alli_data Ciera Martinez July 11, 2017

Purpose: The purpose is to to correlate compounds to oviposition index. Mike wants to use multivariable regression or decision/regression to predict behavior. He also said to use linear or nonparametric.

Library Prereqs
library(lme4)

##

```
## Warning: package 'lme4' was built under R version 3.3.2
## Loading required package: Matrix
library(ggplot2)
## Warning: package 'ggplot2' was built under R version 3.3.2
library(languageR)
library(xlsx)
## Loading required package: rJava
## Loading required package: xlsxjars
library(reshape2)
## Functions
## modelcheck <- function(model, h = 8, w = 10.5) { ## because plot(lmer.obj) doesn't work rs <- residu
Read in Data
aq_DF <- read.csv("../data/output/combinedData.csv", row.names = 1)</pre>
dim(aq_DF)
## [1] 12 40
summary(aq_DF)
##
                 Fly.Line X.eggs.on.yeast.side X.eggs.on.CTL.side
        yeast
              RW1005:12 Min. : 66.0
## Yeast.1:6
                                                Min. : 3.00
  Yeast.2:6
                            1st Qu.:134.5
                                                1st Qu.: 7.25
```

Median :10.00

Median :192.0

```
##
                          Mean :173.7
                                              Mean :19.00
##
                          3rd Qu.:212.0
                                              3rd Qu.:14.00
                          Max.
##
                               :231.0
                                             Max.
                                                    :96.00
##
     Total.eggs
                  Oviposition.index X1.hexanol..2.ethyl_1765
## Min. : 71.0
                 Min.
                         :0.4056
                                   Min.
                                         :0
## 1st Qu.:143.0
                 1st Qu.:0.8513
                                   1st Qu.:0
## Median :205.0 Median :0.8754
                                   Median:0
## Mean :192.7
                  Mean :0.8348
                                   Mean :0
                                   3rd Qu.:0
## 3rd Qu.:239.2
                  3rd Qu.:0.9267
## Max. :323.0
                  Max. :0.9516
                                   Max. :0
## X1..3.dioxolane..2.4.5.trimethyl_347
## Min. :0.3499
## 1st Qu.:0.3499
## Median :0.3833
## Mean
         :0.3833
## 3rd Qu.:0.4167
## Max.
         :0.4167
## X2.methoxy.4.vinylphenol..vanilla..coffee..clove._3379
## Min. :0.0
## 1st Qu.:0.0
## Median :0.5
## Mean :0.5
## 3rd Qu.:1.0
## Max.
        :1.0
## X3.2H..Thiophenone..dihydro.2.methyl..blackberry._1514
## Min.
         :0.0
## 1st Qu.:0.0
## Median :0.5
## Mean :0.5
## 3rd Qu.:1.0
## Max.
        :1.0
## X7.octenoic.acid..ethyl.ester_2692 acetic.acid..very.tiny._199
## Min. :0.0
                                    Min. :0.1867
## 1st Qu.:0.0
                                    1st Qu.:0.1867
## Median :0.5
                                    Median :0.2157
## Mean
         :0.5
                                    Mean
                                          :0.2157
## 3rd Qu.:1.0
                                    3rd Qu.:0.2448
## Max.
         :1.0
                                    Max.
                                           :0.2448
## acetic.acid..2.phenylethyl.ester._3100
## Min. :0
## 1st Qu.:0
## Median :0
## Mean :0
## 3rd Qu.:0
## Max.
         :0
## acetic.acid..2.phenylethyl.ester_3043
## Min. :0
## 1st Qu.:0
## Median:0
## Mean :0
## 3rd Qu.:0
## Max.
         :0
## acetic.acid..2.phenylethyl.ester_3071 butanoic.acid..ethyl.ester_589
## Min. :0.003214
                                       Min.
                                             :0.0000
```

```
1st Qu.:0.0000
## 1st Qu.:0.003214
## Median :0.003804
                                      Median: 0.4886
## Mean :0.003804
                                      Mean :0.4886
## 3rd Qu.:0.004395
                                      3rd Qu.:0.9772
## Max. :0.004395
                                      Max. :0.9772
## decanoic.acid..ethyl.ester 3810 ethane..1...diethoxy..very.tiny. 357
## Min. :0
                                 Min. :0.3499
                                 1st Qu.:0.3499
## 1st Qu.:0
## Median:0
                                 Median : 0.3833
## Mean :0
                                 Mean :0.3833
                                 3rd Qu.:0.4167
## 3rd Qu.:0
## Max. :0
                                 Max. :0.4167
   ethanol 36
                   ethanol._75
                                   ethyl.acetate_135
## Min. :0.8914
                 Min. :0.6249
                                 Min. :0.1165
## 1st Qu.:0.8914
                  1st Qu.:0.6249
                                  1st Qu.:0.1165
## Median :0.9457
                   Median :0.7307
                                  Median :0.5582
## Mean :0.9457
                   Mean :0.7307
                                  Mean :0.5582
## 3rd Qu.:1.0000
                   3rd Qu.:0.8365
                                  3rd Qu.:1.0000
## Max. :1.0000
                   Max. :0.8365 Max. :1.0000
## Hex.5.enoic.acid..ethyl.ester 1526 Hexanoic.acid..ethyl.ester 1595
                                   Min. :0.0
## Min. :0.0
## 1st Qu.:0.0
                                   1st Qu.:0.0
## Median :0.5
                                   Median:0.5
## Mean :0.5
                                   Mean :0.5
## 3rd Qu.:1.0
                                   3rd Qu.:1.0
## Max. :1.0
                                   Max. :1.0
## isoamyl.acetate..very.tiny._220 isoamyl.acetate..very.tiny._422
## Min. :0.09595
                                 Min. :0
## 1st Qu.:0.09595
                                 1st Qu.:0
## Median :0.11091
                                 Median:0
## Mean :0.11091
                                 Mean :0
## 3rd Qu.:0.12586
                                 3rd Qu.:0
## Max. :0.12586
                                 Max. : 0
## isoamyl.acetate_924 isoamyl.acetate_937 isoamyl.acetate_945
                     Min. :0.002092 Min. :0
## Min. :0.4239
## 1st Qu.:0.4239
                      1st Qu.:0.002092
                                       1st Qu.:0
## Median :0.5785
                     Median :0.002956
                                      Median :0
## Mean :0.5785
                     Mean :0.002956
                                      Mean :0
## 3rd Qu.:0.7331
                      3rd Qu.:0.003820
                                        3rd Qu.:0
                     Max. :0.003820 Max. :0
## Max. :0.7331
## isoamyl.alcohol 373 isobutanol 159 isobutyl.acetate 490
                     Min. :0.2645 Min. :0
## Min. :0.3936
## 1st Qu.:0.3936
                      1st Qu.:0.2645
                                    1st Qu.:0
## Median :0.5815
                      Median :0.2999
                                    Median :0
## Mean :0.5815
                      Mean :0.2999
                                     Mean :0
## 3rd Qu.:0.7695
                      3rd Qu.:0.3352
                                     3rd Qu.:0
## Max. :0.7695
                     Max. :0.3352
                                    Max. :0
## methyl.anthranilate..concord.grapes._3522 Nonanal_2202
## Min. :0.0
                                          Min. :0.8803
## 1st Qu.:0.0
                                          1st Qu.:0.8803
## Median :0.5
                                          Median :0.8987
## Mean :0.5
                                          Mean :0.8987
## 3rd Qu.:1.0
                                          3rd Qu.:0.9170
## Max. :1.0
                                          Max. :0.9170
```

```
3rd Qu.:1.0000
##
                                  3rd Qu.:0.6701
          :1.0000
                                  Max.
                                         :0.6701
##
   phenyethyl.alcohol_2157 phenyethyl.alcohol_2249 phenyethyl.alcohol_2291
## Min.
          :0
                           Min.
                                  :0.3383
                                                   Min.
                                                          :0.0000
##
  1st Qu.:0
                           1st Qu.:0.3383
                                                   1st Qu.:0.0000
## Median:0
                           Median : 0.4627
                                                   Median : 0.3268
## Mean
         :0
                           Mean
                                  :0.4627
                                                   Mean
                                                         :0.3268
                           3rd Qu.:0.5872
##
   3rd Qu.:0
                                                   3rd Qu.:0.6536
                                  :0.5872
                                                          :0.6536
          :0
                           Max.
                                                   Max.
## propanoic.acid..ethyl.ester_308 triacetin_3589
   Min.
         :0.1400
                                   Min.
                                          :0
##
  1st Qu.:0.1400
                                   1st Qu.:0
## Median :0.2606
                                   Median:0
## Mean
         :0.2606
                                   Mean
                                          :0
## 3rd Qu.:0.3812
                                   3rd Qu.:0
## Max.
          :0.3812
                                   Max.
str(aq_DF)
## 'data.frame':
                   12 obs. of 40 variables:
                                                           : Factor w/ 2 levels "Yeast.1", "Yeast.2": 1
## $ yeast
## $ Fly.Line
                                                           : Factor w/ 1 level "RW1005": 1 1 1 1 1 1 1
                                                                  184 204 231 207 227 200 150 230 137
## $ X.eggs.on.yeast.side
                                                           : int
## $ X.eggs.on.CTL.side
                                                                  14 8 8 44 96 12 14 10 10 3 ...
                                                           : int
## $ Total.eggs
                                                                  198 212 239 251 323 212 164 240 147
## $ Oviposition.index
                                                                  0.859 0.925 0.933 0.649 0.406 ...
                                                           : num
## $ X1.hexanol..2.ethyl_1765
                                                                  0 0 0 0 0 0 0 0 0 0 ...
                                                           : int
## $ X1..3.dioxolane..2.4.5.trimethyl_347
                                                           : num 0.35 0.35 0.35 0.35
## $ X2.methoxy.4.vinylphenol..vanilla..coffee..clove._3379: int
                                                                 1 1 1 1 1 1 0 0 0 0 ...
## $ X3.2H..Thiophenone..dihydro.2.methyl..blackberry._1514: int
                                                                  1 1 1 1 1 1 0 0 0 0 ...
## $ X7.octenoic.acid..ethyl.ester 2692
                                                           : int
                                                                  1 1 1 1 1 1 0 0 0 0 ...
                                                           : num 0.187 0.187 0.187 0.187 0.187 ...
## $ acetic.acid..very.tiny._199
## $ acetic.acid..2.phenylethyl.ester._3100
                                                           : int
                                                                  0 0 0 0 0 0 0 0 0 0 ...
   $ acetic.acid..2.phenylethyl.ester_3043
                                                                  0 0 0 0 0 0 0 0 0 0 ...
                                                           : int
## $ acetic.acid..2.phenylethyl.ester_3071
                                                                  0.00321 0.00321 0.00321 0.00321 0.00
                                                           : num
## $ butanoic.acid..ethyl.ester_589
                                                                  0.977 0.977 0.977 0.977 ...
   $ decanoic.acid..ethyl.ester_3810
                                                                  0 0 0 0 0 0 0 0 0 0 ...
                                                           : int
   $ ethane..1...diethoxy..very.tiny._357
##
                                                           : num
                                                                  0.35 0.35 0.35 0.35 ...
                                                                 1 1 1 1 1 ...
##
   $ ethanol_36
                                                           : num
## $ ethanol._75
                                                                  0.836 0.836 0.836 0.836 ...
                                                                  0.116 0.116 0.116 0.116 0.116 ...
## $ ethyl.acetate_135
                                                           : num
   $ Hex.5.enoic.acid..ethyl.ester_1526
                                                                  1 1 1 1 1 1 0 0 0 0 ...
                                                           : int
## $ Hexanoic.acid..ethyl.ester_1595
                                                                 1 1 1 1 1 1 0 0 0 0 ...
                                                           : int
## $ isoamyl.acetate..very.tiny._220
                                                                  0.096 0.096 0.096 0.096 0.096 ...
                                                           : num
## $ isoamyl.acetate..very.tiny._422
                                                           : int
                                                                  0 0 0 0 0 0 0 0 0 0 ...
## $ isoamyl.acetate_924
                                                                  0.733 0.733 0.733 0.733 ...
## $ isoamyl.acetate_937
                                                           : num 0.00382 0.00382 0.00382 0.00382 0.00
## $ isoamyl.acetate_945
                                                           : int 0000000000...
                                                           : num 0.769 0.769 0.769 0.769 ...
## $ isoamyl.alcohol_373
```

octanoic.acid.ethyl.ester_2741 oxime..methoxyphenyl..small._1092

Min.

Mean

:0.0000

:0.3351

1st Qu.:0.0000

Median :0.3351

Min.

:0.3183

:0.6592

1st Qu.:0.3183

Median :0.6592

Mean

```
## $ isobutanol 159
                                                                   0.335 0.335 0.335 0.335 ...
## $ isobutyl.acetate_490
                                                                   0000000000...
                                                            : int
## $ methyl.anthranilate..concord.grapes._3522
                                                                   1 1 1 1 1 1 0 0 0 0 ...
                                                                   0.88 0.88 0.88 0.88 ...
## $ Nonanal_2202
                                                            : num
## $ octanoic.acid.ethyl.ester_2741
                                                            : num
                                                                   1 1 1 1 1 ...
## $ oxime..methoxyphenyl..small. 1092
                                                                  0 0 0 0 0 ...
                                                            : num
  $ phenyethyl.alcohol 2157
                                                                   0 0 0 0 0 0 0 0 0 0 ...
                                                            : int
##
   $ phenyethyl.alcohol_2249
                                                            : num
                                                                   0.587 0.587 0.587 0.587 0.587 ...
   $ phenyethyl.alcohol_2291
                                                            : num
                                                                   0 0 0 0 0 ...
   $ propanoic.acid..ethyl.ester_308
                                                            : num
                                                                  0.14 0.14 0.14 0.14 0.14 ...
                                                                   0 0 0 0 0 0 0 0 0 0 ...
   $ triacetin_3589
# Im'm going to force all into num
colnames(aq_DF)
##
    [1] "yeast"
##
    [2] "Fly.Line"
##
  [3] "X.eggs.on.yeast.side"
## [4] "X.eggs.on.CTL.side"
## [5] "Total.eggs"
   [6] "Oviposition.index"
##
  [7] "X1.hexanol..2.ethyl_1765"
##
## [8] "X1..3.dioxolane..2.4.5.trimethyl_347"
## [9] "X2.methoxy.4.vinylphenol..vanilla..coffee..clove._3379"
## [10] "X3.2H..Thiophenone..dihydro.2.methyl..blackberry._1514"
## [11] "X7.octenoic.acid..ethyl.ester_2692"
## [12] "acetic.acid..very.tiny._199"
## [13] "acetic.acid..2.phenylethyl.ester._3100"
## [14] "acetic.acid..2.phenylethyl.ester_3043"
## [15] "acetic.acid..2.phenylethyl.ester_3071"
## [16] "butanoic.acid..ethyl.ester_589"
## [17] "decanoic.acid..ethyl.ester_3810"
## [18] "ethane..1...diethoxy..very.tiny._357"
## [19] "ethanol 36"
## [20] "ethanol._75"
## [21] "ethyl.acetate 135"
## [22] "Hex.5.enoic.acid..ethyl.ester 1526"
## [23] "Hexanoic.acid..ethyl.ester_1595"
## [24] "isoamyl.acetate..very.tiny._220"
## [25] "isoamyl.acetate..very.tiny._422"
## [26] "isoamyl.acetate_924"
## [27] "isoamyl.acetate_937"
## [28] "isoamyl.acetate_945"
## [29] "isoamyl.alcohol_373"
## [30] "isobutanol_159"
## [31] "isobutyl.acetate_490"
## [32] "methyl.anthranilate..concord.grapes._3522"
## [33] "Nonanal_2202"
## [34] "octanoic.acid.ethyl.ester_2741"
## [35] "oxime..methoxyphenyl..small._1092"
## [36] "phenyethyl.alcohol_2157"
## [37] "phenyethyl.alcohol_2249"
## [38] "phenyethyl.alcohol 2291"
```

[39] "propanoic.acid..ethyl.ester_308"

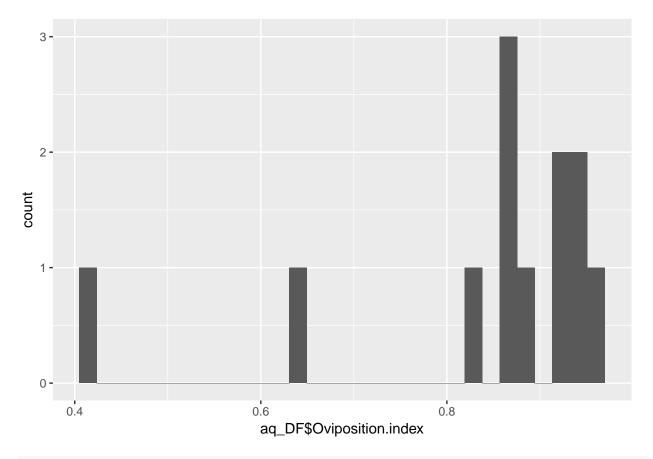
```
## [40] "triacetin_3589"

aq_DF[,7:40] <- apply(aq_DF[,7:40], 2, function(x) as.numeric(as.character(x)))</pre>
```

Visulize Distributions

```
ggplot(aq_DF, aes(aq_DF$Oviposition.index)) +
geom_histogram()
```

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



I think that we need more measurements.