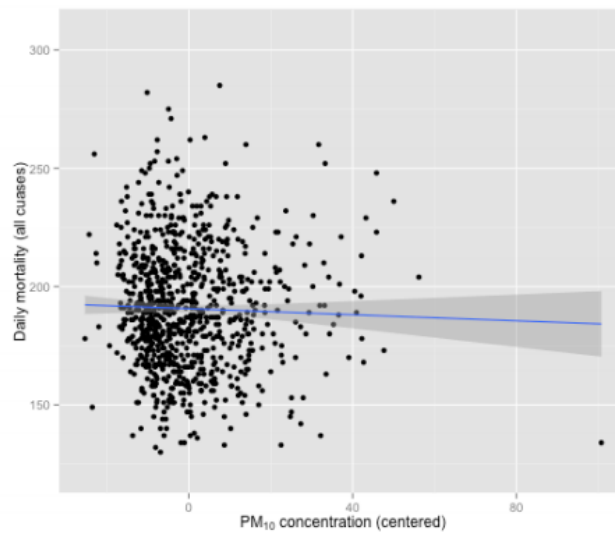
Contents

Principle of Analytic Graphics	3
Exploratory Graphs (examples)	4
One Dimension Summary of Data	4
Two Dimensional Summaries	5
Process of Making a Plot/Considerations	7
Base Plotting	7
Base Graphics Functions and Parameters	8
Base Plot Example	8
Multiple Plot Example	9
Graphics Device	11
<code>lattice</code> Plotting System [<code>library(lattice)</code>]	13
<code>lattice</code> Functions and Parameters	13
<code>lattice</code> Example	14
<code>ggplot2</code> Plotting System [<code>library(ggplot2)</code>]	15
<code>ggplot2</code> Functions and Parameters	15
<code>ggplot2</code> Comprehensive Example	20
Hierarchical Clustering	22
Procedure for Constructing Hierarchical Clusters (<code>hclust</code> function)	22
Approaches for Merging Points/Clusters	22
Characteristics of Hierarchical Clustering Algorithms	23
<code>hclust</code> Function and Example	23
<code>myplcclust</code> Function and Example	24
<code>heatmap</code> Function and Example	25
<code>image</code> Function and Example	25
K-means Clustering	27
Procedure for Constructing K-means Clusters (<code>kmeans</code> function)	27
Characteristics of K-means Clustering Algorithms	28
Dimension Reduction	29
Singular Value Decomposition (SVD)	30
Principal Components Analysis (PCA)	30
SVD and PCA Example	30

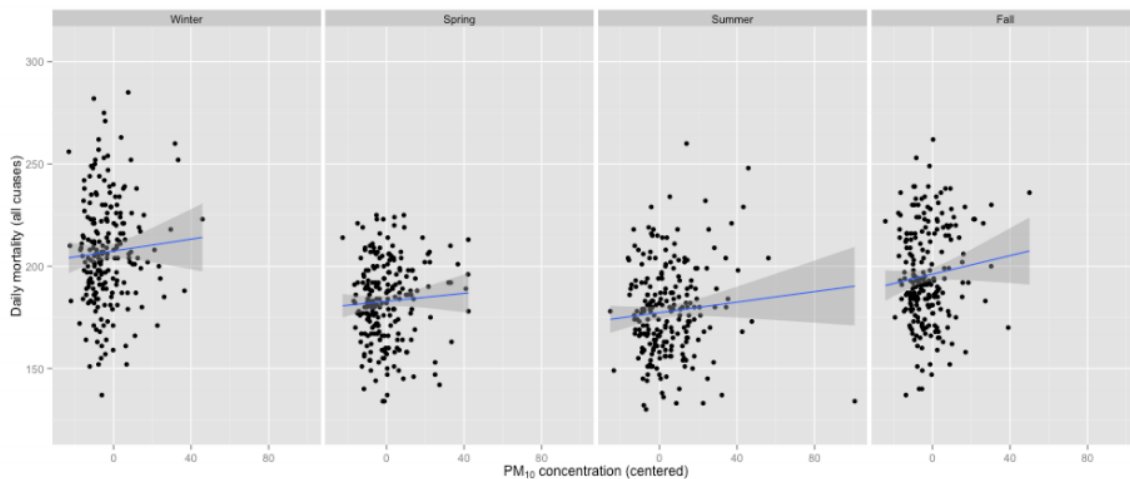
Create Approximations/Data Compression	35
Color Packages in R Plots	37
grDevices Package	37
RColorBrewer Package	38
Case Study: Human Activity Tracking with Smart Phones	41
Case Study: Fine Particle Pollution in the U.S. from 1999 to 2012	49

Principle of Analytic Graphics

- **Principle 1: Show Comparisons**
 - always comparative (compared to what)
 - randomized trial - compare control group to test group
 - evidence for a hypothesis is always relative to another competing hypothesis
- **Principle 2: Show causality/mechanism/explanation/systematic structure**
 - form hypothesis to evidence showing a relationship (causal framework, why something happened)
- **Principle 3: Show multivariate data**
 - more than 2 variables because the real world is multivariate
 - show as much data on a plot as you can
 - *example*



- slightly negative relationship between pollution and mortality



- when split up by season, the relationships are all positive → season = confounding variable
- **Principle 4: Integration of evidence**
 - use as many modes of evidence/displaying evidence as possible (modes of data presentation)
 - integrate words/numbers/images/diagrams (information rich)
 - analysis should drive the tool
- **Principle 5: Describe/document evidence with appropriate labels/scales/sources**
 - add credibility to that data graphic
- **Principle 6: Content is the most important**
 - analytical presentations ultimately stand/fall depending on quality/relevance/integrity of content

Exploratory Graphs ([examples](#))

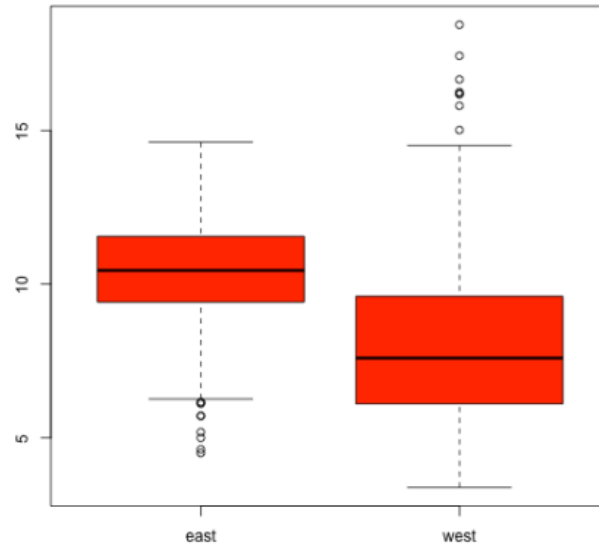
- **Purpose:** understand data properties, find pattern in data, suggest modeling strategies, debug
- **Characteristics:** made quickly, large number produced, gain personal understanding, appearances and presentation are aren't as important

One Dimension Summary of Data

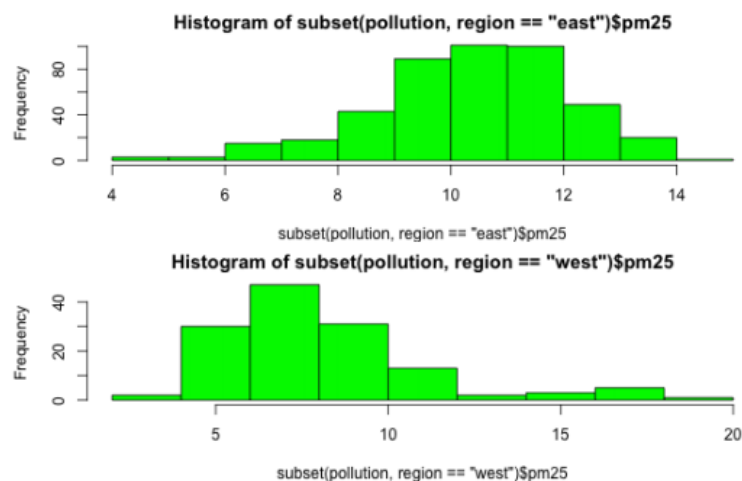
- `summary(data)` = returns min, 1st quartile, median, mean, 3rd quartile, max
- `boxplot(data, col = "blue")` = produces a box with middles 50% highlighted in the specified color
 - `whiskers` = $\pm 1.58IQR/\sqrt{n}$
 - * IQR = interquartile range, $Q_3 - Q_1$
 - `box` = 25%, median, 75%
- `histograms(data, col = "green")` = produces a histogram with specified breaks and color
 - `breaks` = 100 → the higher the number is the smaller/narrower the histogram columns are
- `rug(data)` = density plot, add a strip under the histogram indicating location of each data point
- `barplot(data, col = wheat)` = produces a bar graph, usually for categorical data
- **Overlaying Features**
- `abline(h/v = 12)` = overlays horizontal/vertical line at specified location
 - `col` = "red" → specifies color
 - `lwd` = 4 → line width
 - `lty` = 2 → line type

Two Dimensional Summaries

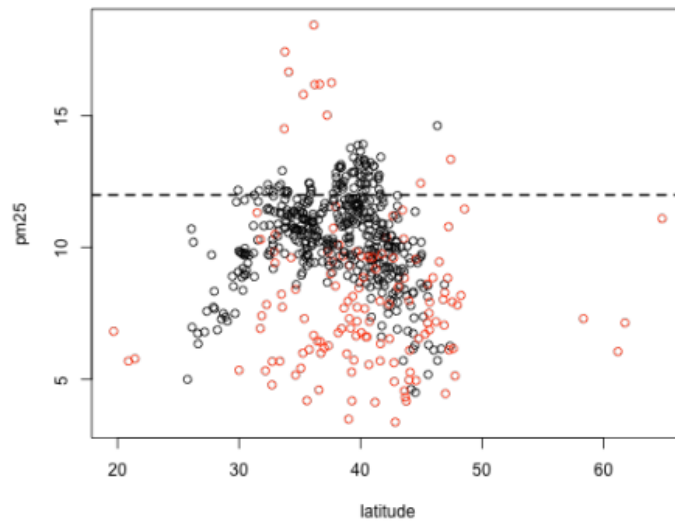
- multiple/overlay 1D plots (using lattice/ggplot2)
- **box plots:** `boxplot(pm25 ~ region, data = pollution, col = "red")`



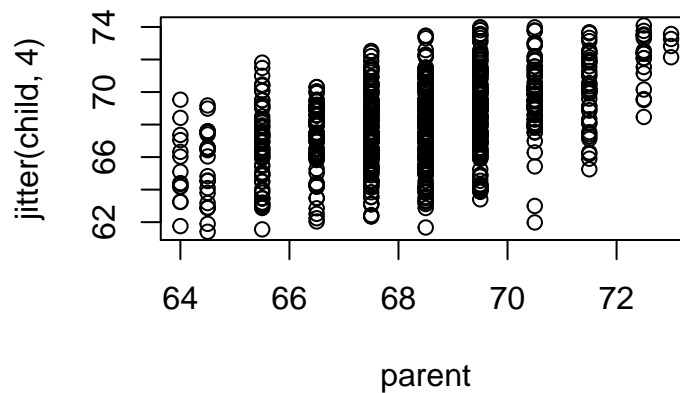
- **histogram:**
 - `par(mfrow = c(2, 1), mar = c(4, 4, 2, 1))` -> set margin
 - `hist(subset(pollution, region == "east")$pm25, col = "green")` -> first histogram
 - `hist(subset(pollution, region == "west")$pm25, col = "green")` -> second histogram



- **scatterplot**
 - `with(pollution, plot(latitude, pm25, col = region))`
 - `abline(h = 12, lwd = 2, lty = 2)` -> plots horizontal dotted line
 - `plot(jitter(child, 4)~parent, galton)` -> spreads out data points at the same position to simulate measurement error/make high frequency more visible

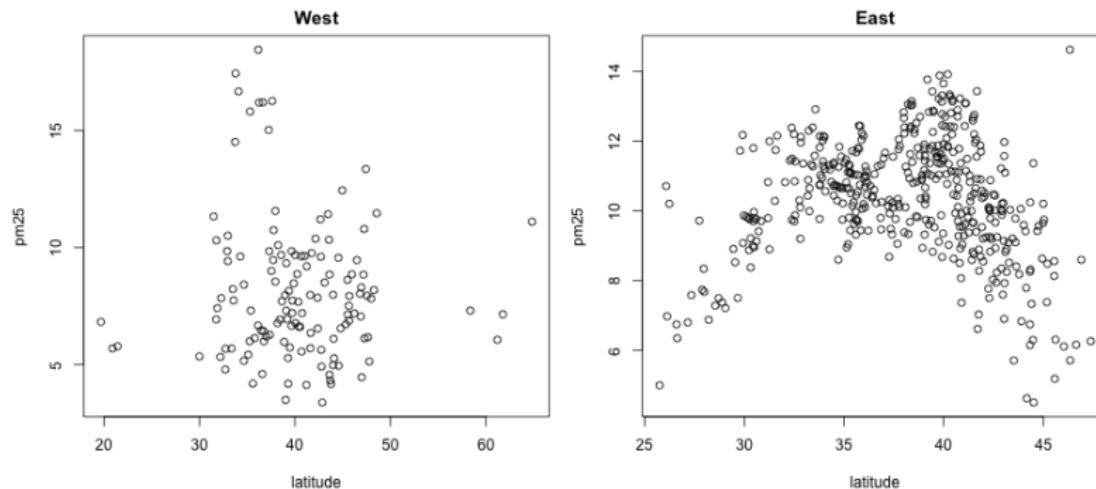


```
## Loading required package: MASS
## Loading required package: HistData
## Loading required package: Hmisc
## Loading required package: lattice
## Loading required package: survival
## Loading required package: splines
## Loading required package: Formula
##
## Attaching package: 'Hmisc'
##
## The following objects are masked from 'package:base':
##
##   format.pval, round.POSIXt, trunc.POSIXt, units
##
## Attaching package: 'UsingR'
##
## The following object is masked from 'package:survival':
##
##   cancer
```



- multiple scatter plots

- `par(mfrow = c(1, 2), mar = c(5, 4, 2, 1))` -> sets margins
- `with(subset(pollution, region == "west"), plot(latitude, pm25, main = "West"))` -> left scatterplot
- `with(subset(pollution, region == "east"), plot(latitude, pm25, main = "East"))` -> right scatterplot



Process of Making a Plot/Considerations

- where will plot be made? screen or file?
- how will plot be used? viewing on screen/web browser/print/presentation?
- large amount of data vs few points?
- need to be able to dynamically resize?
- **plotting system**: base, lattice, ggplot2?

Base Plotting

- blank canvas, “artist’s palette”, start with plot function
- annotations - text, lines, points, axis
- convenient, but cannot go back when started (need to plan ahead)
- everything need to be manually set carefully to be able to achieve the desired effect (margins)
- core plotting/graphics engine in R encapsulated in the following
 - **graphics**: plotting functions for base graphing system (plot, hist, boxplot, text.)
 - **grDevices**: contains all the code implementing the various graphics devices (x11, PDF, PostScript, PNG, etc)
- **Two phase**: initialize, annotate
- calling `plot(x, y)` or `hist(x)` will launch a graphics device and draw a plot on device
 - if no argument specified, default called
 - parameters documented in “`?par`”
 - **Note**: *it is some times necessary to convert column/variable to factor to make plotting easier*

```
* airquality <- transform(airquality, Month = factor(month))
```

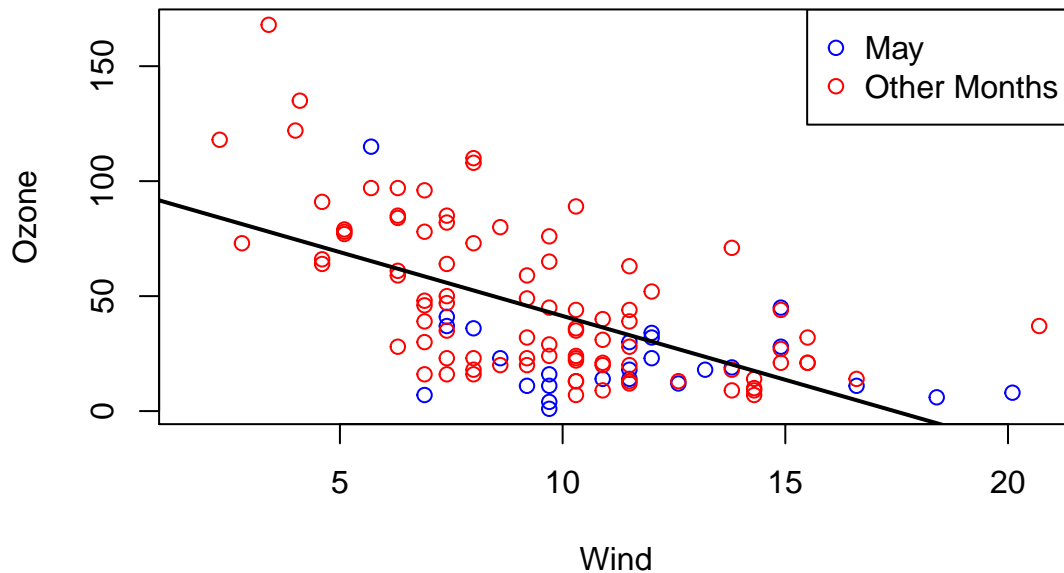
Base Graphics Functions and Parameters

- **arguments**
 - `pch`: plotting symbol (default = open circle)
 - `lty`: line type (default is solid)
 - * 0=blank, 1=solid (default), 2=dashed, 3=dotted, 4=dotdash, 5=longdash, 6=twodash
 - `lwd`: line width (integer)
 - `col`: plotting color (number string or hexcode, `colors()` returns vector of colors)
 - `xlab`, `ylab`: x-y label character strings
 - `cex`: numerical value giving the amount by which plotting text/symbols should be magnified relative to the default
 - * `cex = 0.15 * variable`: plot size as an additional variable
- `par()` function → specifies global graphics parameters, affects all plots in an R session (can be overridden)
 - `las`: orientation of axis labels
 - `bg`: background color
 - `mar`: margin size (order = bottom left top right)
 - `oma`: outer margin size (default = 0 for all sides)
 - `mfrow`: number of plots per row, column (plots are filled row-wise)
 - `mfcol`: number of plots per row, column (plots are filled column-wise)
 - can verify all above parameters by calling `par("parameter")`
- **plotting functions**
 - `lines`: adds lines to a plot, given a vector of x values and corresponding vector of y values
 - `points`: adds a point to the plot
 - `text`: add text labels to a plot using specified x,y coordinates
 - `title`: add annotations to x,y axis labels, title, subtitles, outer margin
 - `mtext`: add arbitrary text to margins (inner or outer) of plot
 - `axis`: specify axis ticks

Base Plot Example

```
library(datasets)
# type = "n" sets up the plot and does not fill it with data
with(airquality, plot(Wind, Ozone, main = "Ozone and Wind in New York City", type = "n"))
# subsets of data are plotted here using different colors
with(subset(airquality, Month == 5), points(Wind, Ozone, col = "blue"))
with(subset(airquality, Month != 5), points(Wind, Ozone, col = "red"))
legend("topright", pch = 1, col = c("blue", "red"), legend = c("May", "Other Months"))
model <- lm(Ozone ~ Wind, airquality)
# regression line is produced here
abline(model, lwd = 2)
```


Ozone and Wind in New York City

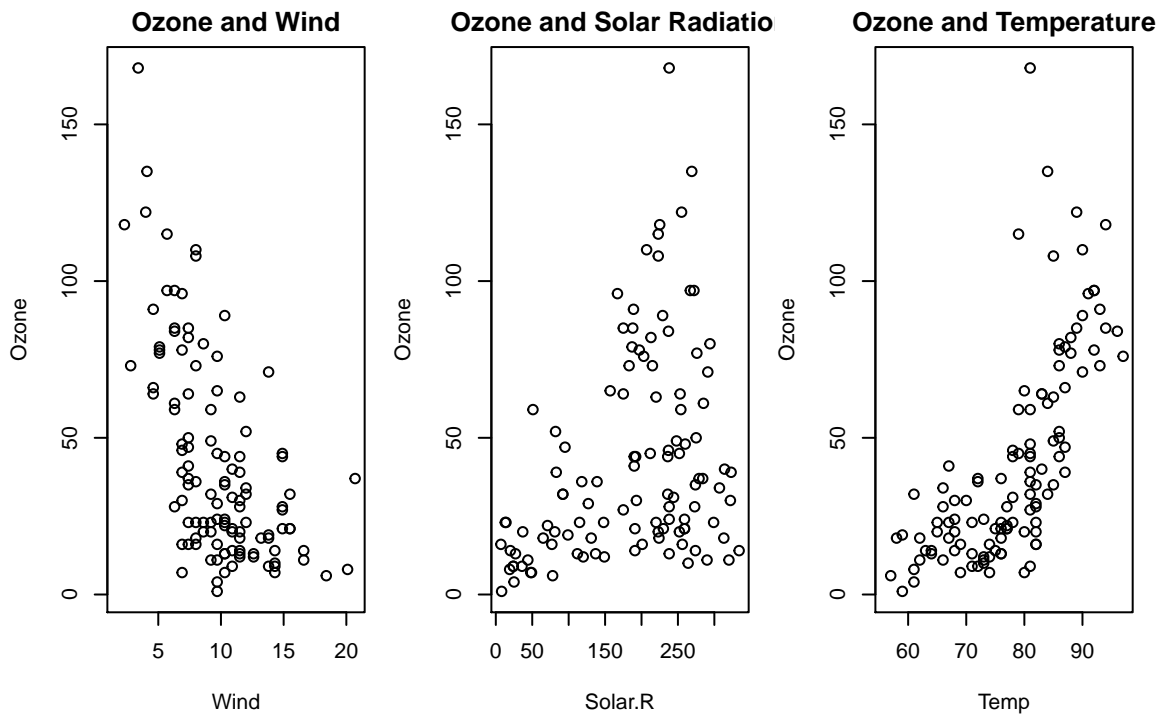


Multiple Plot Example

- *Note: typing `example(points)` in R will launch a demo of base plotting system and may provide some helpful tips on graphing*

```
# this expression sets up a plot with 1 row 3 columns, sets the margin and outer margins
par(mfrow = c(1, 3), mar = c(4, 4, 2, 1), oma = c(0, 0, 2, 0))
with(airquality, {
  # here three plots are filled in with their respective titles
  plot(Wind, Ozone, main = "Ozone and Wind")
  plot(Solar.R, Ozone, main = "Ozone and Solar Radiation")
  plot(Temp, Ozone, main = "Ozone and Temperature")
  # this adds a line of text in the outer margin*
  mtext("Ozone and Weather in New York City", outer = TRUE)}
)
```

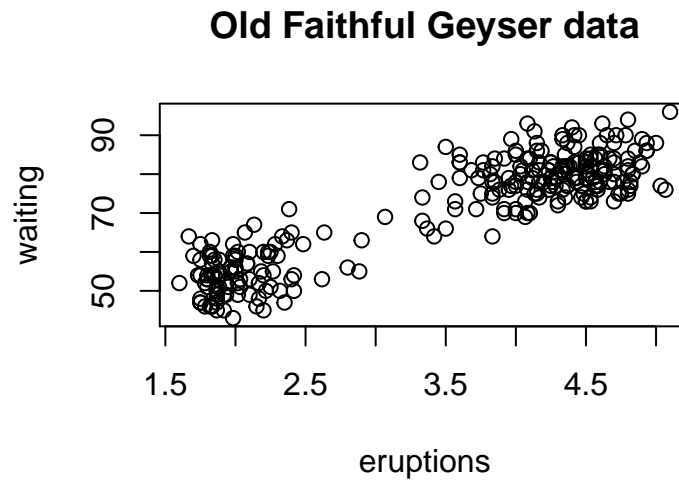
Ozone and Weather in New York City



Graphics Device

- A graphics device is something where you can make a plot appear
 - **window on screen** (screen device) <— quick visualizations and exploratory analysis
 - **pdf** (file device) <— plots that may be printed out or incorporated in to document
 - **PNG/JPEG** (file device) <— plots that may be printed out or incorporated in to document
 - **scalable vector graphics** (SVG)
- When a plot is created in R, it has to be sent to a graphics device
- **Most common is screen device**
 - `quartz()` on Mac, `windows()` on Windows, `x11()` on Unix/Linux
 - `?Devices` = lists devices found
- **Plot creation**
 - screen device
 - * call `plot/xplot/qplot` -> plot appears on screen device -> annotate as necessary -> use
 - file devices
 - * explicitly call graphics device -> plotting function to make plot (write to file) -> annotate as necessary -> explicitly close graphics device with `dev.off()`
- **Graphics File Devices**
 - **Vector Formats** (good for line drawings/plots w/ solid colors, a modest number of points)
 - * **pdf**: useful for line type graphics, resizes well, usually portable, not efficient if too many points
 - * **svg**: XML based scalable vector graphics, support animation and interactivity, web based
 - * **win.metafile**: Windows metafile format
 - * **postscript**: older format, resizes well, usually portable, can create encapsulated postscript file, Windows often don't have postscript viewer (postscript = predecessor of PDF)
 - **Bitmap Formats** (good for plots w/ large number of points, natural scenes/webbased plots)
 - * **png**: Portable Network Graphics, good for line drawings/image with solid colors, uses lossless compression, most web browsers read this natively, good for plotting a lot of data points, does not resize well
 - * **JPEG**: good for photographs/natural scenes/gradient colors, size efficient, uses lossy compression, good for plotting many points, does not resize well, can be read by almost any computer/browser, not great for line drawings (aliasing on edges)
 - * **tiff**: common bitmap format supports lossless compression
 - * **bmp**: native Windows bitmapped format
- **Multiple Open Graphics Devices**
 - possible to open multiple graphics devices (screen, file, or both)
 - plotting occurs only one device at a time
 - `dev.cur()` = returns the currently active device
 - every open graphics device is assigned an integer ≥ 2
 - `dev.set(<integer>)` = change the active graphics device `<integer>` = number associated with the graphics device you want to switch to
- **Copying plots**
 - `dev.copy()` = copy a plot from one device to another
 - `dev.copy2pdf()` = specifically for copying to PDF files
 - **Note**: Copying a plot is not an exact operation, so the result may not be identical to the original
 - **example**

```
## Create plot on screen device
with(faithful, plot(eruptions, waiting))
## Add a main title
title(main = "Old Faithful Geyser data")
```



```
## Copy my plot to a PNG file
dev.copy(png, file = "geyserplot.png")
## Don't forget to close the PNG device!
dev.off()
```

lattice Plotting System [library(lattice)]

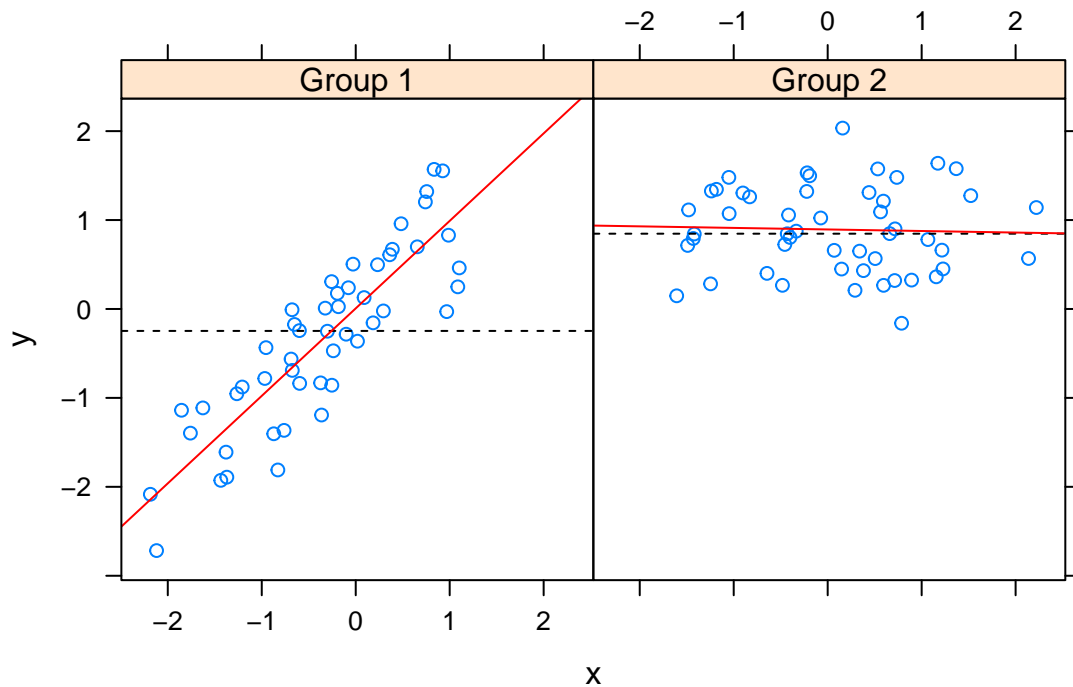
- implemented using the **lattice** and **grid** packages
 - **lattice** package -> contains code for producing **Trellis** graphics (independent from base graphics system)
 - **grid** package -> implements the graphing system; lattice build on top of grid
- all plotting and annotation is done with **single function call**
 - margins/spacing/labels set automatically for entire plot, good for putting multiple on the screen
 - good for conditioning plots -> examining same plots over different conditions how y changes vs x across different levels of z
 - **panel** functions can be specified/customized to modify the subplots
- lattice graphics functions return an object of class “trellis”, where as base graphics functions plot data directly to graphics device
 - print methods for lattice functions actually plots the data on graphics device
 - trellis objects are auto-printed
 - **trellis.par.set()** -> can be used to set global graphic parameters for all trellis objects
- hard to annotate, awkward to specify entire plot in one function call
- cannot add to plot once created, panel/subscript functions hard to prepare

lattice Functions and Parameters

- **Functions**
 - **xyplot()** -> main function for creating scatterplots
 - **bwplot()** -> box and whiskers plots (box plots)
 - **histogram()** -> histograms
 - **stripplot()** -> box plot with actual points
 - **dotplot()** -> plot dots on “violin strings”
 - **sploM()** -> scatterplot matrix (like **pairs()** in base plotting system)
 - **levelplot()/contourplot()** -> plotting image data
- **Arguments for xyplot(y ~ x | f * g, data, layout, panel)**
 - default blue open circles for data points
 - formula notation is used here (~) -> left hand side is the y-axis variable, and the right hand side is the x-axis variable
 - **f/g** = conditioning/categorical variables (optional)
 - * basically creates multi-panelled plots (for different factor levels)
 - * * indicates interaction between two variables
 - * intuitively, the xyplot displays a graph between x and y for every level of **f** and **g**
 - **data** = the data frame/list from which the variables should be looked up
 - * if nothing is passed, the parent frame is used (searching for variables in the workspace)
 - * if no other arguments are passed, defaults will be used
 - **layout** = specifies how the different plots will appear
 - * **layout = c(5, 1)** -> produces 5 subplots in a horizontal fashion
 - * padding/spacing/margin automatically set
 - [optional] **panel** function can be added to control what is plotted inside each panel of the plot
 - * **panel** functions receive x/y coordinates of the data points in their panel (along with any additional arguments)
 - * **?panel.xyplot** -> brings up documentation for the panel functions
 - * **Note:** no base plot functions can be used for lattice plots

lattice Example

```
library(lattice)
set.seed(10)
x <- rnorm(100)
f <- rep(0:1, each = 50)
y <- x + f - f * x + rnorm(100, sd = 0.5)
f <- factor(f, labels = c("Group 1", "Group 2"))
## Plot with 2 panels with custom panel function
xyplot(y ~ x | f, panel = function(x, y, ...) {
  # call the default panel function for xyplot
  panel.xyplot(x, y, ...)
  # adds a horizontal line at the median
  panel.abline(h = median(y), lty = 2)
  # overlays a simple linear regression line
  panel.lmline(x, y, col = 2)
})
```



ggplot2 Plotting System [library(ggplot2)]

- implementation of Grammar of Graphics by Leland Wilkinson, written by Hadley Wickham (created RStudio)
 - “In brief, the grammar tells us that a statistical graphic is a mapping from data to aesthetic attributes (color, 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”
- grammar graphics plot, splits the different between base and lattice systems
- automatically sets spacings/text/tiles but also allows annotations to be added
- default makes a lot of choices, but still customizable

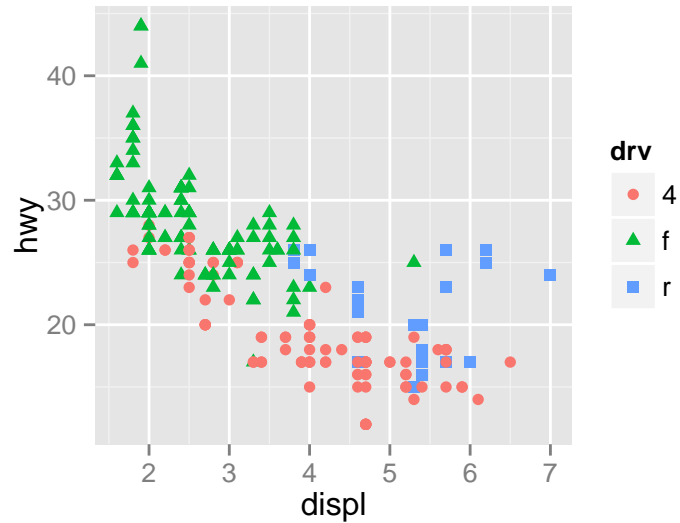
ggplot2 Functions and Parameters

- **basic components** of a ggplot2 graphic
 - **data frame** -> source of data
 - **aesthetic mappings** -> how data are mapped to color/size (x vs y)
 - **geoms** -> geometric objects like points/lines/shapes to put on page
 - **facets** -> conditional plots using factor variables/multiple panels
 - **stats** -> statistical transformations like binning/quantiles/smoothing
 - **scales** -> scale aesthetic map uses (i.e. male = red, female = blue)
 - **coordinate system** -> system in which data are plotted
- **qplot(x, y, data, color, geom)** -> quick plot, analogous to base system's plot() function
 - **default style**: gray background, white gridlines, x and y labels automatic, and solid black circles for data points
 - data always comes from data frame (in unspecified, function will look for data in workspace)
 - plots are made up of aesthetics (size, shape, color) and geoms (points, lines)
 - **Note**: *capable of producing quick graphics, but difficult to customize in detail*
- **factor variables**: important for graphing subsets of data -> they should be labelled with specific information, and not just 1, 2, 3
 - **color = factor1** -> use the factor variable to display subsets of data in different colors on the same plot (legend automatically generated)
 - **shape = factor2** -> use the factor variable to display subsets of data in different shapes on the same plot (legend automatically generated)
 - **example**

```
library(ggplot2)
```

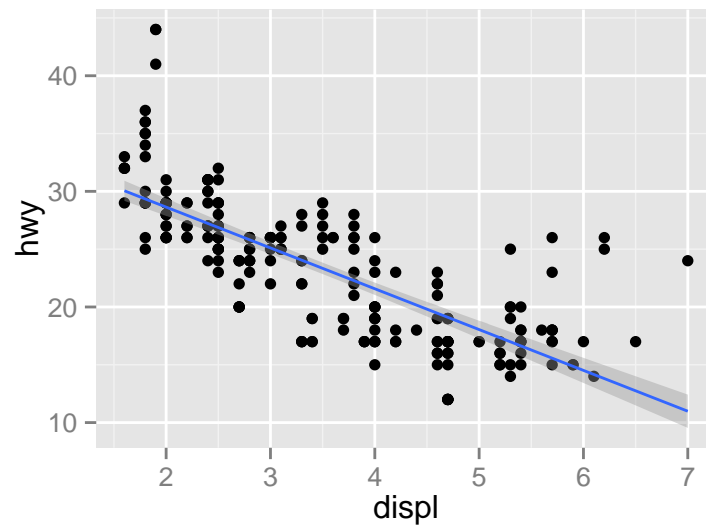
```
##  
## Attaching package: 'ggplot2'  
##  
## The following object is masked from 'package:UsingR':  
##  
## movies
```

```
qplot(displ, hwy, data = mpg, color = drv, shape = drv)
```



- **adding statistics:** `geom = c("points", "smooth")` -> add a smoother/“low S”
 - “points” plots the data themselves, “smooth” plots a smooth mean line in blue with an area of 95% confidence interval shaded in dark gray
 - `method = "lm"` -> additional argument method can be specified to create different lines/confidence intervals
 - * `lm` = linear regression
 - *example*

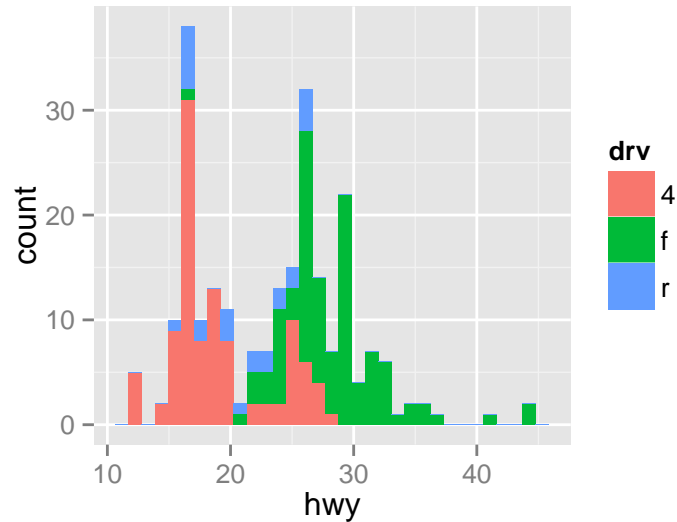
```
qplot(displ, hwy, data = mpg, geom = c("point", "smooth"), method="lm")
```



- **histograms:** if only one value is specified, a histogram is produced
 - `fill = factor1` -> can be used to fill the histogram with different colors for the subsets (legend automatically generated)
 - *example*

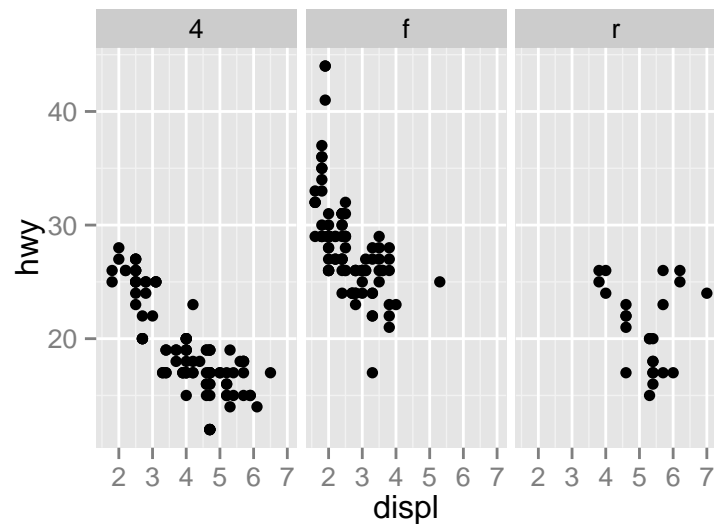

```
qplot(hwy, data = mpg, fill = drv)
```

stat_bin: binwidth defaulted to range/30. Use 'binwidth = x' to adjust this.

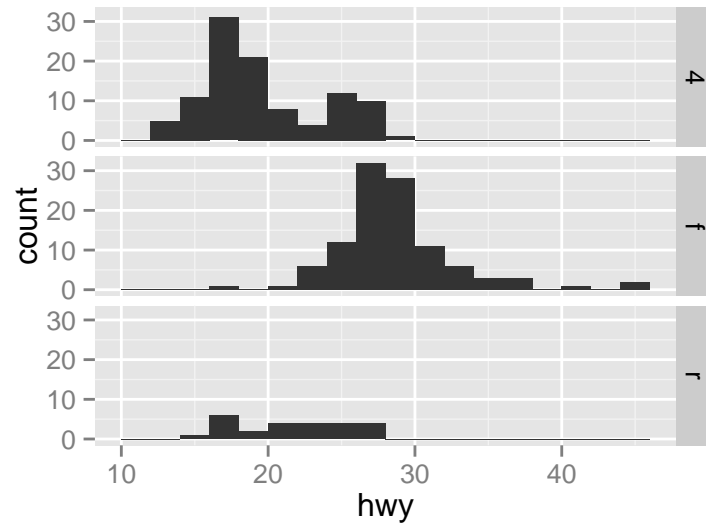


- **facets**: similar to panels in lattice, split data according to factor variables
 - `facets = rows ~ columns` -> produce different subplots by factor variables specified (rows/columns)
 - `"."` indicates there are no addition row or column
 - `facets = . ~ columns` -> creates 1 by col subplots
 - `facets = row ~ .` -> creates row row by 1 subplots
 - labels get generated automatically based on factor variable values
 - *example*

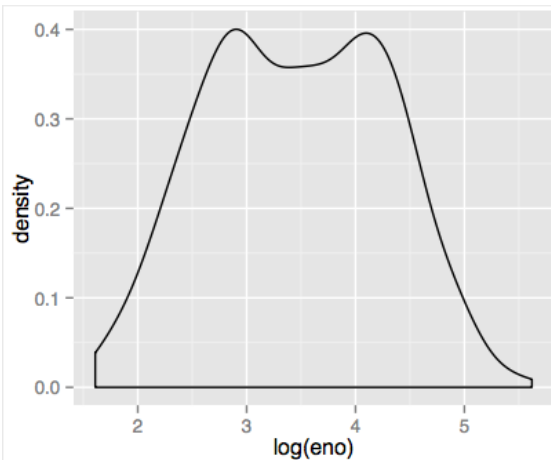
```
qplot(displ, hwy, data = mpg, facets = . ~ drv)
```



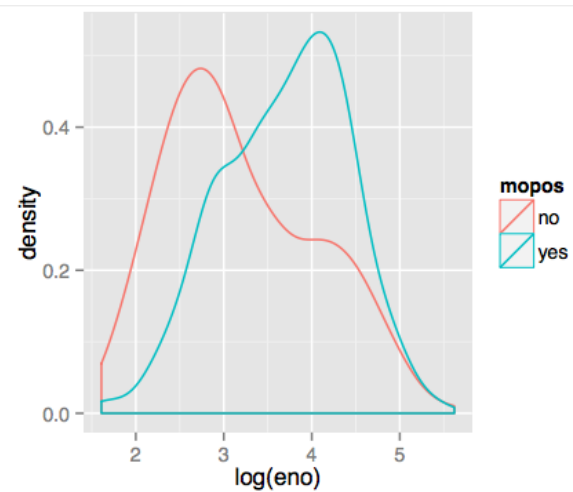
```
qplot(hwy, data = mpg, facets = drv ~ ., binwidth = 2)
```



- **density smooth:** smooths the histograms into a line tracing its shape
 - `geom = "density"` -> replaces the default scatterplot with density smooth curve
 - *example*



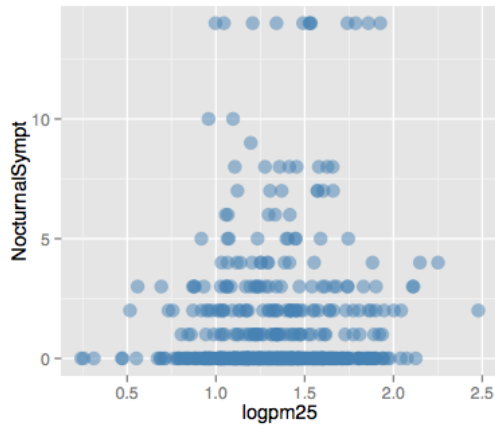
```
qplot(log(eno), data = maacs, geom = "density")
```



```
qplot(log(eno), data = maacs, geom = "density", color = mopos)
```

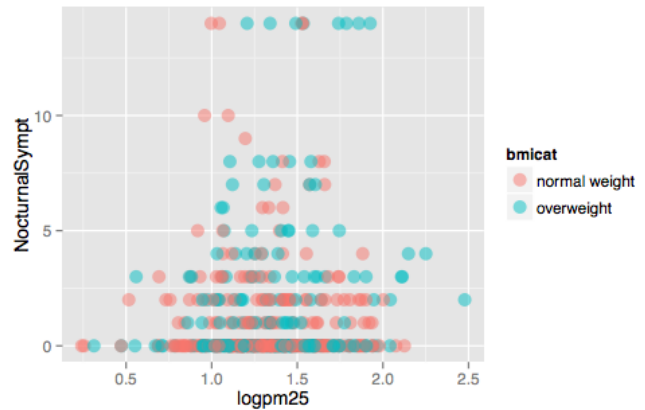
- **ggplot()**
 - built up in layers/modularly (similar to base plotting system)
 - * data -> overlay summary -> metadata/annotation
 - `g <- ggplot(data, aes(var1, var2))`
 - * initiates call to `ggplot` and specifies the data frame that will be used
 - * `aes(var1, var2)` -> specifies aesthetic mapping, or `var1` = x variable, and `var2` = y variable
 - * `summary(g)` -> displays summary of `ggplot` object

- * `print(g)` -> returns error ("no layer on plot") which means the plot does know how to draw the data yet
- `g + geom_point()` -> takes information from g object and produces scatter plot
- `+ geom_smooth()` -> adds low S mean curve with confidence interval
 - * `method = "lm"` -> changes the smooth curve to be linear regression
 - * `size = 4, linetype = 3` -> can be specified to change the size/style of the line
 - * `se = FALSE` -> turns off confidence interval
- `+ facet_grid(row ~ col)` -> splits data into subplots by factor variables (see facets from `qplot()`)
 - * conditioning on continuous variables is possible through cutting/making a new categorical variable
 - * `cutPts <- quantiles(df$cVar, seq(0, 1, length=4), na.rm = TRUE)` -> creates quantiles where the continuous variable will be cut
 - `seq(0, 1, length=4)` -> creates 4 quantile points
 - `na.rm = TRUE` -> removes all NA values
 - * `df$newFactor <- cut(df$cVar, cutPts)` -> creates new categorical/factor variable by using the cutpoints
 - creates n-1 ranges from n points -> in this case 3
- **annotations:**
 - * `xlab(), ylab(), labs(), ggtitle()` -> for labels and titles
 - `labs(x = expression("log " * PM[2.5]), y = "Nocturnal")` -> specifies x and y labels
 - `expression()` -> used to produce mathematical expressions
 - * geom functions -> many options to modify
 - * `theme()` -> for global changes in presentation
 - *example:* `theme(legend.position = "none")`
 - * two standard themes defined: `theme_gray()` and `theme_bw()`
 - * `base_family = "Times"` -> changes font to Times
- **aesthetics**
 - * `+ geom_point(color, size, alpha)` -> specifies how the points are supposed to be plotted on the graph (style)
 - *Note:* this translates to `geom_line()/other forms of plots`
 - `color = "steelblue"` -> specifies color of the data points
 - `aes(color = var1)` -> wrapping color argument this way allows a factor variable to be assigned to the data points, thus subsetting it with different colors based on factor variable values
 - `size = 4` -> specifies size of the data points
 - `alpha = 0.5` -> specifies transparency of the data points
 - * *example*



```
g + geom_point(color = "steelblue",
size = 4, alpha = 1/2)
```

Constant values



```
g + geom_point(aes(color = bmicat),
size = 4, alpha = 1/2)
```

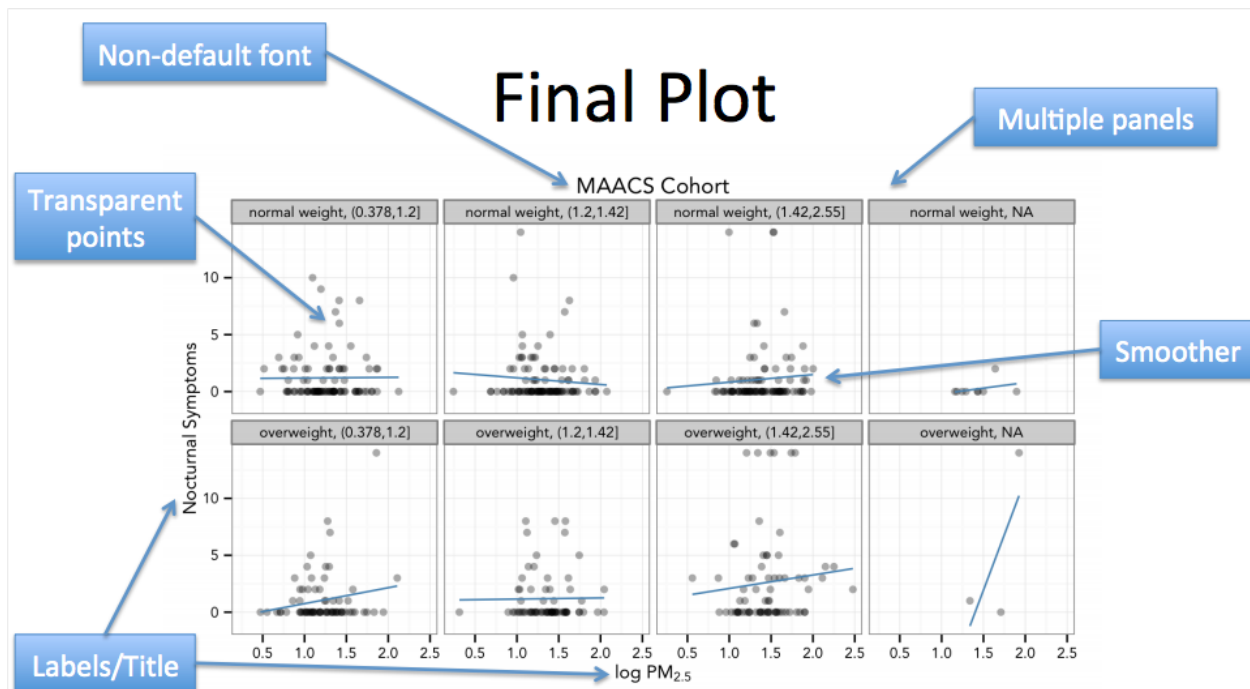
Data variable

– axis limits

- * + `ylim(-3, 3)` → limits the range of y variable to a specific range
 - *Note: ggplot will exclude (not plot) points that fall outside of this range (outliers), potentially leaving gaps in plot*
- * + `coord_cartesian(ylim(-3, 3))` → this will limit the visible range but plot all points of the data

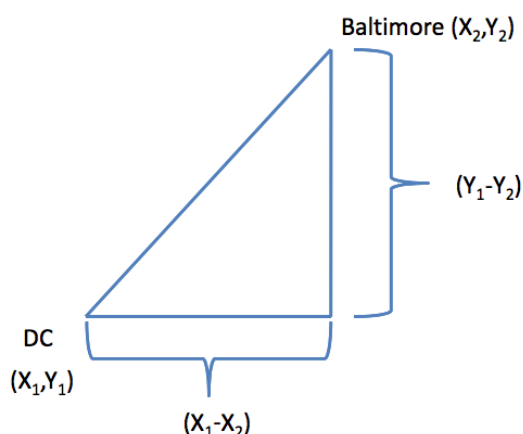
ggplot2 Comprehensive Example

```
# initiates ggplot
g <- ggplot(maacs, aes(logpm25, NocturnalSympt))
g + geom_point(alpha = 1/3)                                # adds points
+ facet_wrap(bmicat ~ no2dec, nrow = 2, ncol = 4)          # make panels
+ geom_smooth(method="lm", se=FALSE, col="steelblue")      # adds smoother
+ theme_bw(base_family = "Avenir", base_size = 10)        # change theme
+ labs(x = expression("log " * PM[2.5]))                  # add labels
+ labs(y = "Nocturnal Symptoms")
+ labs(title = "MAACS Cohort")
```

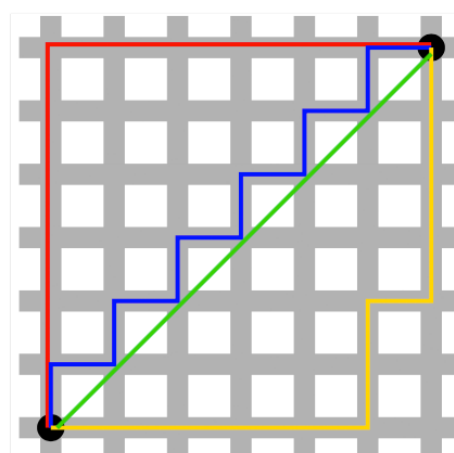


Hierarchical Clustering

- useful for visualizing high dimensional data, organizes things that are close into groups
- **agglomerative approach** (most common) — bottom up
 1. start with data
 2. find closest pairs, put them together (create “super point” and remove original data)
 3. find the next closest
 4. repeat = yields a tree showing order of merging (dendrogram)
 - requires
 - * **merging approach**: how to merge two points
 - * **distance metric**: calculating distance between two points
 - * **continuous** - *Euclidean distance* $\rightarrow \sqrt{(A_1 - A_2)^2 + (B_1 - B_2)^2 + \dots + (Z_1 - Z_2)^2}$
 - * **continuous** - *correlation similarity* \rightarrow how correlated two data points are
 - * **binary** - *manhattan distance* (“city block distance”) $\rightarrow |A_1 - A_2| + |B_1 - B_2| + \dots + |Z_1 - Z_2|$



Euclidean Distance



Binary Distance

Procedure for Constructing Hierarchical Clusters (hclust function)

1. calculate all pair wise distances between all points to see which points are closest together
 - `dist(data.frame(x=x, y=y) \rightarrow returns pair wise distances for all of the (x,y) coordinates`
 - **Note:** `dist()` function uses Euclidean distance by default
2. group two closest points from the calculated distances and merge them to a single point
3. find the next two closest points and merge them, and repeat
4. order of clustering is shown in the dendrogram

Approaches for Merging Points/Clusters

- the approach is specified in the argument `method = "complete"` or `"average"` in `hclust()` function
- **average linkage** \rightarrow taking average of the x and y coordinates for both points/clusters (center of mass effectively)

- **complete linkage** → to measure distance of two clusters, take the two points in the clusters that are the furthest apart
- **Note:** two approaches may produce different results so it's a good idea to use both approaches to validate results

Characteristics of Hierarchical Clustering Algorithms

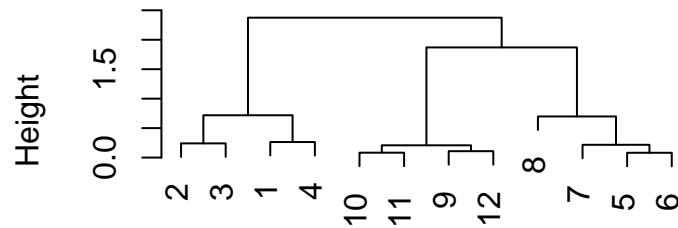
- clustering result/plot maybe **unstable**
 - changing few points/outliers could lead to large changes
 - change different distance metrics to see how sensitive the clustering is
 - change merging strategy
 - scaling of variables could affect the clustering (if one unit/measurement is much larger than another)
- **deterministic** → running the hclust function with same parameters and the same data will produce the same plot
- determining how many clusters there are (where to cut) may **not always be clear**
- **primarily used for exploratory data analysis**, to see over all pattern in data if there is any at all

hclust Function and Example

- `hh <- hclust(dist(dataFrame))` function → produces a hierarchical cluster object based on pair wise distances from a data frame of x and y values
 - `dist()` → defaults to Euclidean, calculates the distance/similarity between two observations; when applied to a data frame, the function applies the $\sqrt{(A_1 - A_2)^2 + (B_1 - B_2)^2 + \dots + (Z_1 - Z_2)^2}$ formula to every pair of rows of data to construct a matrix of distances between the rows
 - * order of the hierarchical cluster is derived from the distance
 - `plot(hh)` → plots the dendrogram
 - automatically sorts column and row according to cluster
 - `names(hh)` → returns all parameters of the hclust object
 - * `hh$order` → returns the order of the rows/clusters from the dendrogram
 - * `hh$dist.method` → returns method for calculating distance/similarity
- **Note:** dendrogram that gets generated **DOES NOT** show how many clusters there are, so cutting (at 2.0 level for example) must be done to determine number of clusters — must be a convenient and sensible point
- **hclust Example**

```
set.seed(1234)
x <- rnorm(12,mean=rep(1:3,each=4),sd=0.2)
y <- rnorm(12,mean=rep(c(1,2,1),each=4),sd=0.2)
dataFrame <- data.frame(x=x,y=y)
distxy <- dist(dataFrame)
hClustering <- hclust(distxy)
plot(hClustering)
```

Cluster Dendrogram



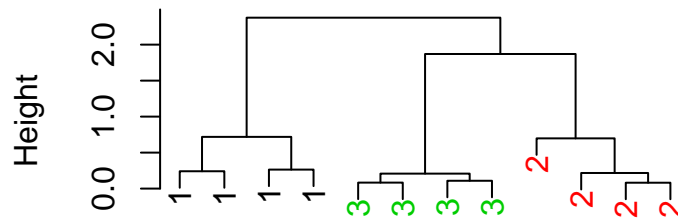
distxy
hclust (*, "complete")

myplcclust Function and Example

- *Note: myplcclust = a function to plot hclust objects in color (clusters labelled 1 2 3 etc.), but must know how many clusters there are initially*

```
myplcclust <- function(hclust, lab = hclust$labels,
  lab.col = rep(1, length(hclust$labels)), hang = 0.1, ...) {
  ## modification of plclust for plotting hclust objects *in colour*! Copyright
  ## Eva KF Chan 2009 Arguments: hclust: hclust object lab: a character vector
  ## of labels of the leaves of the tree lab.col: colour for the labels;
  ## NA=default device foreground colour hang: as in hclust & plclust Side
  ## effect: A display of hierarchical cluster with coloured leaf labels.
  y <- rep(hclust$height, 2)
  x <- as.numeric(hclust$merge)
  y <- y[which(x < 0)]
  x <- x[which(x < 0)]
  x <- abs(x)
  y <- y[order(x)]
  x <- x[order(x)]
  plot(hclust, labels = FALSE, hang = hang, ...)
  text(x = x, y = y[hclust$order] - (max(hclust$height) * hang), labels = lab[hclust$order],
  col = lab.col[hclust$order], srt = 90, adj = c(1, 0.5), xpd = NA, ...)
}
# example
dataFrame <- data.frame(x = x, y = y)
distxy <- dist(dataFrame)
hClustering <- hclust(distxy)
myplcclust(hClustering, lab = rep(1:3, each = 4), lab.col = rep(1:3, each = 4))
```


Cluster Dendrogram



```
distxy
hclust (*, "complete")
```

heatmap Function and Example

- `heatmap(data.matrix)` function -> similar to `image(t(x))`
 - good for visualizing high-dimension matrix data, runs hierarchical analysis on rows and columns of table
 - yellow = high value, red = low value
 - **Note:** the input must be a numeric matrix, so `as.matrix(data.frame)` can be used to convert if necessary
- *example*

```
set.seed(12345)
data <- matrix(rnorm(400), nrow = 40)
heatmap(data)
```

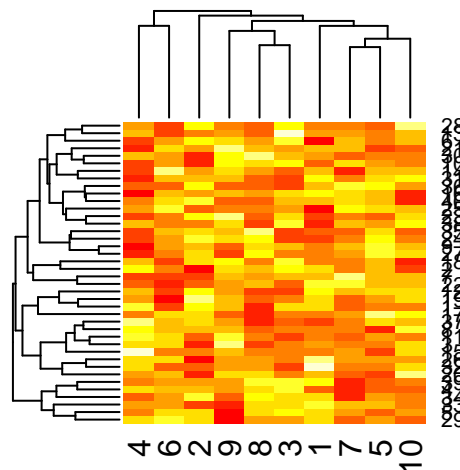
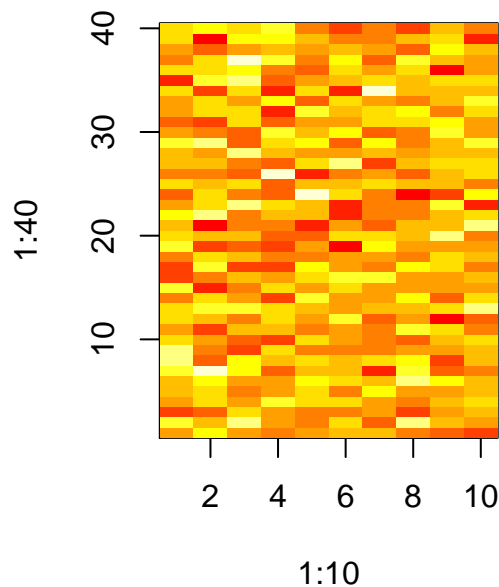


image Function and Example

- `image(x, y, t(dataMatrix)[, nrow(dataMatrix):1])` -> produces similar color grid plot as the `heatmap()` without the dendrograms

- `t(dataMatrix)[, nrow(dataMatrix)]`
 - * `t(dataMatrix)` -> transpose of dataMatrix, this is such that the plot will be displayed in the same fashion as the matrix (rows as values on the y axis and columns as values on the x axis)
 - *example* 40 x 10 matrix will have graph the 10 columns as x values and 40 rows as y values
 - * `[, nrow(dataMatrix)]` -> subsets the data frame in reverse column order; when combined with the `t()` function, it reorders the rows of data from 40 to 1, such that the data from the matrix is displayed in order from top to bottom
 - *Note: without this statement the rows will be displayed in order from bottom to top, as that is in line with the positive y axis*
- `x, y` -> used to specify the values displayed on the x and y axis
 - * *Note: must be in increasing order*
- *example*

```
image(1:10, 1:40, t(data)[, nrow(data):1])
```



K-means Clustering

- similar to hierarchical clustering, focuses on finding things that are close together
 - define close, groups, visualizing/interpreting grouping
- **partitioning approach**
 1. set number of clusters initially
 2. find centroids for each cluster
 3. assign points to the closest centroid
 4. recalculate centroid
 5. repeat = yields estimate of cluster centroids and which cluster each point belongs to
 - **requires**
 - * distance metric
 - * initial number of clusters
 - * initial guess as to where the cluster centroids are

Procedure for Constructing K-means Clusters (`kmeans` function)

1. choose three random points as the starting centroids
2. take each of the data points and assign it to the closest centroid (creating a cluster around each starting point)
3. take each cluster and recalculate the centroid (taking the mean) with its enclosed data points
4. repeat step 2 and 3 (reassign points to centroids and update centroid locations) until a stable result is achieved

- *example*

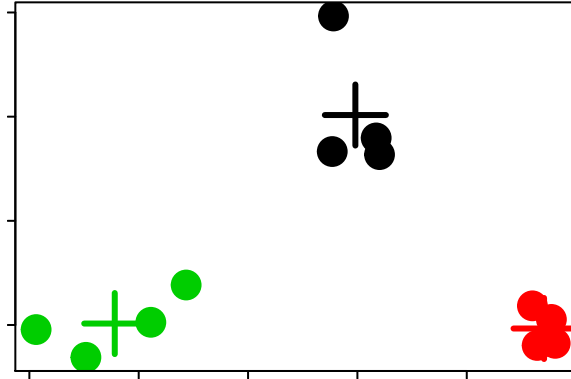
```
set.seed(1234)
x <- rnorm(12,mean=rep(1:3,each=4),sd=0.2)
y <- rnorm(12,mean=rep(c(1,2,1),each=4),sd=0.2)
dataFrame <- data.frame(x=x,y=y)
# specifies initial number of clusters to be 3
kmeansObj <- kmeans(dataFrame,centers=3)
names(kmeansObj)
```

```
## [1] "cluster"      "centers"      "totss"       "withinss"
## [5] "tot.withinss" "betweenss"   "size"       "iter"
## [9] "ifault"
```

```
# returns cluster assignments
kmeansObj$cluster
```

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

```
par(mar=rep(0.2,4))
plot(x,y,col=kmeansObj$cluster,pch=19,cex=2)
points(kmeansObj$centers,col=1:3,pch=3,cex=3,lwd=3)
```



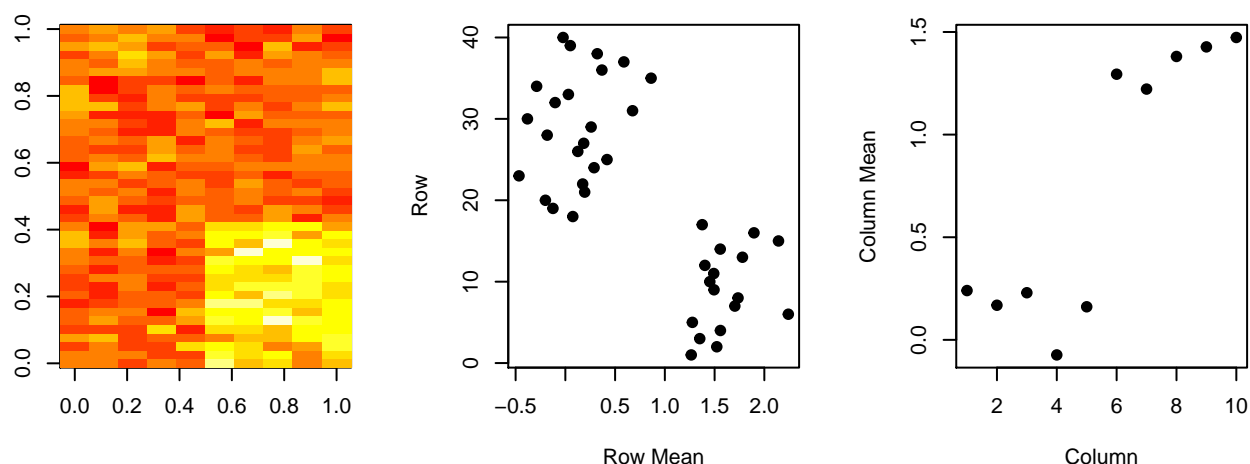
Characteristics of K-means Clustering Algorithms

- requires number of clusters initially
 - pick by eye/intuition
 - pick by cross validation/information theory, etc. [\[link\]](#)
- not deterministic (starting points chosen at random)
 - useful to run the algorithms a few times with different starting points to validate results

Dimension Reduction

- two kinds of problems that relate to high-dimension dataset/matrix with many variables
 1. find a new set (smaller) of variables that are uncorrelated and explain as much variance of data as possible
 - normally many variables are not independent (i.e. height vs weight)
 - statistical problem, commonly solved with PCA
 2. find a lower rank matrix (best matrix created with fewer variables) that still explains the data
 - data compression problem, commonly solved SVD
- *example*
 - **Note:** we are arbitrarily introduced pattern in data: we flip a coin and if the it is heads, we replace the row with $[0, 0, 0, 0, 0, 3, 3, 3, 3, 3]$
 - here we plot the patterns in rows and columns (already sorted)

```
for(i in 1:40){  
  # flip a coin  
  coinFlip <- rbinom(1,size=1,prob=0.5)  
  # if coin is heads add a common pattern to that row  
  if(coinFlip){  
    data[i,] <- data[i,] + rep(c(0,3),each=5)  
  }  
}  
  
# hierarchical clustering  
hh <- hclust(dist(data))  
dataOrdered <- data[hh$order,]  
# create 1 x 3 panel plot  
par(mfrow=c(1,3))  
# heat map (sorted)  
image(t(dataOrdered)[,nrow(dataOrdered):1])  
# row means (40 rows)  
plot(rowMeans(dataOrdered),40:1,,xlab="Row Mean",ylab="Row",pch=19)  
# column means (10 columns)  
plot(colMeans(dataOrdered),xlab="Column",ylab="Column Mean",pch=19)
```



Singular Value Decomposition (SVD)

- Let X = matrix which each variable in column (measurement) and each observation in row (subject)
- SVD in this case is a **matrix decomposition** process, in which X is divided into *three* separate matrices as follows:

$$X = UDV^T$$

- U = left singular vector, orthogonal matrix (columns independent of each other)
- D = singular values, diagonal matrix
- V = right singular vector, orthogonal matrix (columns independent of each other)
- **Note:** *orthogonal implies that a matrix is always invertible [$A^{-1} = A^T$] and that the product of the matrix and its transpose equals the identity matrix [$AA^T = I$]*
 - * when a orthogonal matrices, A , is multiplied by another matrix, B , it is effectively a linear transformation in that the length and angles of B are preserved
- **Note:** *diagonal implies that any value outside of the main diagonal (\searrow) = 0*
 - * example

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{bmatrix}$$

- **Note:** *scale of data matters for SVD/PCA (scaling the data may help), patterns detected maybe mixed together, and computation is intensive for these operations*

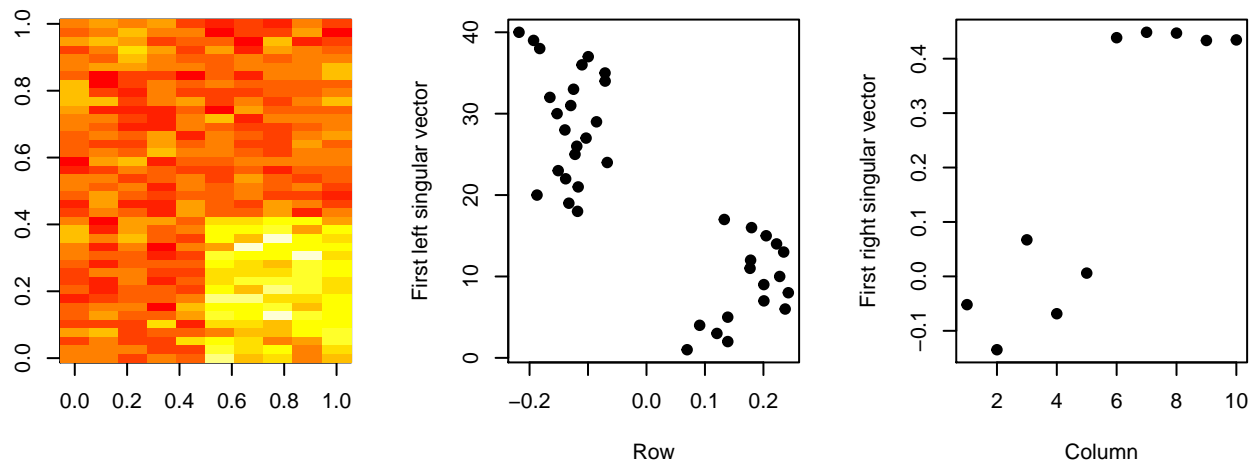
Principal Components Analysis (PCA)

- first scale the variables and run SVD on normalized matrix
 - **scaling** = subtract each column by its mean and divide by its standard deviation
- **principal components** = the right singular values or the V matrix

SVD and PCA Example

- **U and V Matrices**
 - `s <- svd(data)` = performs SVD on data ($n \times m$ matrix) and splits it into u , v , and d matrices
 - * `s$u` = $n \times m$ matrix \rightarrow horizontal variation
 - * `s$d` = $1 \times m$ vector \rightarrow vector of the singular/diagonal values
 - `diag(s$d)` = $m \times m$ diagonal matrix
 - * `s$v` = $m \times m$ matrix \rightarrow vertical variation
 - * `s$u %*% diag(s$d) %*% t(s$v)` returns the original data $\rightarrow X = UDV^T$
 - `scale(data)` = scales the original data by subtracting each datapoint by its column mean and dividing by its column standard deviation

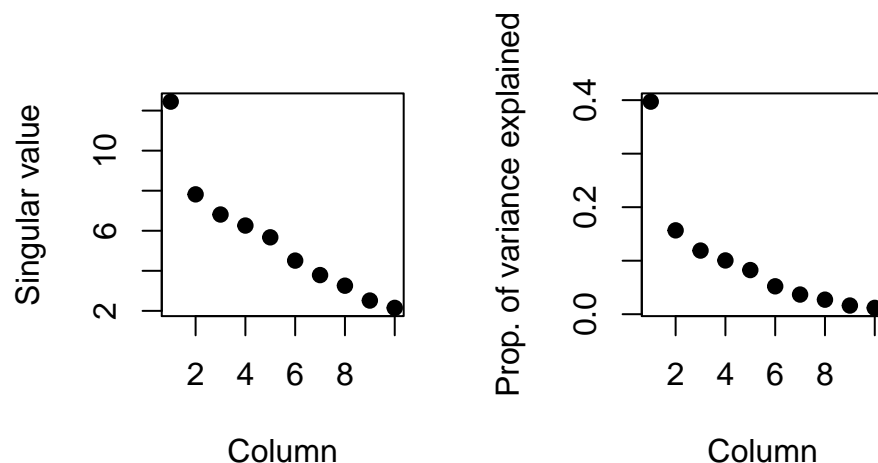
```
# running svd
svd1 <- svd(scale(dataOrdered))
# create 1 by 3 panel plot
par(mfrow=c(1,3))
# data heatmap (sorted)
image(t(dataOrdered)[,nrow(dataOrdered):1])
# U Matrix - first column
plot(svd1$u[,1],40:1,,xlab="Row",ylab="First left singular vector",pch=19)
# V vector - first column
plot(svd1$v[,1],xlab="Column",ylab="First right singular vector",pch=19)
```



- **D Matrix and Variance Explained**

- *d* matrix (`s$d` vector) captures the singular values, or *variation in data that is explained by that particular component* (variable/column/dimension)
- **proportion of variance Explained** = converting the singular values to variance (square the values) and divide by the total variance (sum of the squared singular values)
 - * effectively the same pattern as the singular values, just converted to percentage
 - * in this case, the first component/dimension, which captures the shift in means (see previous plot) of SVD captures about 40% of the variation

```
# create 1 x 2 panel plot
par(mfrow=c(1,2))
# plot singular values
plot(svd1$d, xlab="Column", ylab="Singular value", pch=19)
# plot proportion of variance explained
plot(svd1$d^2/sum(svd1$d^2), xlab="Column", ylab="Prop. of variance explained", pch=19)
```

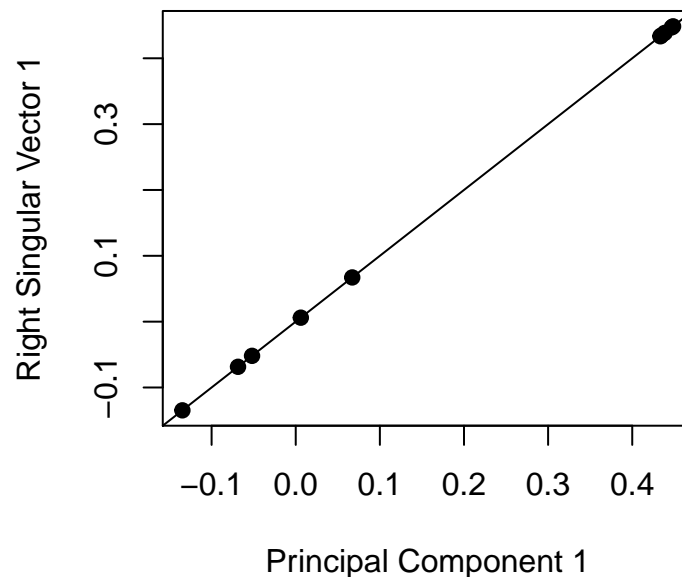


- **Relationship to PCA**

- `p <- prcomp(data, scale = TRUE)` = performs PCA on data specified
 - * `scale = TRUE` = scales the data before performing PCA
 - * returns `prcomp` object

- * `summary(p)` = prints out the principal component's standard deviation, proportion of variance, and cumulative proportion
- PCA's rotation vectors are equivalent to their counterparts in the V matrix from the SVD

```
# SVD
svd1 <- svd(scale(dataOrdered))
# PCA
pca1 <- prcomp(dataOrdered,scale=TRUE)
# Plot the rotation from PCA (Principal Components) vs v vector from SVD
plot(pca1$rotation[,1],svd1$v[,1],pch=19,xlab="Principal Component 1",
     ylab="Right Singular Vector 1")
abline(c(0,1))
```



```
# summarize PCA
summary(pca1)
```

```
## Importance of components:
##          PC1      PC2      PC3      PC4      PC5      PC6      PC7
## Standard deviation  1.9930  1.2518  1.0905  1.0024  0.90836  0.72211  0.60630
## Proportion of Variance 0.3972  0.1567  0.1189  0.1005  0.08251  0.05214  0.03676
## Cumulative Proportion 0.3972  0.5539  0.6728  0.7733  0.85582  0.90797  0.94473
##          PC8      PC9      PC10
## Standard deviation  0.52145  0.40286  0.34423
## Proportion of Variance 0.02719  0.01623  0.01185
## Cumulative Proportion 0.97192  0.98815  1.00000
```

• More Complex Patterns

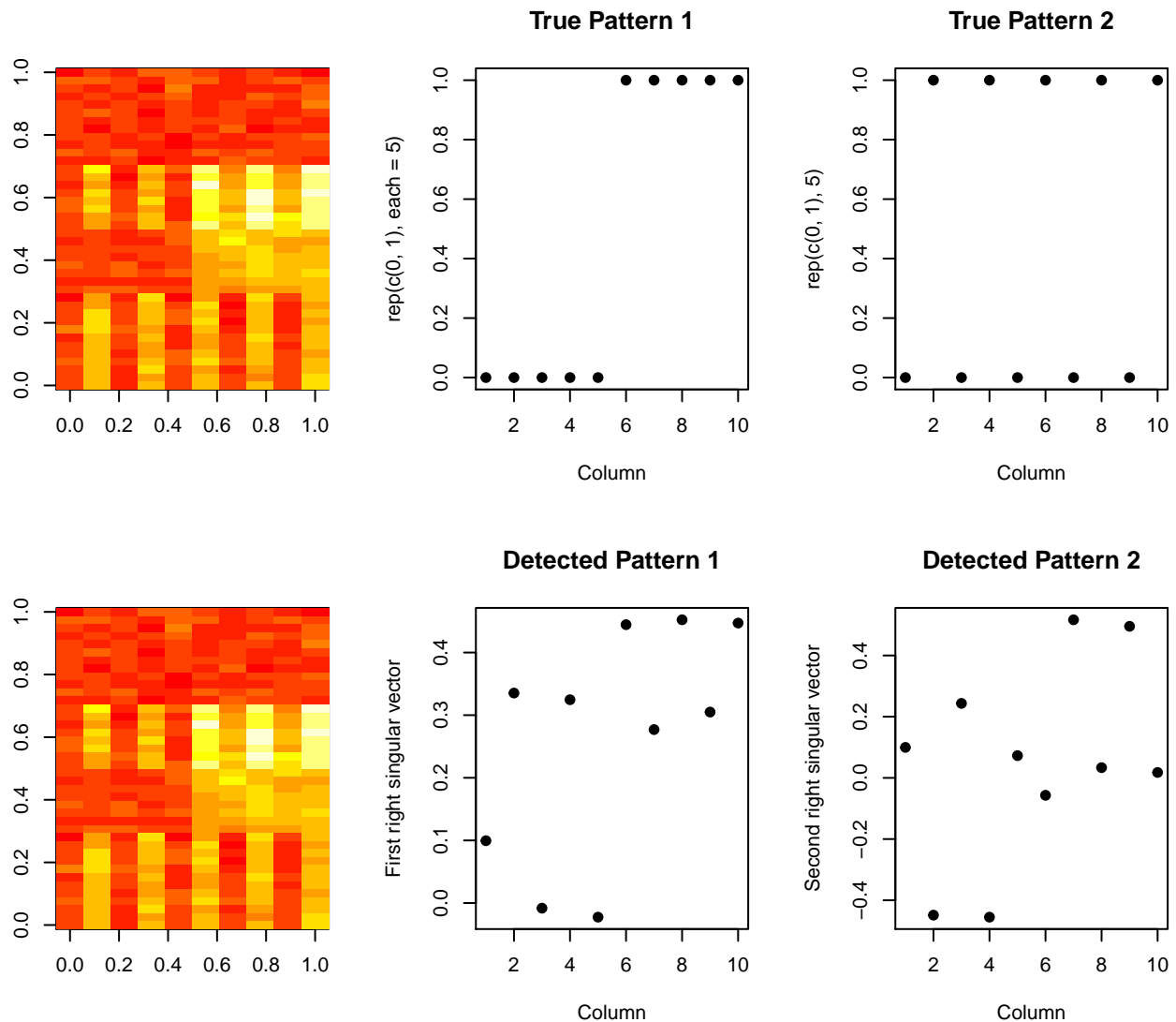
- SVD can be used to *detect unknown patterns* within the data (we rarely know the true distribution/pattern about the population we're analyzing)
- however, it may be hard to pinpoint exact patterns as the principal components may confound each other
 - * in the example below, you can see that the two principal components that capture the most variation have both horizontal shifts and alternating patterns captured in them


```

set.seed(678910)
# setting pattern
data <- matrix(rnorm(400), nrow = 40)
for(i in 1:40){
  # flip a coin
  coinFlip1 <- rbinom(1,size=1,prob=0.5)
  coinFlip2 <- rbinom(1,size=1,prob=0.5)
  # if coin is heads add a common pattern to that row
  if(coinFlip1){
    data[i,] <- data[i,] + rep(c(0,5),each=5)
  }
  if(coinFlip2){
    data[i,] <- data[i,] + rep(c(0,5),5)
  }
}
hh <- hclust(dist(data)); dataOrdered <- data[hh$order,]

# perform SVD
svd2 <- svd(scale(dataOrdered))
par(mfrow=c(2,3))
image(t(dataOrdered)[,nrow(dataOrdered):1])
plot(rep(c(0,1),each=5),pch=19,xlab="Column", main="True Pattern 1")
plot(rep(c(0,1),5),pch=19,xlab="Column",main="True Pattern 2")
image(t(dataOrdered)[,nrow(dataOrdered):1])
plot(svd2$v[,1],pch=19,xlab="Column",ylab="First right singular vector",
     main="Detected Pattern 1")
plot(svd2$v[,2],pch=19,xlab="Column",ylab="Second right singular vector",
     main="Detected Pattern 2")

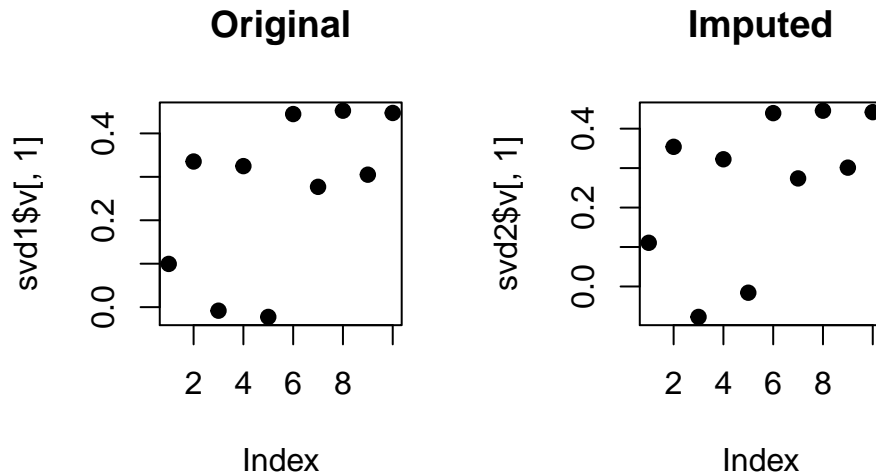
```



• Missing Data

- SVD cannot be performed on dataset with NA values
- `impute` package from [Bioconductor](http://bioconductor.org) can help approximate missing values from surrounding values
 - * `impute.knn` function takes the missing row and imputes the data using the k nearest neighbors to that row
 - $k=10$ = default value (take the nearest 10 rows)

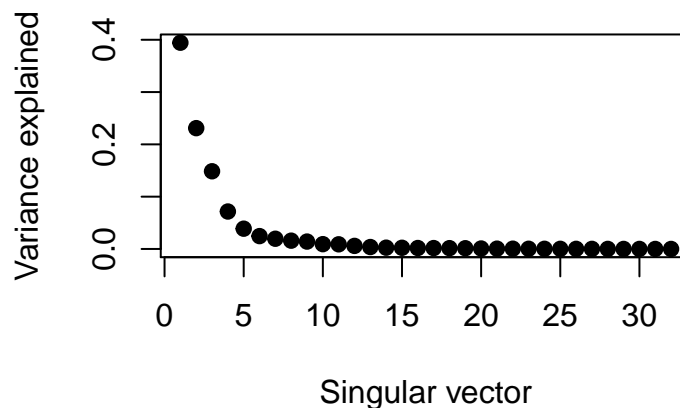
```
library(impute) ## Available from http://bioconductor.org
data2 <- dataOrdered
# set random samples = NA
data2[sample(1:100,size=40,replace=FALSE)] <- NA
data2 <- impute.knn(data2)$data
svd1 <- svd(scale(dataOrdered)); svd2 <- svd(scale(data2))
par(mfrow=c(1,2))
plot(svd1$v[,1],pch=19, main="Original")
plot(svd2$v[,1],pch=19, main="Imputed")
```



Create Approximations/Data Compression

- SVD can be used to create lower rank representation, or compressed representation of data
- if we look at the variance explained plot below, *most of the variation* is explained by the *first few principal components*

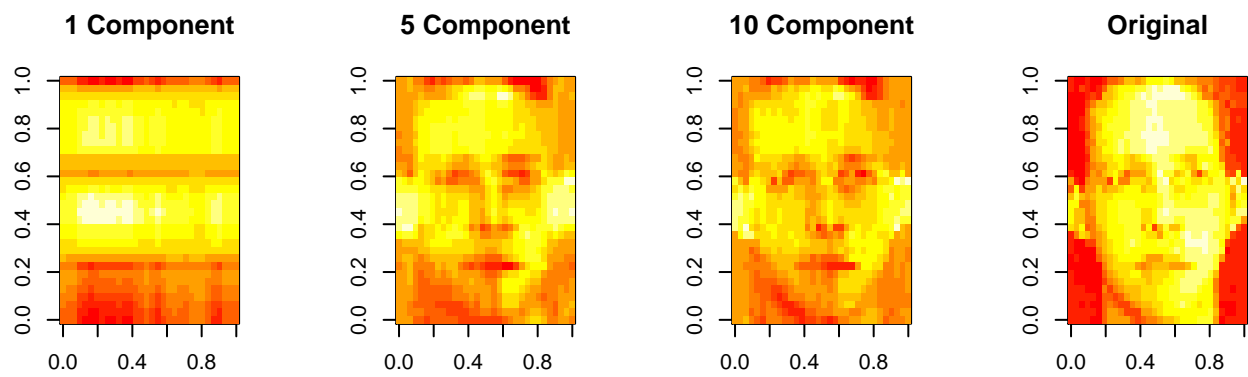
```
# load faceData
load("figures/face.rda")
# perform SVD
svd3 <- svd(scale(faceData))
plot(svd3$d^2/sum(svd3$d^2), pch=19, xlab="Singular vector", ylab="Variance explained")
```



- approximations can thus be created by taking the first few components and using matrix multiplication with the corresponding U , V , and D components

```
approx1 <- svd3$u[,1] %*% t(svd3$v[,1]) * svd3$d[1]
approx5 <- svd3$u[,1:5] %*% diag(svd3$d[1:5]) %*% t(svd3$v[,1:5])
approx10 <- svd3$u[,1:10] %*% diag(svd3$d[1:10]) %*% t(svd3$v[,1:10])
# create 1 x 4 panel plot
par(mfrow=c(1,4))
# plot original facedata
image(t(approx1)[,nrow(approx1):1], main = "1 Component")
image(t(approx5)[,nrow(approx5):1], main = "5 Component")
```

```
image(t(approx10)[,nrow(approx10):1], main = "10 Component")  
image(t(faceData)[,nrow(faceData):1], main = "Original")
```



Color Packages in R Plots

- proper use of color can help convey the message by improving clarity/contrast of data presented
- default color schemes for most plots in R are fairly terrible, so some external packages are helpful

grDevices Package

- `colors()` function = lists names of colors available in any plotting function
- **colorRamp function**
 - takes any set of colors and return a function that takes values between 0 and 1, indicating the extremes of the color palette (e.g. see the `gray` function)
 - `pal <- colorRamp(c("red", "blue"))` = defines a `colorRamp` function
 - `pal(0)` returns a 1 x 3 matrix containing values for RED, GREEN, and BLUE values that range from 0 to 255
 - `pal(seq(0, 1, len = 10))` returns a 10 x 3 matrix of 10 colors that range from RED to BLUE (two ends of spectrums defined in the object)
 - *example*

```
# define colorRamp function
pal <- colorRamp(c("red", "blue"))
# create a color
pal(0.67)
```

```
##      [,1] [,2] [,3]
## [1,] 84.15  0 170.85
```

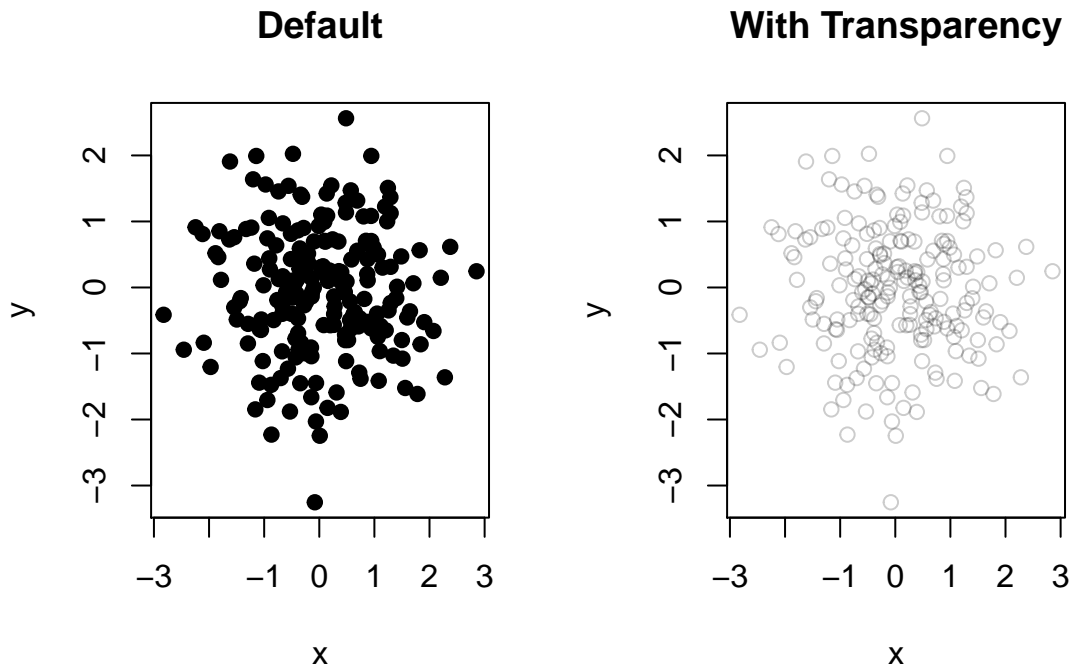
- **colorRampPalette function**
 - takes any set of colors and return a function that takes integer arguments and returns a vector of colors interpolating the palette (like `heat.colors` or `topo.colors`)
 - `pal <- colorRampPalette(c("red", "yellow"))` defines a `colorRampPalette` function
 - `pal(10)` returns 10 interpolated colors in hexadecimal format that range between the defined ends of spectrums
 - *example*

```
# define colorRampPalette function
pal <- colorRampPalette(c("red", "yellow"))
# create 10 colors
pal(10)
```

```
## [1] "#FF0000" "#FF1C00" "#FF3800" "#FF5500" "#FF7100" "#FF8D00" "#FFAA00"
## [8] "#FFC600" "#FFE200" "#FFFF00"
```

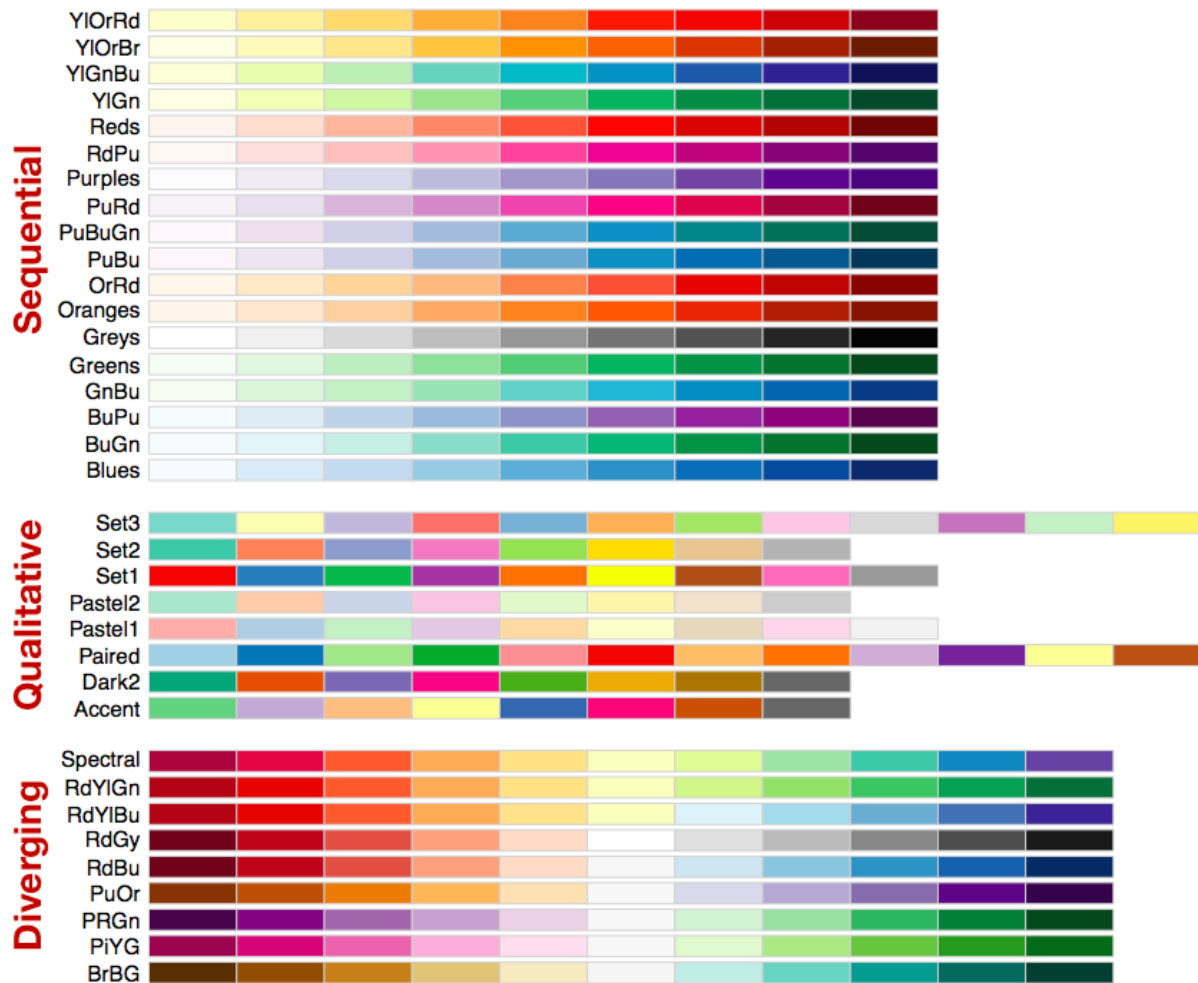
- **rgb function**
 - `red`, `green`, and `blue` arguments = values between 0 and 1
 - `alpha = 0.5` = transparency control, values between 0 and 1
 - returns hexadecimal string for color that can be used in `plot/image` commands
 - `colorspace` package can be used for different control over colors
 - *example*

```
x <- rnorm(200); y <- rnorm(200)
par(mfrow=c(1,2))
# normal scatter plot
plot(x, y, pch = 19, main = "Default")
# using transparency shows data much better
plot(x, y, col = rgb(0, 0, 0, 0.2), main = "With Transparency")
```



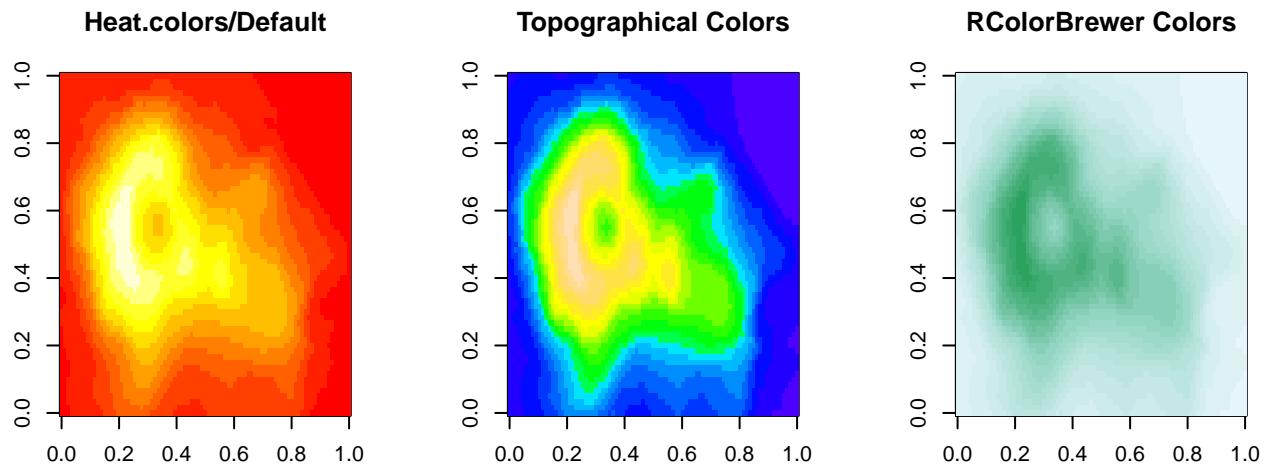
RColorBrewer Package

- can be found on CRAN that has predefined color palettes
 - `library(RColorBrewer)`
- **types of palettes**
 - *Sequential* = numerical/continuous data that is ordered from low to high
 - *Diverging* = data that deviate from a value, increasing in two directions (i.e. standard deviations from the mean)
 - *Qualitative* = categorical data/factor variables
- palette information from the RColorBrewer package can be used by `colorRamp` and `colorRampPalette` functions
- available colors palletes



- `brewer.pal(n, "BuGn")` function
 - `n` = number of colors to generated
 - "BuGn" = name of palette
 - * `?brewer.pal` list all available palettes to use
 - returns list of `n` hexadecimal colors
- *example*

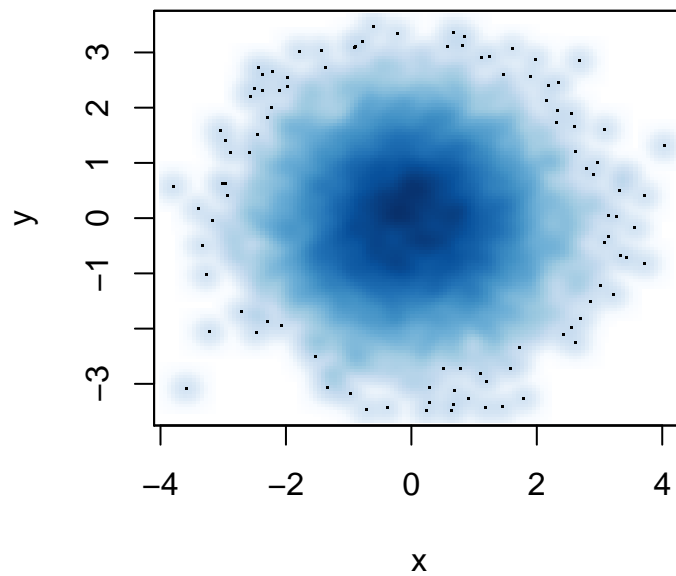
```
library(RColorBrewer)
# generate 3 colors using brewer.pal function
cols <- brewer.pal(3, "BuGn")
pal <- colorRampPalette(cols)
par(mfrow=c(1,3))
# heat.colors/default
image(volcano, main = "Heat.colors/Default")
# topographical colors
image(volcano, col = topo.colors(20), main = "Topographical Colors")
# RColorBrewer colors
image(volcano, col = pal(20), main = "RColorBrewer Colors")
```



- **smoothScatter** function

- used to plot large quantities of data points
- creates 2D histogram of points and plots the histogram
- default color scheme = “Blues” palette from RColorBrewer package
- *example*

```
x <- rnorm(10000); y <- rnorm(10000)
smoothScatter(x, y)
```



Case Study: Human Activity Tracking with Smart Phones

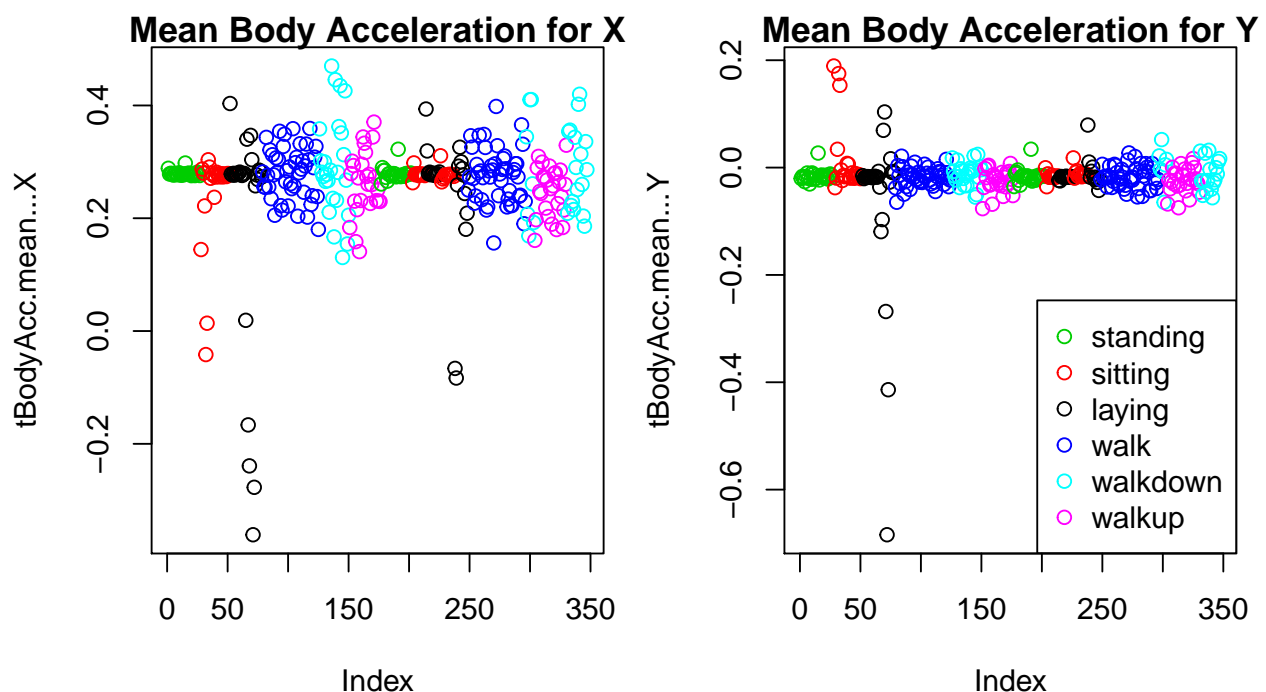
Loading Training Set of Samsung S2 Data from [UCI Repository](#)

```
# load data frame provided
load("samsungData.rda")
# table of 6 types of activities
table(samsungData$activity)
```

```
##
##   laying  sitting standing   walk walkdown  walkup
##    1407    1286    1374    1226     986    1073
```

Plotting Average Acceleration for First Subject

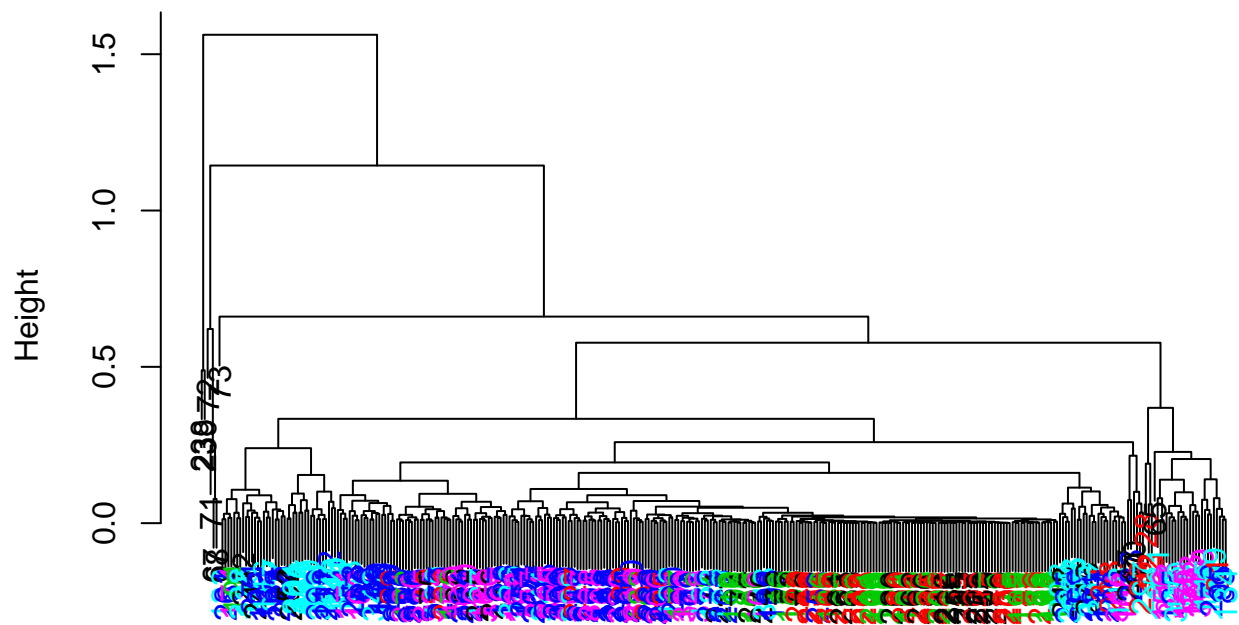
```
# set up 1 x 2 panel plot
par(mfrow=c(1, 2), mar = c(5, 4, 1, 1))
# converts activity to a factor variable
samsungData <- transform(samsungData, activity = factor(activity))
# find only the subject 1 data
sub1 <- subset(samsungData, subject == 1)
# plot mean body acceleration in X direction
plot(sub1[, 1], col = sub1$activity, ylab = names(sub1)[1],
     main = "Mean Body Acceleration for X")
# plot mean body acceleration in Y direction
plot(sub1[, 2], col = sub1$activity, ylab = names(sub1)[2],
     main = "Mean Body Acceleration for Y")
# add legend
legend("bottomright", legend=unique(sub1$activity), col=unique(sub1$activity), pch = 1)
```



Clustering Based on Only Average Acceleration

```
# load myplclust function
source("myplclust.R")
# calculate distance matrix
distanceMatrix <- dist(sub1[,1:3])
# form hclust object
hclustering <- hclust(distanceMatrix)
# run myplclust on data
myplclust(hclustering, lab.col = unclass(sub1$activity))
```

Cluster Dendrogram

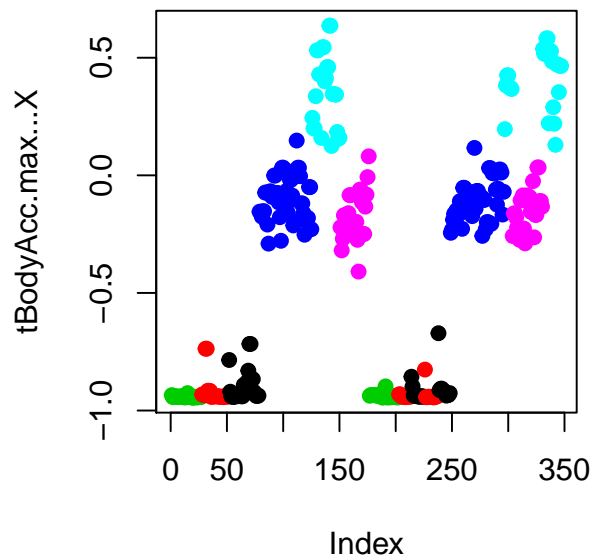


distanceMatrix
hclust (*, "complete")

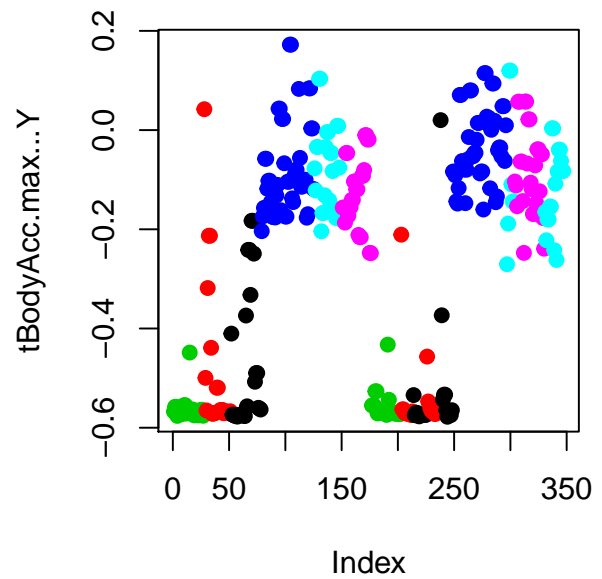
Plotting Max Acceleration for the First Subject

```
# create 1 x 2 panel
par(mfrow=c(1,2))
# plot max accelerations in x and y direction
plot(sub1[,10], pch=19, col=sub1$activity, ylab=names(sub1)[10],
     main = "Max Body Acceleration for X")
plot(sub1[,11], pch=19, col = sub1$activity, ylab=names(sub1)[11],
     main = "Max Body Acceleration for Y")
```

Max Body Acceleration for X



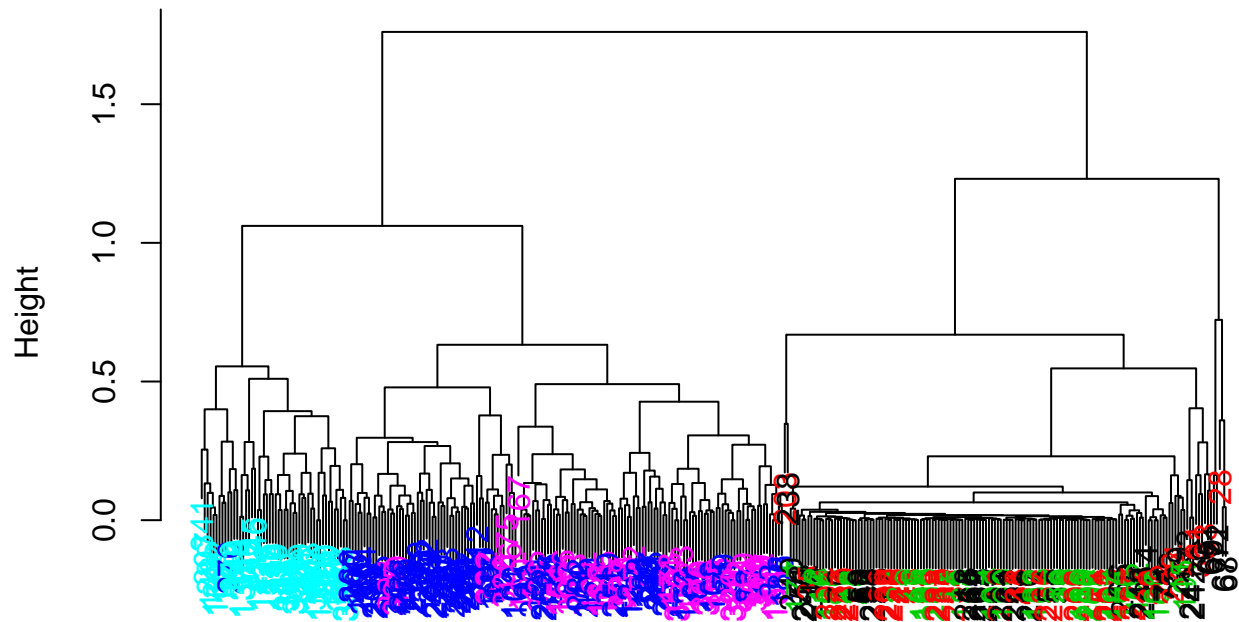
Max Body Acceleration for Y



Clustering Based on Maximum Acceleration

```
# calculate distance matrix for max distances
distanceMatrix <- dist(sub1[,10:12])
hclustering <- hclust(distanceMatrix)
myplclust(hclustering, lab.col=unclass(sub1$activity))
```

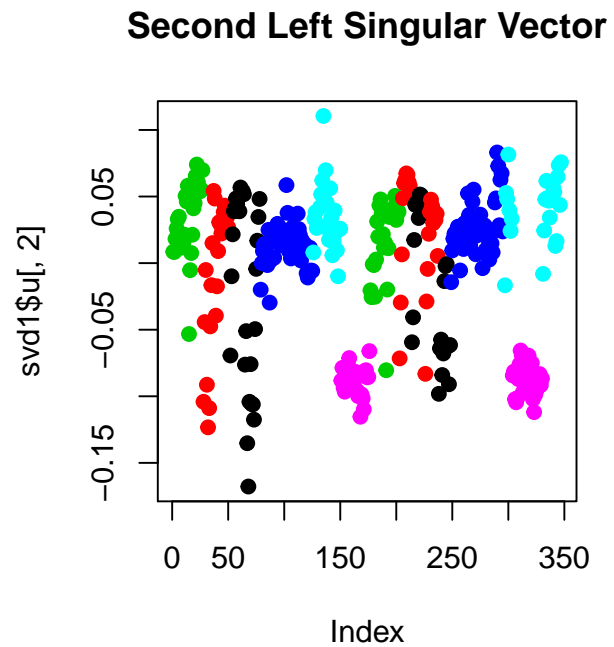
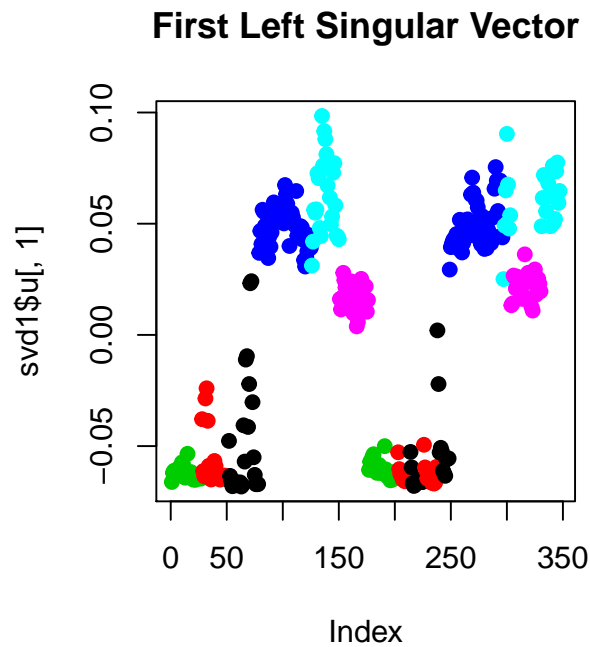
Cluster Dendrogram



distanceMatrix
hclust (*, "complete")

Singular Value Decomposition

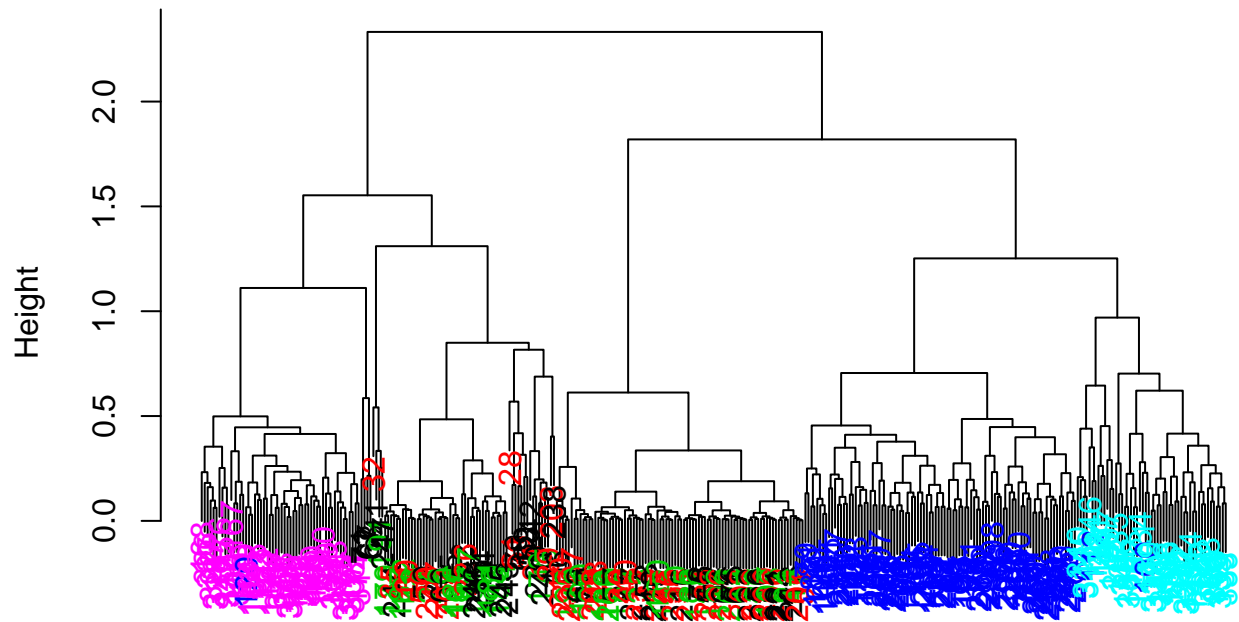
```
# perform SVD minus last two columns (subject and activity)
svd1 = svd(scale(sub1[, -c(562, 563)]))
# create 1 x 2 panel plot
par(mfrow=c(1, 2))
# plot first two left singular vector
# separate moving from non moving
plot(svd1$u[, 1], col=sub1$activity, pch=19, main = "First Left Singular Vector")
plot(svd1$u[, 2], col=sub1$activity, pch=19, main = "Second Left Singular Vector")
```



New Clustering with Maximum Contributors

```
# find the max contributing feature
maxContrib <- which.max(svd1$v[,2])
# recalculate distance matrix
distanceMatrix <- dist(sub1[, c(10:12,maxContrib)])
hclustering <- hclust(distanceMatrix)
myplclust(hclustering,lab.col=unclass(sub1$activity))
```

Cluster Dendrogram



distanceMatrix
hclust (*, "complete")

```
# name of max contributing factor
names(samsungData)[maxContrib]
```

```
## [1] "fBodyAcc.meanFreq...Z"
```

K-means Clustering (nstart=1, first try)

```
# specify 6 centers for data
kClust <- kmeans(sub1[, -c(562, 563)], centers=6)
# tabulate 6 clusteres against 6 activity but many clusters contain multiple activities
table(kClust$cluster, sub1$activity)
```

```
##
##      laying sitting standing walk walkdown walkup
##  1         0         0         0    95         0         0
##  2        16        12         7     0         0         0
##  3        24        33        46     0         0         0
##  4        10         2         0     0         0         0
##  5         0         0         0     0        49         0
##  6         0         0         0     0         0        53
```

K-means clustering (nstart=100, first try)

```
# run k-means algorithm 100 times
kClust <- kmeans(sub1[, -c(562, 563)], centers=6, nstart=100)
# tabulate results
table(kClust$cluster, sub1$activity)
```

```
##
##      laying sitting standing walk walkdown walkup
##  1         0      37       51    0         0      0
##  2         3        0        0    0         0     53
##  3        18       10        2    0         0      0
##  4         0        0        0    0        49      0
##  5        29        0        0    0         0      0
##  6         0        0        0   95         0      0
```

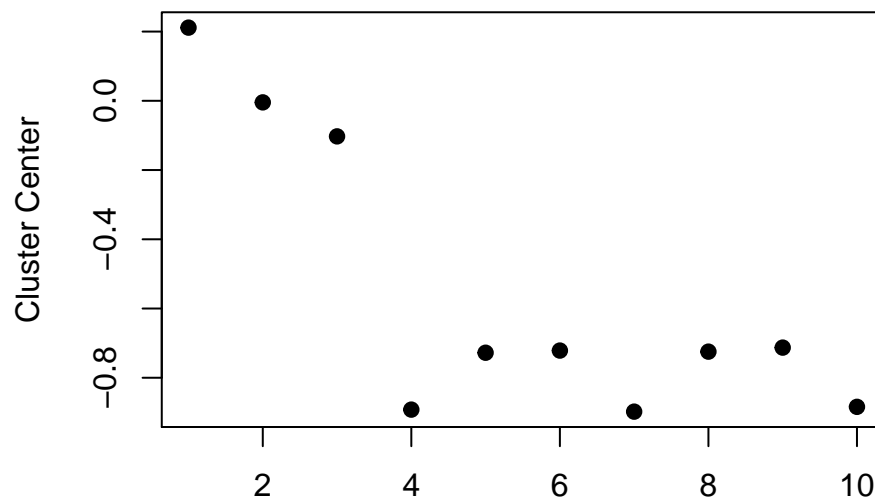
K-means clustering (nstart=100, second try)

```
# run k-means algorithm 100 times
kClust <- kmeans(sub1[, -c(562, 563)], centers=6, nstart=100)
# tabulate results
table(kClust$cluster, sub1$activity)
```

```
##
##      laying sitting standing walk walkdown walkup
##  1        18       10        2    0         0      0
##  2         0        0        0    0        49      0
##  3        29        0        0    0         0      0
##  4         0       37       51    0         0      0
##  5         0        0        0   95         0      0
##  6         3        0        0    0         0     53
```

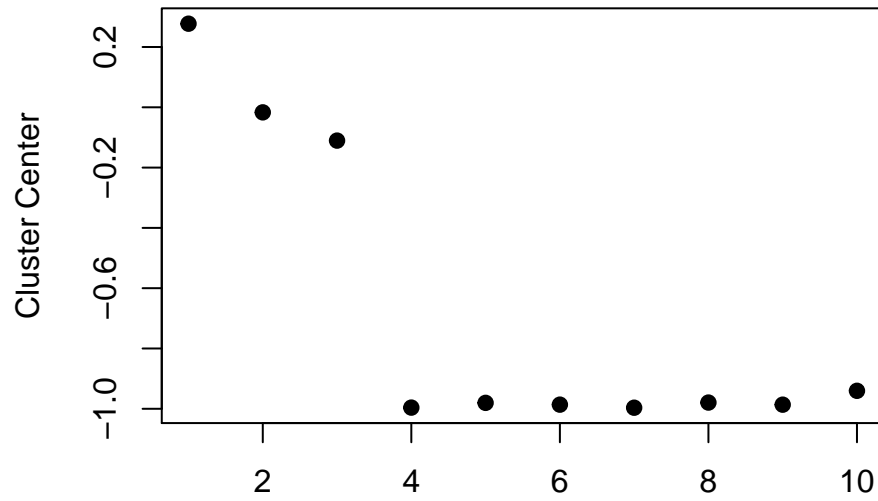
Cluster 1 Variable Centers (Laying)

```
# plot first 10 centers of k-means for laying to understand which features drive the activity
plot(kClust$center[1, 1:10], pch=19, ylab="Cluster Center", xlab="")
```



Cluster 2 Variable Centers (Walking)

```
# plot first 10 centers of k-means for laying to understand which features drive the activity  
plot(kClust$center[4,1:10],pch=19,ylab="Cluster Center",xlab="")
```



Case Study: Fine Particle Pollution in the U.S. from 1999 to 2012

Read Raw Data from 1999 and 2012

```
# read in raw data from 1999
pm0 <- read.table("pm25_data/RD_501_88101_1999-0.txt", comment.char = "#", header = FALSE, sep = "|", na
# read in headers/column labels
cnames <- readLines("pm25_data/RD_501_88101_1999-0.txt", 1)
# convert string into vector
cnames <- strsplit(substring(cnames, 3), "|", fixed = TRUE)
# make vector the column names
names(pm0) <- make.names(cnames[[1]])
# we are interested in the pm2.5 readings in the "Sample.Value" column
x0 <- pm0$Sample.Value
# read in the data from 2012
pm1 <- read.table("pm25_data/RD_501_88101_2012-0.txt", comment.char = "#", header = FALSE, sep = "|",
  na.strings = "", nrow = 1304290)
# make vector the column names
names(pm1) <- make.names(cnames[[1]])
# take the 2012 data for pm2.5 readings
x1 <- pm1$Sample.Value
```

Summaries for Both Periods

```
# generate 6 number summaries
summary(x1)
```

```
##      Min. 1st Qu.  Median    Mean 3rd Qu.    Max.     NA's
## -10.00    4.00    7.63    9.14   12.00   909.00   73133
```

```
summary(x0)
```

```
##      Min. 1st Qu.  Median    Mean 3rd Qu.    Max.     NA's
##      0.00    7.20   11.50   13.74   17.90   157.10   13217
```

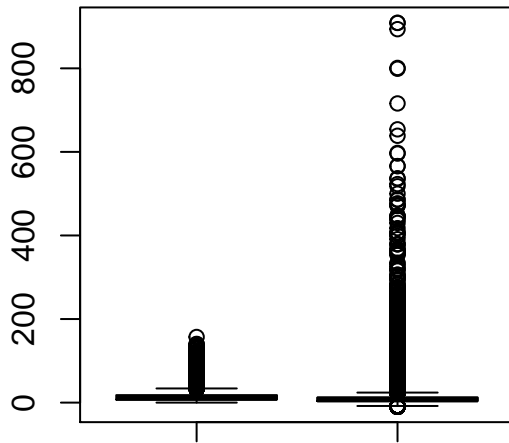
```
# calculate % of missing values, Are missing values important here?
data.frame(NA.1990 = mean(is.na(x0)), NA.2012 = mean(is.na(x1)))
```

```
##      NA.1990    NA.2012
## 1 0.1125608 0.05607125
```

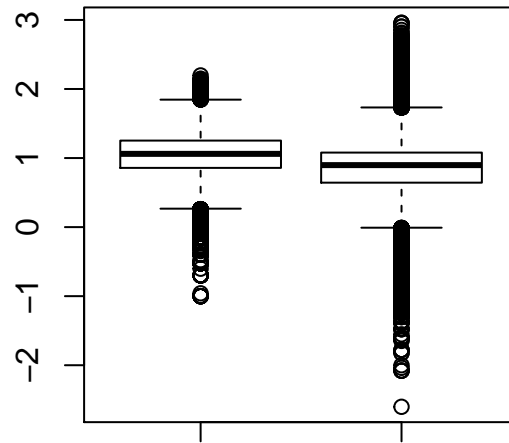
Make a boxplot of both 1999 and 2012

```
par(mfrow = c(1,2))
# regular boxplot, data too right skewed
boxplot(x0, x1, main = "Regular Boxplot")
# log boxplot, significant difference in means, but more spread
boxplot(log10(x0), log10(x1), main = "log Boxplot")
```

Regular Boxplot



log Boxplot



Check for Negative Values in 'x1'

```
# summary again
summary(x1)
```

```
##      Min. 1st Qu.  Median    Mean 3rd Qu.    Max.     NA's
## -10.00   4.00   7.63   9.14  12.00  909.00   73133
```

```
# create logical vector for
negative <- x1 < 0
# count number of negatives
sum(negative, na.rm = T)
```

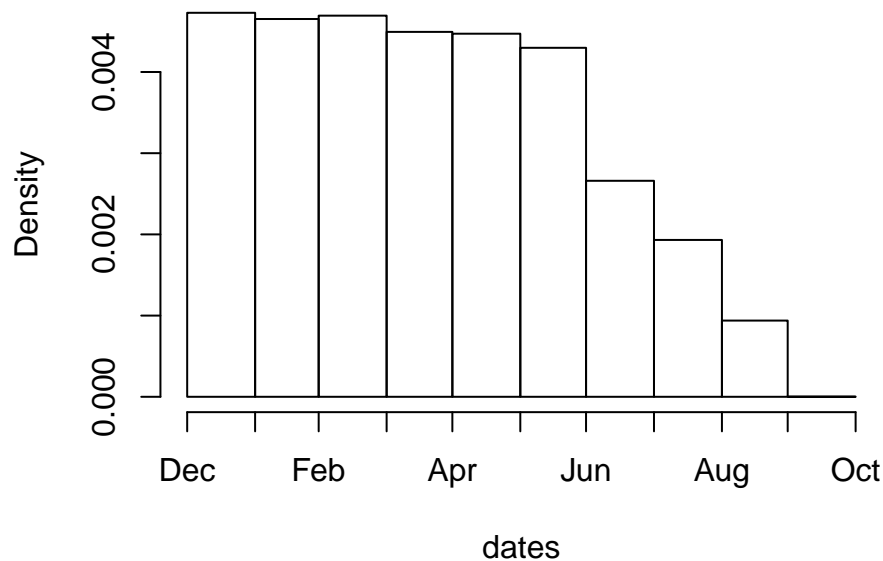
```
## [1] 26474
```

```
# calculate percentage of negatives
mean(negative, na.rm = T)
```

```
## [1] 0.0215034
```

```
# capture the date data
dates <- pm1$Date
dates <- as.Date(as.character(dates), "%Y%m%d")
# plot the histogram
hist(dates, "month") ## Check what's going on in months 1--6
```

Histogram of dates



Check Same New York Monitors at 1999 and 2012

```
# find unique monitors in New York in 1999
site0 <- unique(subset(pm0, State.Code == 36, c(County.Code, Site.ID)))
# find unique monitors in New York in 2012
site1 <- unique(subset(pm1, State.Code == 36, c(County.Code, Site.ID)))
# combine country codes and siteIDs of the monitors
site0 <- paste(site0[,1], site0[,2], sep = ".")
site1 <- paste(site1[,1], site1[,2], sep = ".")
# find common monitors in both
both <- intersect(site0, site1)
# print common monitors in 1999 and 2012
print(both)
```

```
## [1] "1.5"      "1.12"     "5.80"     "13.11"    "29.5"     "31.3"     "63.2008"
## [8] "67.1015" "85.55"    "101.3"
```

Find how many observations available at each monitor

```
# add columns for combined county/site for the original data
pm0$county.site <- with(pm0, paste(County.Code, Site.ID, sep = "."))
pm1$county.site <- with(pm1, paste(County.Code, Site.ID, sep = "."))
# find subsets where state = NY and county/site = what we found previously
cnt0 <- subset(pm0, State.Code == 36 & county.site %in% both)
cnt1 <- subset(pm1, State.Code == 36 & county.site %in% both)
# split data by the county/site values and count observations
sapply(split(cnt0, cnt0$county.site), nrow)
```

```
##      1.12      1.5      101.3      13.11      29.5      31.3      5.80 63.2008 67.1015
##       61      122      152       61       61      183       61      122      122
##    85.55
##       7
```

```
supply(split(cnt1, cnt1$county.site), nrow)
```

```
##      1.12      1.5    101.3    13.11     29.5     31.3     5.80 63.2008 67.1015
##       31       64       31       31       33       15       31       30       31
##    85.55
##       31
```

Choose Monitor where County = 63 and Side ID = 2008

```
# filter data by state/county/siteID
pm1sub <- subset(pm1, State.Code == 36 & County.Code == 63 & Site.ID == 2008)
pm0sub <- subset(pm0, State.Code == 36 & County.Code == 63 & Site.ID == 2008)
# there are 30 observations from 2012, and 122 from 1999
dim(pm1sub)
```

```
## [1] 30 29
```

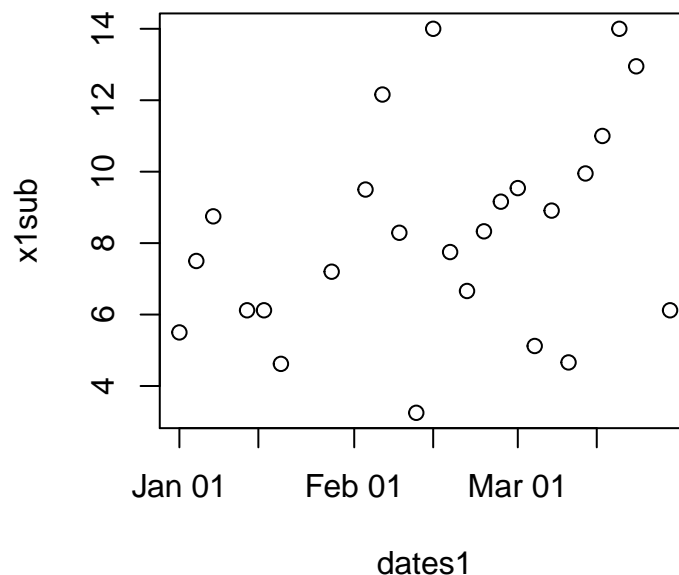
```
dim(pm0sub)
```

```
## [1] 122 29
```

Plot Data for 2012

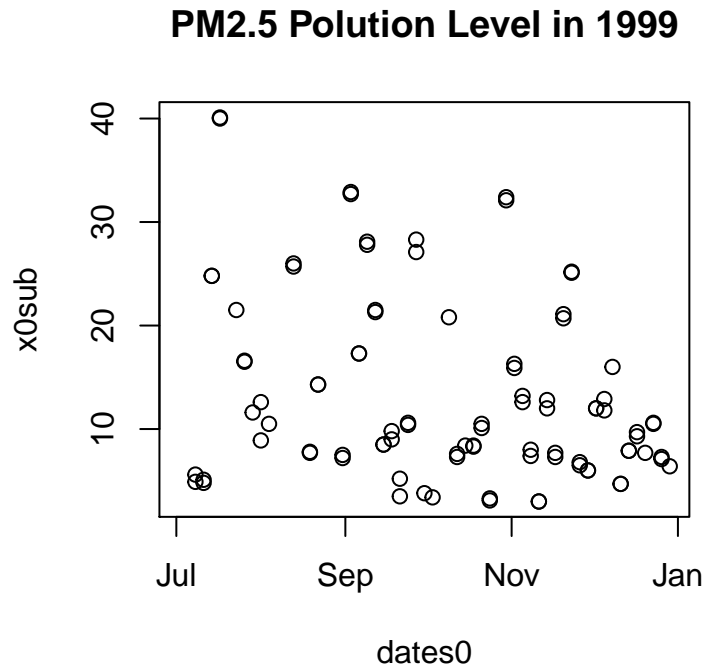
```
# capture the dates of the subset of data
dates1 <- pm1sub$Date
# capture measurements for the subset of data
x1sub <- pm1sub$Sample.Value
# convert dates to appropriate format
dates1 <- as.Date(as.character(dates1), "%Y%m%d")
# plot pm2.5 value vs time
plot(dates1, x1sub, main = "PM2.5 Polution Level in 2012")
```

PM2.5 Polution Level in 2012



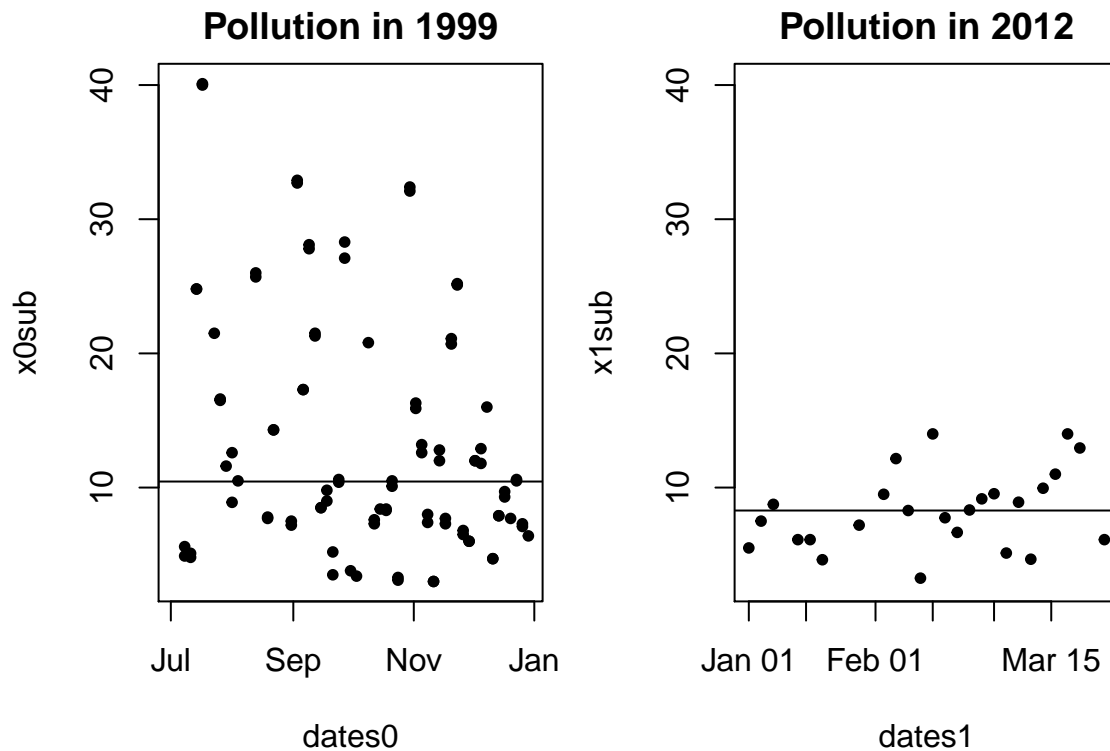
Plot data for 1999

```
# capture the dates of the subset of data
dates0 <- pm0sub$Date
# convert dates to appropriate format
dates0 <- as.Date(as.character(dates0), "%Y%m%d")
# capture measurements for the subset of data
x0sub <- pm0sub$Sample.Value
# plot pm2.5 value vs time
plot(dates0, x0sub, main = "PM2.5 Pollution Level in 1999")
```



Panel Plot for Both Years

```
# find max range for data
rng <- range(x0sub, x1sub, na.rm = T)
# create 1 x 2 panel plot
par(mfrow = c(1, 2), mar = c(4, 4, 2, 1))
# plot time series plot for 1999
plot(dates0, x0sub, pch = 20, ylim = rng, main="Pollution in 1999")
# plot the median
abline(h = median(x0sub, na.rm = T))
# plot time series plot for 2012
plot(dates1, x1sub, pch = 20, ylim = rng, main="Pollution in 2012")
# plot the median
abline(h = median(x1sub, na.rm = T))
```



Find State-wide Means and Trend

```
# divide data by state and find the mean of pollution level for 1999
mn0 <- with(pm0, tapply(Sample.Value, State.Code, mean, na.rm = T))
# divide data by state and find the mean of pollution level for 1999
mn1 <- with(pm1, tapply(Sample.Value, State.Code, mean, na.rm = T))
# convert to data frames while preserving state names
d0 <- data.frame(state = names(mn0), mean = mn0)
d1 <- data.frame(state = names(mn1), mean = mn1)
# merge the 1999 and 2012 means by state
mrg <- merge(d0, d1, by = "state")
# dimension of combined data frame
dim(mrg)
```

```
## [1] 52 3
```

```
# first few lines of data
head(mrg)
```

```
##   state   mean.x   mean.y
## 1     1 19.956391 10.126190
## 2    10 14.492895 11.236059
## 3    11 15.786507 11.991697
## 4    12 11.137139  8.239690
## 5    13 19.943240 11.321364
## 6    15  4.861821  8.749336
```

```

# plot the pollution levels data points for 1999
with(mrg, plot(rep(1, 52), mrg[, 2], xlim = c(.8, 2.2), ylim = c(3, 20),
  main = "PM2.5 Pollution Level by State for 1999 & 2012",
  xlab = "", ylab = "State-wide Mean PM"))
# plot the pollution levels data points for 2012
with(mrg, points(rep(2, 52), mrg[, 3]))
# connected the dots
segments(rep(1, 52), mrg[, 2], rep(2, 52), mrg[, 3])
# add 1999 and 2012 labels
axis(1, c(1, 2), c("1999", "2012"))

```

PM2.5 Pollution Level by State for 1999 & 2012

