Data Screening

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Introduction

This Data Screenining notebook follows the GUide to STatistical Analysis in Microbial Ecology (GUSTA ME). The purpose is to inspect the variables that we'll be using to test for hypotheses later on, and check whether they follow typical assumptions made in parametric tests such as normality, freedom from heteroskedasticity (difference in variability btw. two+ variables) and outliers.

Reference:

https://sites.google.com/site/mb3gustame/home Buttigieg PL, Ramette A (2014) A Guide to Statistical Analysis in Microbial Ecology: a community-focused, living review of multivariate data analyses. FEMS Microbiol Ecol. 90: 543-550.

Packages

```
library(sm)
library(vioplot)

library(dplyr)
library(tidyr)
library(zoo)
library(reshape)
library(ggplot2)
library("ggrepel")

library("plotly")
library("cowplot")
library("gridExtra")
library("Cairo")
library("GGally")
library("scales")

# Stats
library("vegan")
library("cluster")

# Saving a xlxs file
# library(xlsx)
```

Lab parameters

```
# Initial signature measured in tank
initialDelta = d13Co = -31.2144
```

```r
# Define initial concentration (for Raleigh plots)
#Co <- 8 # ug/g dry soil (based on Corn applications)
Co <- 6.53 # ug/g dry soil (based on Max conc. measured in soils)

epsilon_lab = -1.75
```

Missing values

1. Missing chemical and isotope data due to machine failure or automatic sampling servicing program.

These have been considered to be Values Missing Completely at Random (MCAR) as they are associated to the end of the automatic sampler's capacity for a certain number of events where servicing was inadequate for the discharge amounts seen during a sampling week. Here the values' missingess is not related to any other value in the data set.

2. Isotope data for both soil and water samples due to concentration value being below the limit of detection.

These values must be considered to be Missing at Random (MAR) as the missing value has no relation to the value that 'should' be there, but does depend on other variables in the data set. Thus, other variables must be taken into account for MAR data to be considered random (i.e. missing data is "conditioned by" other data in the data set).

Import soils

Convert to single time observation for merging with water observation.

```r
# Soils
soils = read.csv2("Data/MassBalance_R.csv",
                        na.strings=c('#DIV/0!', '', 'NA'), header = TRUE)
colnames(soils)[colnames(soils) == "ti"] <- "Date.ti"
soils$Date.ti <- as.POSIXct(strptime(soils$Date.ti,
                                             "%Y-%m-%d %H:%M", tz="EST")) # csv typos, option 1
sum(is.na(soils$Date.ti)) == 0
```

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

```r
initialDelta
```

```
## [1] -31.2144
```

```r
# Get rid of imputed values to avoid unwanted bias
soils$DD13C.North <- (ifelse(!is.na(soils$comp.d13C.SD.North), soils$comp.d13C.North - (initialDelta), I
soils$DD13C.Talweg <- (ifelse(!is.na(soils$comp.d13C.SD.Talweg), soils$comp.d13C.Talweg - (initialDelta
soils$DD13C.South <- (ifelse(!is.na(soils$comp.d13C.SD.South), soils$comp.d13C.South - (initialDelta), I



dropSoil <- c("WeekSubWeek", # "Event",
              "B.diss", "B.filt", "CumOutDiss.g", "CumOutFilt.g", "CumOutAppMass.g",  "CumOutMELsm.g",
              # "CumAppMass.g",
              "ID.N", "ID.T",  "Area.N", "Area.T", "Area.S",
              "comp.d13C.SE.North", "comp.d13C.SE.Talweg", "comp.d13C.SE.South",
              "f.max.comp", "f.mean.comp", "f.min.comp", "ngC.SD","ngC.SE", "N_compsoil", "N_ngC")
soils <- soils[ , !(names(soils) %in% dropSoil)]
```

```
timeApps <- soils[ , c("Date.ti", "timeSinceApp", "Event")]

# Quasi-Molten SOILS
soilGroups = read.csv2("Data/WeeklySoils_Rng.csv",
                       na.strings=c('#DIV/0!', '', 'NA'), header = TRUE)
soilGroups$Date.ti <- as.POSIXct(strptime(soilGroups$Date.ti,
                                          "%Y-%m-%d %H:%M", tz="EST")) # csv typos, option 1
sum(is.na(soilGroups$Date.ti)) == 0
```

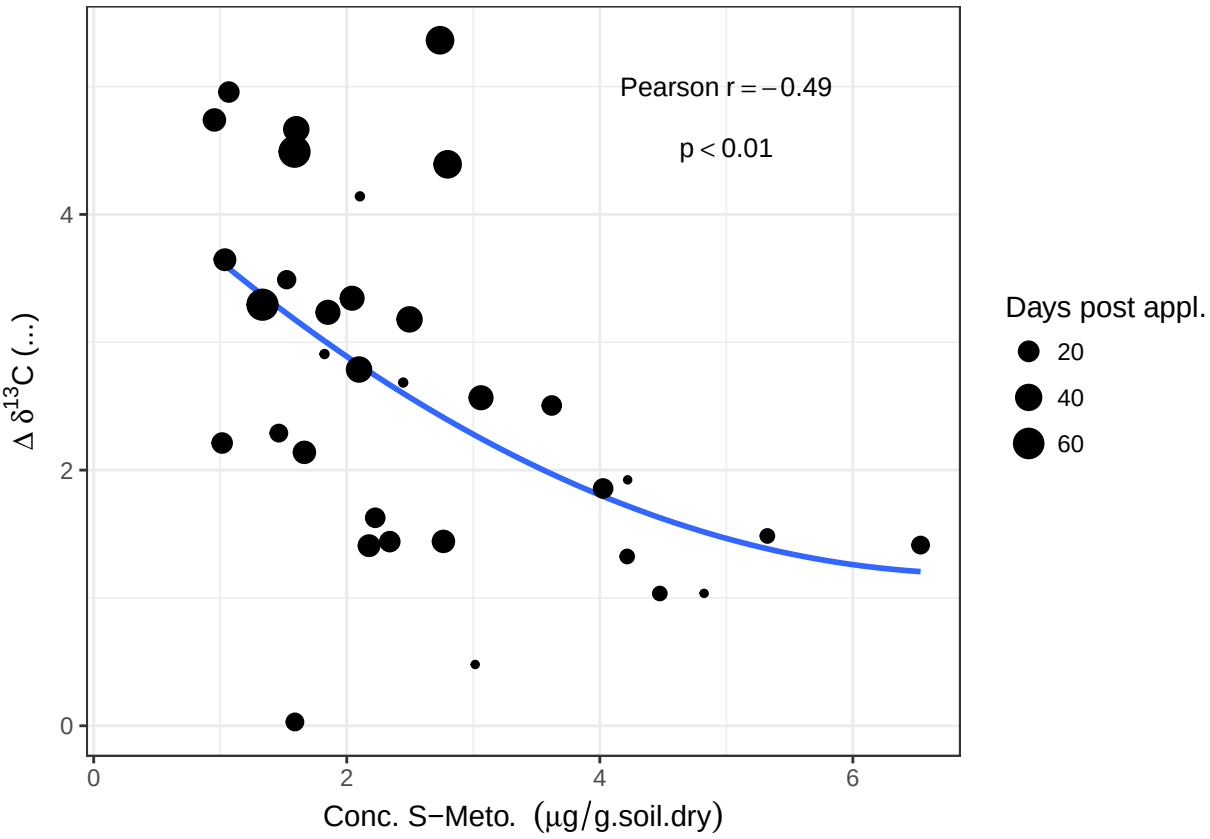
```
## [1] TRUE
```

```
soilGroups$comp.d13C <- ifelse(is.na(soilGroups$comp.d13C.SD), NA, soilGroups$comp.d13C)
soilGroups$ngC.Label <- ifelse(soilGroups$ngC.mean < 10, "< 10 ng", "> 10 ng")

#str(soils)

soilGrApp <- merge(soilGroups, timeApps, by = "Date.ti", all = F)
soilGrApp <- soilGrApp[complete.cases(soilGrApp[ , "timeSinceApp"]),]

soilGrApp$DD13C.comp <- ifelse(is.na(soilGrApp$comp.d13C.SD), NA, soilGrApp$DD13C.comp)

cor.test(soilGroups$comp.d13C, soilGroups$Conc.mug.g.dry.soil)
```

```
##
##  Pearson's product-moment correlation
##
## data:  soilGroups$comp.d13C and soilGroups$Conc.mug.g.dry.soil
## t = -3.221, df = 32, p-value = 0.002931
## alternative hypothesis: true correlation is not equal to 0
## 95 percent confidence interval:
##  -0.7135739 -0.1881206
## sample estimates:
##        cor
## -0.4948086
```

```
pearson_r <- cor.test(soilGroups$comp.d13C, soilGroups$Conc.mug.g.dry.soil)[4]
r_label <- sprintf("Pearson~r == %0.2f", pearson_r)
p_value <- cor.test(soilGroups$comp.d13C, soilGroups$Conc.mug.g.dry.soil)[3]

if (p_value < 0.0001){
  p_label <- "(p < 0.0001)"
} else if (p_value < 0.001) {
  p_label <- "(p < 0.001)"
} else if (p_value < 0.015) {
  p_label <- ("p < 0.01")
} else {
  p_label <- "Check significance"
}

soilGrApp$Source <- ifelse(soilGrApp$Transect == "T", "Valley", "Plateau")
soilGrApp$Source <- as.factor(soilGrApp$Source)

p <- ggplot(data = subset(soilGrApp, !is.na(ngC.Label)), aes(x=Conc.mug.g.dry.soil, y=DD13C.comp))+
  stat_smooth(data = subset(soilGrApp, !is.na(ngC.Label)),
```

```
            aes(x=Conc.mug.g.dry.soil, y=DD13C.comp), method = "lm", formula = y ~ poly(x, 2), se=F) +
  geom_point(aes(group = Source, size = timeSinceApp)) + # , colour = Source)) +  # , shape = ngC.Label)
  theme_bw() +
  labs(size="Days post appl.", colour="Source" ) + #, shape = "Mass Carbon") +
  ylab(expression(paste({Delta~delta}^"13","C", ' (\u2030)'))) +
  xlab(expression(paste("Conc. S-Meto.  ", {({mu}*g / g.soil.dry)}))) +
  annotate("text", x = 5, y = 5, label = as.character(r_label), parse = T, size = 3.5) +
  annotate("text", x = 5, y = 4.5, label = p_label, parse = T, size = 3.5) +
  scale_size_continuous(range = c(1, 5))

  #scale_color_hue("Group") +
  #scale_fill_manual(
  #  "CI horizontal line", values=rep(1,4),
  #  guide=guide_legend(override.aes = list(colour=c("orange", "darkred"))),
  #  labels=c("CI of 95%", "CI of 99%")
  #)
  #geom_text_repel(data = subset(soilGrApp, (!is.na(ngC.Label) & Wnum > 10) ), aes(label=Wnum),
  #                arrow = arrow(length = unit(0.005, 'npc'), type = "closed"),
  #                force = 1,
  #                point.padding = unit(1.0, 'lines'),
  #                max.iter = 2e3,
  #                nudge_x = .2)
p
```




```
#ggsave(p, filename = "DDvsConc_soils.png", width = 8, height = 5, units = "in", scale = 1)

#ggplotly(p)
```

```
  #stat_smooth(method = "lm", formula = y ~ poly(x, 2)) +
  #stat_smooth(method = "lm", formula = y~x, se=F)
```

Raleigh plot

$$ln(\frac{1000+\delta^{13}C_0+\Delta\delta^{13}C}{1000+\delta^{13}C_0}) = (\alpha-1)\cdot lnf = \frac{\epsilon}{1000}\cdot lnf$$

$$f = \frac{C_t}{C_0}$$

```
soilGrApp$iniCo <- ifelse(soilGrApp$Transect == "N", 4.82,
                          ifelse(soilGrApp$Transect == "T", 5.32,
                                 ifelse(soilGrApp$Transect == "S", 6.53, NA)))
#soilGrApp$iniCo <- 8

soilGrApp$yRaleigh <- log((1000+d13Co+soilGrApp$DD13C.comp)/(1000+d13Co))
soilGrApp$xRaleigh <- log(soilGrApp$Conc.mug.g.dry.soil/soilGrApp$iniCo)

# model<-lm(yRaleigh~xRaleigh, data= soilGrApp, subset=(Wnum < 12 & !is.na(ngC.Label)))
model<-lm(yRaleigh~xRaleigh, data= soilGrApp, subset=(!is.na(ngC.Label))) # & ngC.mean >= 5))
cof <- as.numeric(coef(model)[2]*1000)
se <- summary(model)$coef[[4]]*1000
lab <- sprintf(" epsilon == %0.2f ", cof)
labSE <- sprintf("\u00B1 %0.2f ", se)
labSE2 <- sprintf("± %0.2f ", se)

labSE3 <- paste(" '' %+-%  ' 0.43' ")
lab1 <- paste(lab, labSE3)

summary(model)
```

```
##
## Call:
## lm(formula = yRaleigh ~ xRaleigh, data = soilGrApp, subset = (!is.na(ngC.Label)))
##
## Residuals:
##        Min         1Q     Median         3Q        Max
## -3.019e-03 -8.602e-04  6.753e-05  7.700e-04  3.141e-03
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  0.0013771  0.0004145   3.323 0.002241 **
## xRaleigh    -0.0015079  0.0004064  -3.710 0.000785 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.001196 on 32 degrees of freedom
##   (3 observations deleted due to missingness)
## Multiple R-squared:  0.3008, Adjusted R-squared:  0.2789
## F-statistic: 13.76 on 1 and 32 DF,  p-value: 0.0007848
```

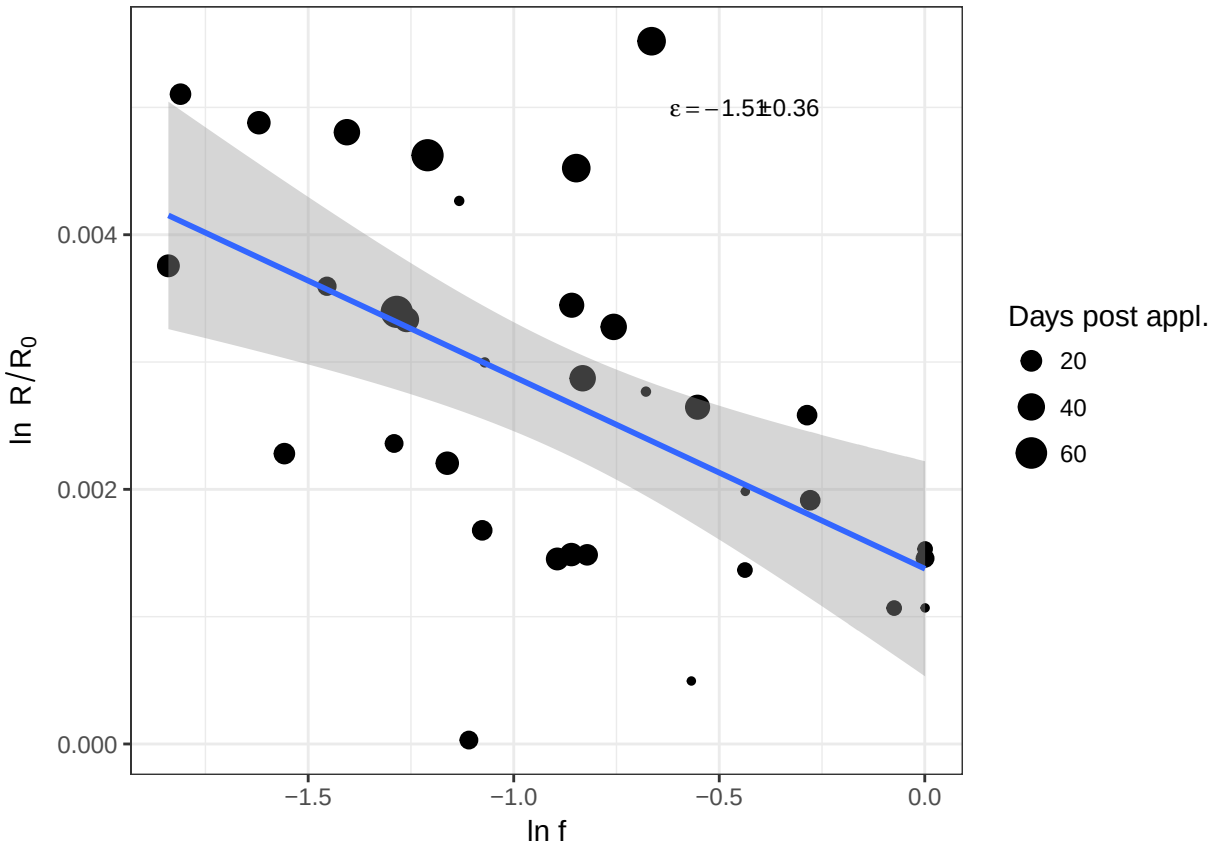
```
# Compre to each transect
modelTalweg<-lm(yRaleigh~xRaleigh, data=soilGrApp, subset=(Wnum < 12 & !is.na(ngC.Label) & Transect == '
eT <- coef(modelTalweg)[2]*1000

modelNorth<-lm(yRaleigh~xRaleigh, data=soilGrApp, subset=(Wnum < 12 & !is.na(ngC.Label) & Transect == "I
eN <- coef(modelNorth)[2]*1000

modelSouth<-lm(yRaleigh~xRaleigh, data=soilGrApp, subset=(Wnum < 12 & !is.na(ngC.Label) & Transect == "S
eS <- coef(modelSouth)[2]*1000

sd(c(coef(modelSouth)[2]*1000 , coef(modelNorth)[2]*1000 , coef(modelTalweg)[2]*1000))
```

```
## [1] 0.6369918
```

```
mean(c(coef(modelSouth)[2]*1000 , coef(modelNorth)[2]*1000 , coef(modelTalweg)[2]*1000))
```

```
## [1] -1.272724
```

```
#modelFull<-lm(yRaleigh~xRaleigh, data=soilGroups, subset=(Wnum < 16))
#summary(modelFull)

raleigh <- ggplot(data = subset(soilGrApp, ( Wnum > 0 & !is.na(ngC.Label) & !is.na(yRaleigh) )), aes(x=x
  geom_point(aes(group = Source, size = timeSinceApp ))+ #, colour = Source)) +  #, shape = ngC.Label))
  theme_bw() +
  scale_size_continuous(range = c(1, 5)) +
  labs(size="Days post appl.", colour="Source") + #, shape = "Mass Carbon") +
  xlab("ln f") +
  ylab("ln R/Ro") +
  ylab(expression(paste("ln  ",  R / R['0'] ))) +
  stat_smooth(data= subset(soilGrApp , ( Wnum > 0 & !is.na(ngC.Label) & !is.na(yRaleigh) )) , method = '
  annotate("text", x = -0.5, y = 0.005,
           # label = as.character(expression(paste( "\u0190", " \u2030", " = ", cof))), parse = T, size
           label = lab, parse = T, size = 3.0) +
  annotate("text", x = -0.33, y = 0.005,
           label = as.character(expression(paste( "\u00B1" , 0.36))), parse = T, size = 3.0) # +

  #geom_text_repel(data = subset(soilGrApp, (!is.na(ngC.Label) & Wnum > 7 & Wnum < 12) ), aes(label=Wnu
  #                arrow = arrow(length = unit(0.005, 'npc'), type = "closed"),
  #                force = 1,
  #                point.padding = unit(1.0, 'lines'),
  #                max.iter = 2e3,
  #                nudge_x = .2)




  #geom_text_repel(aes(label=Wnum),
   #              arrow = arrow(length = unit(0.005, 'npc'), type = "closed"),
    #              force = 1,
     #             point.padding = unit(1.0, 'lines'),
      #            max.iter = 2e3,
       #           nudge_x = .2)
raleigh
```




```
# ggsave(raleigh, filename = "lnDDvslnConc_soils.png", width = 8, height = 5, units = "in", scale = 1)
```

Import waters

Compare mass balance, theoretical and CSIA

```
waters = read.csv2("Data/WeeklyHydroContam_R.csv")
waters$ti <- as.POSIXct(strptime(waters$ti, "%Y-%m-%d %H:%M", tz="EST"))
colnames(waters)[colnames(waters) == "ti"] <- "Date.ti"
waters$Events <- factor(waters$Events, levels = unique(waters$Events))
waters$Event <- factor(waters$Event, levels = unique(waters$Event))

dropWater <- c("N.x", "N.y",
               "Markers" , "TimeDiff",
               "se.d13C", "MES.mg.L", "MES.sd", "MO.mg.L", "filt.se.d13C", "f.diss", "f.filt",
               # "Appl.Mass.g",
               "DissSmeto.mg", "DissSmeto.mg.SD",
               "DissOXA.mg", "DissOXA.mg.SD",
               "DissESA.mg", "DissESA.mg.SD",
               "FiltSmeto.mg", "DissSmeto.mg.SD",
               "TotSMout.mg", "TotSMout.mg.SD",
               "FracDiss", "FracFilt")
waters <- waters[ , !(names(waters) %in% dropWater)]
```

```r
# Half-life calculations (days)
median_half <- 29
max_half <- 12
min_half <- 46


waters$No_First <- ifelse(waters$Appl.Mass.g == 0, NA, waters$Appl.Mass.g)
waters$No_Second <- waters$No_First
waters$No_Second[1] <- 0
waters$No_Third <- waters$No_Second
waters$No_Second[which(!is.na(waters$No_Second))[3]] <- NA
waters$No_Third[which(!is.na(waters$No_Second))[2]] <- NA

waters$No_First <- na.locf( waters$No_First )
waters$No_Second <- na.locf(waters$No_Second)
waters$No_Third <- na.locf(waters$No_Third)

# Compute cumulative time for first, second and third applications
waters$CumDays_First <- cumsum(waters$Duration)/24

waters$dt_Second <- ifelse(waters$No_Second == 0, 0, waters$Duration)
waters$CumDays_Second <- cumsum(waters$dt_Second)/24
waters$dt_Second <- NULL

waters$dt_Third <- ifelse(waters$No_Third == 0, 0 , waters$Duration)
waters$CumDays_Third <- cumsum(waters$dt_Third)/24
waters$dt_Third <- NULL

waters$remain_1st_29d <- waters$No_First*(0.5)^(waters$CumDays_First/median_half)
waters$remain_2nd_29d <- waters$No_Second*(0.5)^(waters$CumDays_Second/median_half)
waters$remain_3rd_29d <- waters$No_Third*(0.5)^(waters$CumDays_Third/median_half)

waters$remain_1st_46d <- waters$No_First*(0.5)^(waters$CumDays_First/min_half)
waters$remain_2nd_46d <- waters$No_Second*(0.5)^(waters$CumDays_Second/min_half)
waters$remain_3rd_46d <- waters$No_Third*(0.5)^(waters$CumDays_Third/min_half)

waters$remain_1st_12d <- waters$No_First*(0.5)^(waters$CumDays_First/max_half)
waters$remain_2nd_12d <- waters$No_Second*(0.5)^(waters$CumDays_Second/max_half)
waters$remain_3rd_12d <- waters$No_Third*(0.5)^(waters$CumDays_Third/max_half)

waters$remainMedTheo_prc <- ((waters$remain_1st_29d + waters$remain_2nd_29d + waters$remain_3rd_29d)/wa
waters$remainMinTheo_prc <- ((waters$remain_1st_46d + waters$remain_2nd_46d + waters$remain_3rd_46d)/wa
waters$remainMaxTheo_prc <- ((waters$remain_1st_12d + waters$remain_2nd_12d + waters$remain_3rd_12d)/wa

colnames(waters)
```

```
##  [1] "Date.ti"               "WeekSubWeek"
##  [3] "tf"                    "iflux"
##  [5] "fflux"                 "changeflux"
##  [7] "maxQ"                  "minQ"
##  [9] "dryHrs"                "Duration.Hrs"
## [11] "chExtreme"             "Peak"
## [13] "AveDischarge.m3.h"     "Volume.m3"
## [15] "Sampled.Hrs"           "Sampled"
```

```
## [17] "Conc.mug.L"              "Conc.SD"
## [19] "OXA_mean"                "OXA_SD"
## [21] "ESA_mean"                "ESA_SD"
## [23] "diss.d13C"               "SD.d13C"
## [25] "N_ngC.diss"              "ngC.mean.diss"
## [27] "ngC.SD.diss"             "Conc.Solids.mug.gMES"
## [29] "Conc.Solids.ug.gMES.SD" "filt.d13C"
## [31] "filt.SD.d13C"            "N_ngC.fl"
## [33] "ngC.mean.fl"             "ngC.SD.fl"
## [35] "DD13C.diss"              "DD13C.filt"
## [37] "B.diss"                  "B.filt"
## [39] "NH4.mM"                  "TIC.ppm.filt"
## [41] "Cl.mM"                   "NO3...mM"
## [43] "PO4..mM"                 "NPOC.ppm"
## [45] "TIC.ppm.unfilt"          "TOC.ppm.unfilt"
## [47] "ExpMES.Kg"               "Appl.Mass.g"
## [49] "timeSinceApp"            "CumAppMass.g"
## [51] "DissSmeto.g"             "DissSmeto.g.SD"
## [53] "DissOXA.g"               "DissOXA.g.SD"
## [55] "DissESA.g"               "DissESA.g.SD"
## [57] "FiltSmeto.mg.SD"         "FiltSmeto.g"
## [59] "FiltSmeto.g.SD"          "TotSMout.g"
## [61] "TotSMout.g.SD"           "MELsm.g"
## [63] "MELsm.g.SD"              "CumOutDiss.g"
## [65] "CumOutFilt.g"            "CumOutSmeto.g"
## [67] "CumOutMELsm.g"           "BalMassDisch.g"
## [69] "prctMassOut"             "FracDeltaOut"
## [71] "Events"                  "Weeks"
## [73] "Event"                   "No_First"
## [75] "No_Second"               "No_Third"
## [77] "CumDays_First"           "CumDays_Second"
## [79] "CumDays_Third"           "remain_1st_29d"
## [81] "remain_2nd_29d"          "remain_3rd_29d"
## [83] "remain_1st_46d"          "remain_2nd_46d"
## [85] "remain_3rd_46d"          "remain_1st_12d"
## [87] "remain_2nd_12d"          "remain_3rd_12d"
## [89] "remainMedTheo_prc"       "remainMinTheo_prc"
## [91] "remainMaxTheo_prc"
```

```
dropWater2 <- c("No_First", "No_Second" ,"No_Third",
                "CumDays_First", "CumDays_Second", "CumDays_Third",
                "remain_1st_29d", "remain_2nd_29d", "remain_3rd_29d",
                "remain_1st_46d", "remain_2nd_46d", "remain_3rd_46d",
                "remain_1st_12d", "remain_2nd_12d", "remain_3rd_12d")

waters <- waters[ , !(names(waters) %in% dropWater2)]

keepWaterMB <- c("Date.ti", "CumAppMass.g",
                 # MB
                 "CumOutSmeto.g", "CumOutMELsm.g" ,
                 "remainMedTheo_prc", "remainMinTheo_prc", "remainMaxTheo_prc",
                 # CSIA
                 "B.diss", "SD.d13C")
```

```r
# Get last 5 rows, omit NA's, will return rows only where B.diss was not NA
watersMassBal <- na.omit(waters[ , (names(waters) %in% keepWaterMB)])
watersMassBal <- subset(watersMassBal, SD.d13C < 1)

watersMassBal$SMout_prc <- (watersMassBal$CumOutSmeto.g/watersMassBal$CumAppMass.g)*100
watersMassBal$TPout_prc <- (watersMassBal$CumOutMELsm.g/watersMassBal$CumAppMass.g)*100
watersMassBal$f <- 100 - (watersMassBal$B.diss + watersMassBal$SMout_prc)
watersMassBal$SD.d13C <- NULL


mayBal <- subset(watersMassBal, (Date.ti > as.POSIXct("2016-04-01 00:00:00", tz = "EST")
                 & Date.ti < as.POSIXct("2016-05-01 00:00:00", tz = "EST")) )
juneBal <- subset(watersMassBal, (Date.ti > as.POSIXct("2016-06-07 00:00:00", tz = "EST")
                 & Date.ti <= as.POSIXct("2016-06-24 14:52:00", tz = "EST")) )

B.mean.may <- mean(mayBal$B.diss)
B.sd.may <- sd(mayBal$B.diss)
f.mean.may <- mean(mayBal$f)
f.sd.may <- sd(mayBal$f)

B.mean.june <- mean(juneBal$B.diss)
B.sd.june <- sd(juneBal$B.diss)
f.mean.june <- mean(juneBal$f)
f.sd.june <- sd(juneBal$f)

mayBal <- tail(mayBal, n=1)
mayBal$B.mean <- B.mean.may
mayBal$B.sd1 <- B.mean.may-B.sd.may
mayBal$B.sd2 <- B.mean.may+B.sd.may
mayBal$f.mean <- f.mean.may
mayBal$f.sd1 <- f.mean.may-f.sd.may
mayBal$f.sd2 <- f.mean.may+f.sd.may
mayBal$DegMed <- 100 - mayBal$remainMedTheo_prc
mayBal$DegLow <- 100 - mayBal$remainMinTheo_prc
mayBal$DegHigh <- 100 - mayBal$remainMaxTheo_prc
mayBal$Month <- "April"

juneBal <- tail(juneBal, n=1)
juneBal$B.mean <- B.mean.june
juneBal$B.sd1 <- B.mean.june-B.sd.june
juneBal$B.sd2 <- B.mean.june+B.sd.june
juneBal$f.mean <- f.mean.june
juneBal$f.sd1 <- f.mean.june-f.sd.june
juneBal$f.sd2 <- f.mean.june+f.sd.june
juneBal$DegMed <- 100 - juneBal$remainMedTheo_prc
juneBal$DegLow <- 100 - juneBal$remainMinTheo_prc
juneBal$DegHigh <- 100 - juneBal$remainMaxTheo_prc
juneBal$Month <- "June"


bal <- rbind(mayBal, juneBal)
bal$SMout.SD1 <- NA
bal$SMout.SD2 <- NA
```

```
bal$TPout.SD1 <- NA
bal$TPout.SD2 <- NA

bal$B.diss <- NULL
bal$f <- NULL
bal$Date.ti <- NULL
bal$CumAppMass.g <- NULL
bal$CumOutSmeto.g <- NULL
bal$CumOutMELsm.g <- NULL


names(bal)
```

```
##  [1] "remainMedTheo_prc" "remainMinTheo_prc" "remainMaxTheo_prc"
##  [4] "SMout_prc"         "TPout_prc"         "B.mean"
##  [7] "B.sd1"             "B.sd2"             "f.mean"
## [10] "f.sd1"             "f.sd2"             "DegMed"
## [13] "DegLow"            "DegHigh"           "Month"
## [16] "SMout.SD1"         "SMout.SD2"         "TPout.SD1"
## [19] "TPout.SD2"
```

```
bal <- bal[c("Month",
             "B.mean" , "B.sd1" ,  "B.sd2",
              "f.mean" , "f.sd1" , "f.sd2",
             "DegMed", "DegLow", "DegHigh",
             "remainMedTheo_prc", "remainMinTheo_prc", "remainMaxTheo_prc",
             "SMout_prc",  "SMout.SD1", "SMout.SD2",
             "TPout_prc", "TPout.SD1", "TPout.SD2")]

names(bal) <- c("Month",
             "B.measure" , "B.SD1" ,  "B.SD2",
              "f.measure" , "f.SD1" , "f.SD2",
             "Deg.measure", "Deg.SD1", "Deg.SD2",
             "Rem.measure", "Rem.SD1", "Rem.SD2",
             "SMout.measure",  "SMout.SD1", "SMout.SD2",
             "TPout.measure", "TPout.SD1", "TPout.SD2")

balTidy <- bal %>%
  gather(measure, value, -Month) %>% # Melts data frame
  separate(measure, into = c("Sink", "temporary_var")) %>% # parses the sep = "." into...
  spread(temporary_var, value) # Moves molten temporary variable to own column

type <- rep(c("CSIA", "DT50", "CSIA", "DT50", "MB", "MB"), 2)

balTidyType <- cbind(balTidy, type)

balTidyType$Sink <- as.factor(balTidyType$Sink)
balTidyType$Month <- as.factor(balTidyType$Month)
balTidyType$Sink <- factor(balTidyType$Sink, levels = c("B" , "TPout",  "Deg" ,"f" ,"SMout", "Rem"))
levels(balTidyType$type)
```

```
## [1] "CSIA" "DT50" "MB"
```

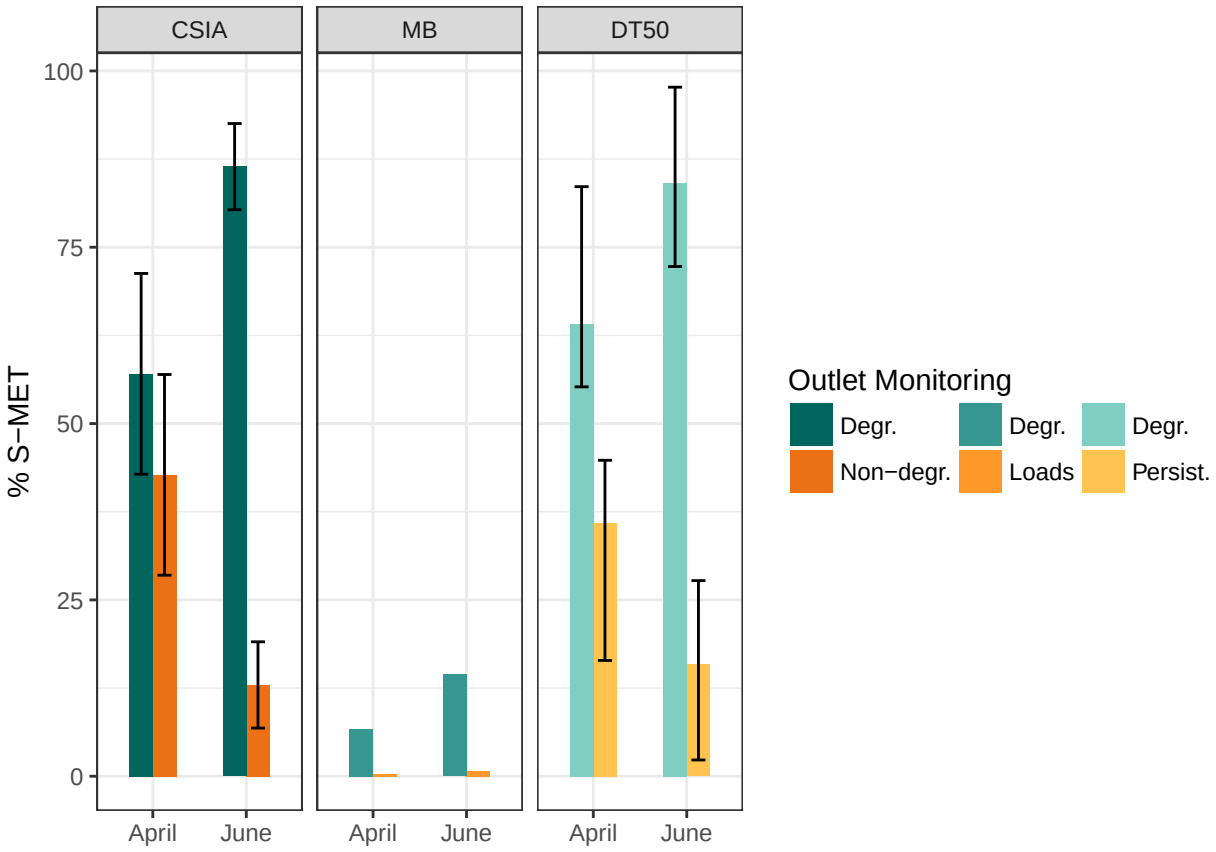
```
balTidyType$type <- factor(balTidyType$type, levels = c("CSIA" , "MB", "DT50"))
levels(balTidyType$Sink)
```

```
## [1] "B"     "TPout" "Deg"   "f"     "SMout" "Rem"
```

```
levels(balTidyType$Month)
```

```
## [1] "April" "June"
```

```
OutBars <- ggplot(data = balTidyType , aes(x=Month, y=measure, fill = Sink, ymin=SD1, ymax=SD2))+
  geom_bar(stat = "identity", position = "dodge", width = 0.5) +
  geom_errorbar(#aes(ymin=SD1, ymax=SD2),
                  width=.3 , # ) + #,                    # Width of the error bars
                  position=position_dodge(.5)) +
  theme_bw() +
  ylab("% S-MET") +
  theme(axis.title.x = element_blank() ) +
  #xlab("Month") +
  facet_wrap(~type) +
  scale_fill_manual(values = c("#01665e", "#35978f", "#80cdc1", "#ec7014", "#fe9929", "#fec44f" ), # bl
                    #values = c("#238b45", "#41ab5d", "#74c476", "#40004b", "#762a83", "#9970ab" ), # g
                    #values = c("#238b45", "#41ab5d", "#74c476", "#ec7014", "#fe9929", "#fec44f" ), # g
                    #values = c("#80cdc1", "#018571", "#a6611a", "#dfc27d", "#80cdc1", "#018571"),
                    name= "Outlet Monitoring" ,# element_blank(), #"Mass Balance", # \n
                       breaks=c("B", "f" ,
                                "TPout" , "SMout" ,
                                "Deg", "Rem"
                                ),
                       labels=c("Degr.", "Non-degr.",
                                "Degr.", "Loads",
                                "Degr." , "Persist."
                                 )) +
  guides(fill=guide_legend(ncol=3))

OutBars
```



Compare to Catchment soils

```
names(soils)
```

```
##  [1] "Date.ti"             "Event"               "timeSinceApp"
##  [4] "diss.d13C"           "SD.d13C"             "CumAppMass.g"
##  [7] "B.mean.comp.North"   "B.max.comp.North"    "B.min.comp.North"
## [10] "MassSoil.g.North"    "comp.d13C.North"     "comp.d13C.SD.North"
## [13] "B.mean.comp.Talweg"  "B.max.comp.Talweg"   "B.min.comp.Talweg"
## [16] "MassSoil.g.Talweg"   "comp.d13C.Talweg"    "comp.d13C.SD.Talweg"
## [19] "B.mean.comp.South"   "B.max.comp.South"    "B.min.comp.South"
## [22] "MassSoil.g.South"    "comp.d13C.South"     "comp.d13C.SD.South"
## [25] "ID.S"                "CatchMassSoil.g"     "BulkMass.g"
## [28] "BulkCatch.d13"       "BulkCatch.d13.SD"    "f.mean.bulk"
## [31] "B.mean.bulk"         "DD13C.North"         "DD13C.Talweg"
## [34] "DD13C.South"
```

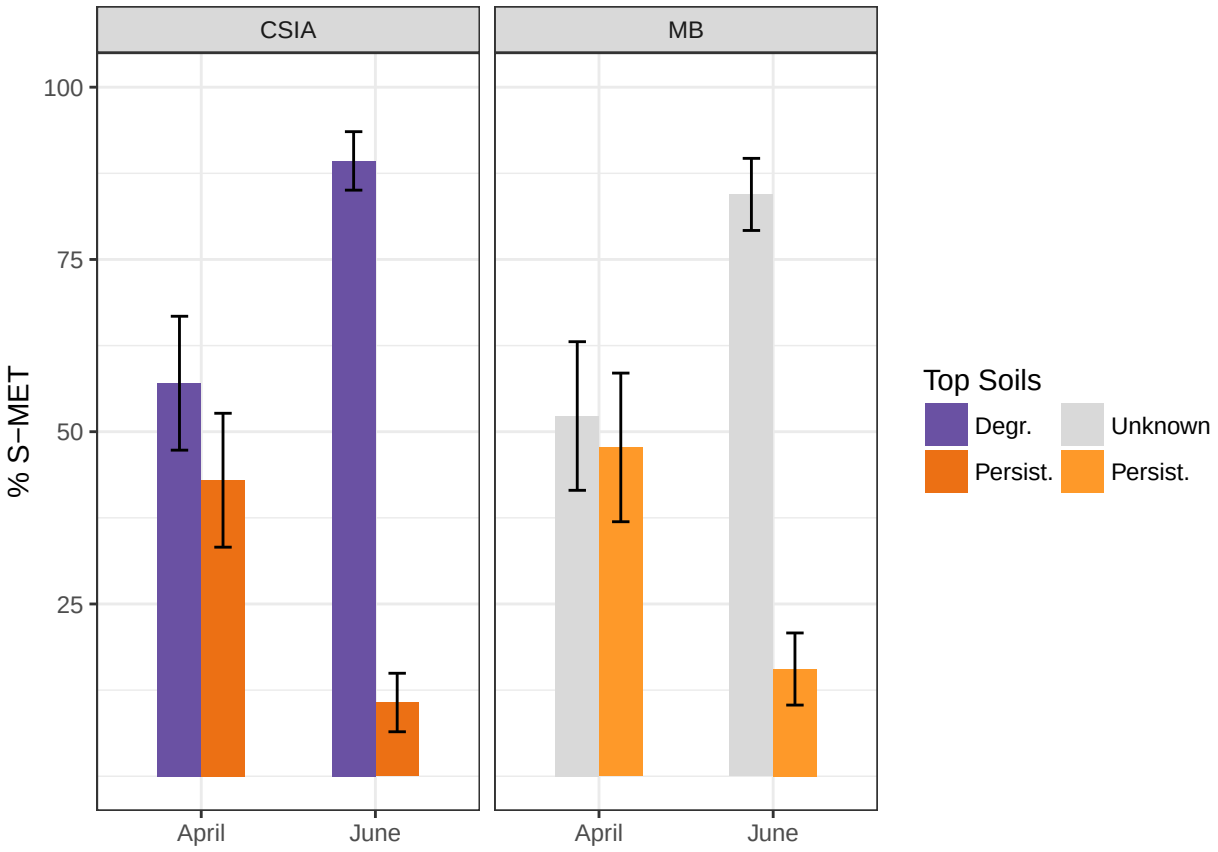
```
keepMB <- c("Date.ti", "CumAppMass.g", "CatchMassSoil.g",
            "f.mean.bulk", "B.mean.bulk")


soilsMB <- soils[, (names(soils) %in% keepMB)]

soilsMB$Rem.measure <- (soilsMB$CatchMassSoil.g/soilsMB$CumAppMass.g)*100
soilsMB$Unk.measure <- 100 - soilsMB$Rem.measure
soilsMB$CatchMassSoil.g <- NULL
```

```r
soilsMB$CumAppMass.g <- NULL

soils.April <- subset(soilsMB, (Date.ti > as.POSIXct("2016-04-01 00:00:00", tz = "EST")
                & Date.ti < as.POSIXct("2016-05-01 00:00:00", tz = "EST")))
soils.April <- na.omit(soils.April)

soils.June <- subset(soilsMB, (Date.ti > as.POSIXct("2016-06-07 00:00:00", tz = "EST")
                & Date.ti <= as.POSIXct("2016-06-28 14:52:00", tz = "EST")) )
soils.June <- na.omit(soils.June)

B.mean.maySol <- mean(soils.April$B.mean.bulk)
B.sd.maySol <- sd(soils.April$B.mean.bulk)
f.mean.maySol <- mean(soils.April$f.mean.bulk*100)
f.sd.maySol <- sd(soils.April$f.mean.bulk*100)
Rem.mean.maySol <- mean(soils.April$Rem.measure)
Rem.sd.maySol <- sd(soils.April$Rem.measure)
Unk.mean.maySol <- mean(soils.April$Unk.measure)
Unk.sd.maySol <- sd(soils.April$Unk.measure)

B.mean.juneSol <- mean(soils.June$B.mean.bulk)
B.sd.juneSol <- sd(soils.June$B.mean.bulk)
f.mean.juneSol <- mean(soils.June$f.mean.bulk*100)
f.sd.juneSol <- sd(soils.June$f.mean.bulk*100)
Rem.mean.juneSol <- mean(soils.June$Rem.measure)
Rem.sd.juneSol <- sd(soils.June$Rem.measure)
Unk.mean.juneSol <- mean(soils.June$Unk.measure)
Unk.sd.juneSol <- sd(soils.June$Unk.measure)


Month <- c("April", "June")
balSol <- data.frame(Month)
balSol$B.measure <- c(B.mean.maySol, B.mean.juneSol)
balSol$B.SD1 <- c(B.mean.maySol-B.sd.maySol , B.mean.juneSol-B.sd.juneSol)
balSol$B.SD2 <- c(B.mean.maySol+B.sd.maySol , B.mean.juneSol+B.sd.juneSol)
balSol$f.measure <- c(f.mean.maySol, f.mean.juneSol)
balSol$f.SD1 <- c(f.mean.maySol-f.sd.maySol, f.mean.juneSol-f.sd.juneSol)
balSol$f.SD2 <- c(f.mean.maySol+f.sd.maySol, f.mean.juneSol+f.sd.juneSol)

balSol$Unk.measure <- c(Unk.mean.maySol, Unk.mean.juneSol)
balSol$Unk.SD1 <- c(Unk.mean.maySol-Unk.sd.maySol, Unk.mean.juneSol-Unk.sd.juneSol)
balSol$Unk.SD2 <- c(Unk.mean.maySol+Unk.sd.maySol, Unk.mean.juneSol+Unk.sd.juneSol)

balSol$Rem.measure <- c(Rem.mean.maySol, Rem.mean.juneSol)
balSol$Rem.SD1 <- c(Rem.mean.maySol-Rem.sd.maySol, Rem.mean.juneSol-Rem.sd.juneSol)
balSol$Rem.SD2 <- c(Rem.mean.maySol+Rem.sd.maySol, Rem.mean.juneSol+Rem.sd.juneSol)

solTidy <- balSol %>%
  gather(measure, value, -Month) %>% # Melts data frame
  separate(measure, into = c("Sink", "temporary_var")) %>% # parses the sep = "." into...
  spread(temporary_var, value) # Moves molten temporary variable to own column

type <- rep(c("CSIA", "CSIA", "MB", "MB"), 2)
```

```r
balTidySol <- cbind(solTidy, type)
balTidySol$Sink <- as.factor(balTidySol$Sink)

levels(balTidySol$Sink)
```

```
## [1] "B"   "f"   "Rem" "Unk"
```

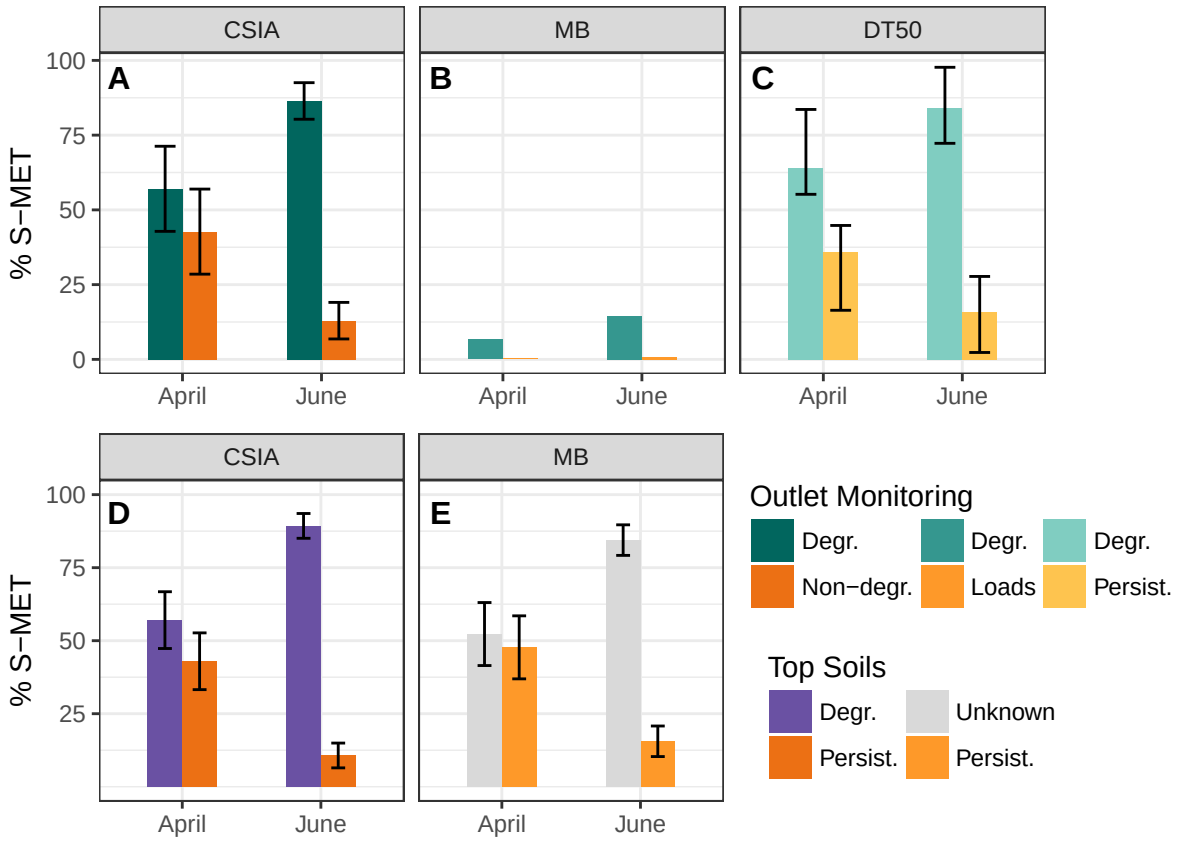
```r
balTidySol$Sink <- factor(balTidySol$Sink, levels = c("B" , "f" ,"Unk", "Rem"))

SoilBars <- ggplot(data = balTidySol , aes(x=Month, y=measure, fill = Sink, ymin=SD1, ymax=SD2))+
  geom_bar(stat = "identity", position = "dodge", width = 0.5) +
  geom_errorbar(#aes(ymin=SD1, ymax=SD2),
                  width=.2 , # ) + #,                    # Width of the error bars
                  position=position_dodge(.5)) +
  theme_bw() +
  ylab("% S-MET") +
  theme(axis.title.x = element_blank() ) +
  xlab("Month") +
  facet_wrap(~type) +
  scale_y_continuous( breaks=c(25, 50, 75, 100), limits = c(0, 100) )+ #expand=c(0, 10, 0, 0)) +
  scale_fill_manual(#values = c("#6a51a3" , "#ec7014", "#807dba", "#fe9929"), # purple-orange
                    values = c("#6a51a3" , "#ec7014", "#d9d9d9", "#fe9929"), # Unknown as grey
                    name= "Top Soils" ,# element_blank(), #"Mass Balance", # \n
                    breaks=c("B", "f" ,
                                "Unk" , "Rem"
                                ),
                    labels=c("Degr.", "Persist.",
                                "Unknown", "Persist." ))+
  guides(fill=guide_legend(ncol=2))

SoilBars
```



Merge both Outlet and Soils - BARS

```
#balAll <- rbind(balTidyType,  balTidySol)

OutBars_noLeg <- OutBars + theme(legend.position = 'none')
OutBars_Leg <- get_legend(OutBars)

SoilBars_noLeg <- SoilBars + theme(legend.position = 'none')
SoilBars_Leg <- get_legend(SoilBars)

#plot_grid(OutBars_noLeg, SoilBars_noLeg,
#                    ncol =1, nrow = 2, align ="v" )
#,
#                    labels = c("A", "C", "B", "D"))

balAllplot <- ggdraw() +
  draw_plot(OutBars_noLeg, x=0.01, y=.5, width =  0.86, height = .5) +
  draw_plot(SoilBars_noLeg, x=0.01, y = 0.0, width = 0.60, height = 0.5) +
  draw_plot(OutBars_Leg, x=0.74, y = 0.3, width = 0.1, height = 0.1) +
  draw_plot(SoilBars_Leg, x=0.70, y = 0.1, width = 0.1, height = 0.1) +
  draw_label("A", x= 0.11, y = .9, size = 12, fontface = "bold") +
  draw_label("D", x= 0.11, y = .39, size = 12, fontface = "bold") +
  draw_label("B", x= 0.37, y = .9, size = 12, fontface = "bold") +
  draw_label("E", x= 0.37, y = .39, size = 12, fontface = "bold") +
  draw_label("C", x= 0.63, y = .9, size = 12, fontface = "bold")
```

```
balAllplot
```




```
ggsave(balAllplot, filename = "MB_CSIA_Bars.png", width = 8, height = 5, units = "in", scale = 1)
```

Water Rayleigh plots

```
#waters$remain_maxHalf
#waters$remain_minHalf

waterCo <- max(waters$Conc.mug.L)
d13Co
```

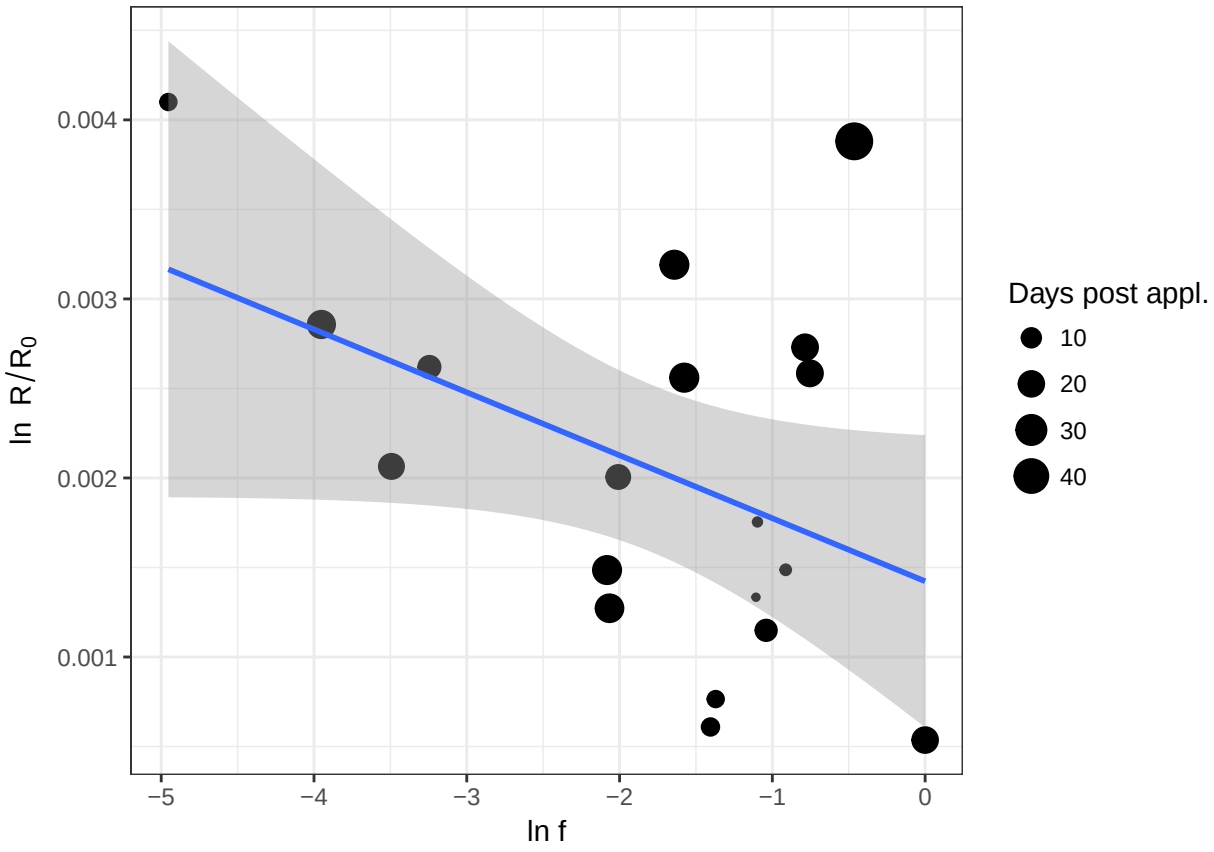
```
## [1] -31.2144
```

```
waters$yRaleigh <- log((1000+d13Co+waters$DD13C.diss)/(1000+d13Co))
waters$xRaleigh <- log(waters$Conc.mug.L/waterCo)
waters$DIa <- waters$maxQ*waters$Volume.m3/waters$Duration.Hrs

waterClean <- subset(waters, Sampled == "Sampled")
waterModel<-lm(yRaleigh~xRaleigh, data= waterClean)
summary(waterModel)
```

```
##
## Call:
## lm(formula = yRaleigh ~ xRaleigh, data = waterClean)
##
```

```
## Residuals:
##        Min         1Q     Median         3Q        Max
## -0.0018789 -0.0008911 -0.0002357  0.0006844  0.0023033
##
## Coefficients:
##               Estimate Std. Error t value Pr(>|t|)
## (Intercept)  0.0019996  0.0004099   4.879  5.1e-05 ***
## xRaleigh    -0.0001201  0.0001413  -0.850    0.403
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.001243 on 25 degrees of freedom
##   (11 observations deleted due to missingness)
## Multiple R-squared:  0.0281, Adjusted R-squared:  -0.01077
## F-statistic: 0.7229 on 1 and 25 DF,  p-value: 0.4033
```

```
cof <- as.numeric(coef(model)[2]*1000)
se <- summary(model)$coef[[4]]*1000



waterRaleigh <- ggplot(data = subset(waterClean, (!is.na(yRaleigh) & xRaleigh > -7 & ngC.mean.diss > 5)
  geom_point(aes(size = timeSinceApp)) +
  theme_bw() +
  scale_size_continuous(range = c(1, 6)) +
  labs(size="Days post appl.") +
  xlab("ln f") +
  ylab("ln R/Ro") +
  ylab(expression(paste("ln  ",  R / R['0'] ))) +
  stat_smooth(data= subset(waterClean, (!is.na(yRaleigh) & xRaleigh > -7  & ngC.mean.diss > 5)), method

waterRaleigh
```




```
# ggsave(waterRaleigh, filename = "lnDDvslnConc_water.png", width = 8, height = 5, units = "in", scale =
# Date conversion correct:
sum(is.na(waters$Date.ti)) == 0
```

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

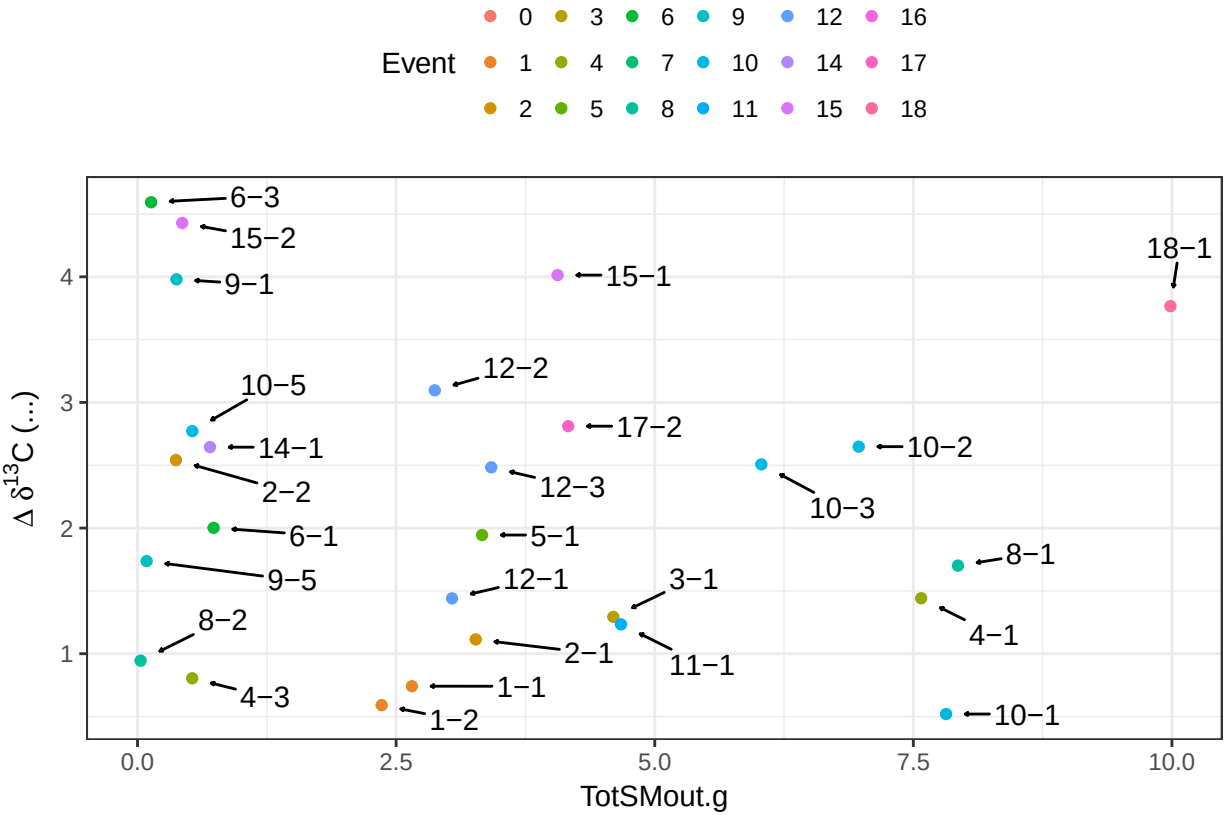
```
str(waters)
```

```
## 'data.frame':    51 obs. of  79 variables:
##  $ Date.ti               : POSIXct, format: "2016-03-25 00:04:00" "2016-03-25 12:04:00" ...
##  $ WeekSubWeek           : Factor w/ 51 levels "W0-0x","W0-1",..: 1 2 3 4 5 6 26 27 28 29 ...
##  $ tf                    : Factor w/ 51 levels "2016-03-25 12:02:00",..: 1 2 3 4 5 6 7 8 9 10 ...
##  $ iflux                 : num  1.25 1.12 1.31 1.46 16.33 ...
##  $ fflux                 : num  1.13 1.31 1.46 16.45 15.18 ...
##  $ changeflux            : num  -0.119 0.189 0.148 14.989 -1.15 ...
##  $ maxQ                  : num  1.25 1.38 1.64 38.4 18.67 ...
##  $ minQ                  : num  1.118 1.082 0.929 1.449 13.201 ...
##  $ dryHrs                : num  0.0167 6.0167 47.3 66.1333 1.65 ...
##  $ Duration.Hrs          : num  12 82.5 37.6 27.3 23.1 ...
##  $ chExtreme             : num  -0.13 0.256 0.33 36.944 -3.133 ...
##  $ Peak                  : int  NA NA NA 1 NA NA 2 NA NA 3 ...
##  $ AveDischarge.m3.h     : num  1.2 1.21 1.28 14.32 15.53 ...
##  $ Volume.m3             : num  14.4 100.2 48.3 390.4 359.2 ...
##  $ Sampled.Hrs           : num  12 82.5 37.6 27.3 23.1 ...
##  $ Sampled               : Factor w/ 2 levels "Not Sampled",..: 1 2 1 2 2 1 2 2 1 2 ...
##  $ Conc.mug.L            : num  0.246 0.246 3.517 6.788 6.561 ...
##  $ Conc.SD               : num  0.0193 0.0193 0.1544 0.2894 0.1906 ...
##  $ OXA_mean              : num  4.82 4.82 17.68 30.53 32.49 ...
```

```
##  $ OXA_SD                : num  1.141 1.141 5.663 10.185 0.243 ...
##  $ ESA_mean              : num  18.1 18.1 32 46 41.3 ...
##  $ ESA_SD                : num  3.497 3.497 3.267 3.037 0.853 ...
##  $ diss.d13C             : num  NA NA NA -30.5 -30.6 ...
##  $ SD.d13C               : num  NA NA NA 0.106 0.151 ...
##  $ N_ngC.diss            : int  NA NA NA 3 3 NA 3 3 NA 3 ...
##  $ ngC.mean.diss         : num  NA NA NA 42.7 54.7 ...
##  $ ngC.SD.diss           : num  NA NA NA 1.92 2.54 ...
##  $ Conc.Solids.mug.gMES  : num  0.645 0.645 0.385 0.126 0.436 ...
##  $ Conc.Solids.ug.gMES.SD: num  0.0232 0.0232 0.0252 0.0271 0.1232 ...
##  $ filt.d13C             : num  NA NA NA NA NA ...
##  $ filt.SD.d13C          : num  NA NA NA NA NA ...
##  $ N_ngC.fl              : int  NA NA NA NA NA NA 3 3 NA NA ...
##  $ ngC.mean.fl           : num  NA NA NA NA NA ...
##  $ ngC.SD.fl             : num  NA NA NA NA NA ...
##  $ DD13C.diss            : num  NA NA NA 0.741 0.59 ...
##  $ DD13C.filt            : num  NA NA NA NA NA ...
##  $ B.diss                : num  NA NA NA 35.4 29.4 ...
##  $ B.filt                : num  NA NA NA NA NA ...
##  $ NH4.mM                : num  NA NA NA 0.05 NA NA NA NA NA NA ...
##  $ TIC.ppm.filt          : num  NA NA NA 51.8 44.8 NA 66.7 52.1 NA 69.4 ...
##  $ Cl.mM                 : num  NA NA NA 1.48 1574 ...
##  $ NO3...mM              : num  NA NA NA 616 778 ...
##  $ PO4..mM               : int  NA NA NA NA NA NA NA NA NA NA ...
##  $ NPOC.ppm              : num  NA NA NA 4 4.4 NA 5.8 3.4 NA 9.1 ...
##  $ TIC.ppm.unfilt        : num  NA NA NA 44.8 26.4 NA 39 32.3 NA 54.8 ...
##  $ TOC.ppm.unfilt        : num  NA NA NA 4.7 5.4 NA 2.7 3.8 NA 3.9 ...
##  $ ExpMES.Kg             : num  5.35 5.35 14.88 24.4 8.08 ...
##  $ Appl.Mass.g           : num  9498 0 0 0 0 ...
##  $ timeSinceApp          : num  0.5 3.9 5.5 6.6 7.6 11.6 12.6 14 20.6 2.2 ...
##  $ CumAppMass.g          : num  9498 9498 9498 9498 9498 ...
##  $ DissSmeto.g           : num  0.00354 0.0246 0.17004 2.64991 2.357 ...
##  $ DissSmeto.g.SD        : num  0.000278 0.001934 0.007463 0.11298 0.068486 ...
##  $ DissOXA.g             : num  0.0695 0.4832 0.8547 11.9184 11.6727 ...
##  $ DissOXA.g.SD          : num  0.0165 0.1143 0.2738 3.976 0.0873 ...
##  $ DissESA.g             : num  0.26 1.81 1.55 17.95 14.83 ...
##  $ DissESA.g.SD          : num  0.0504 0.3503 0.158 1.1855 0.3066 ...
##  $ FiltSmeto.mg.SD       : num  0.124 0.124 0.374 0.66 0.996 ...
##  $ FiltSmeto.g           : num  0.00345 0.00345 0.00573 0.00307 0.00352 ...
##  $ FiltSmeto.g.SD        : num  0.000124 0.000124 0.000374 0.00066 0.000996 ...
##  $ TotSMout.g            : num  0.00699 0.02806 0.17577 2.65298 2.36052 ...
##  $ TotSMout.g.SD         : num  0.000216 0.00137 0.005284 0.07989 0.048432 ...
##  $ MELsm.g               : num  0.302 2.078 2.379 30.241 27.008 ...
##  $ MELsm.g.SD            : num  0.0269 0.1868 0.1789 2.4062 0.1634 ...
##  $ CumOutDiss.g          : num  0.00354 0.02815 0.19818 2.84809 5.2051 ...
##  $ CumOutFilt.g          : num  0.00345 0.0069 0.01263 0.01571 0.01923 ...
##  $ CumOutSmeto.g         : num  0.00699 0.03505 0.21082 2.8638 5.22432 ...
##  $ CumOutMELsm.g         : num  0.302 2.38 4.76 35.001 62.009 ...
##  $ BalMassDisch.g        : num  9498 9495 9493 9463 9436 ...
##  $ prctMassOut           : num  4.98e-05 2.00e-04 1.25e-03 1.89e-02 1.68e-02 ...
##  $ FracDeltaOut          : num  0 0 0 -0.576 -0.515 ...
##  $ Events                : Factor w/ 51 levels "0-1","0-2","0-3",..: 1 2 3 4 5 6 7 8 9 10 ...
##  $ Weeks                 : Factor w/ 16 levels "W0","W1","W10",..: 1 1 1 2 2 2 9 9 9 10 ...
##  $ Event                 : Factor w/ 19 levels "0","1","2","3",..: 1 1 1 2 2 2 3 3 3 4 ...
```

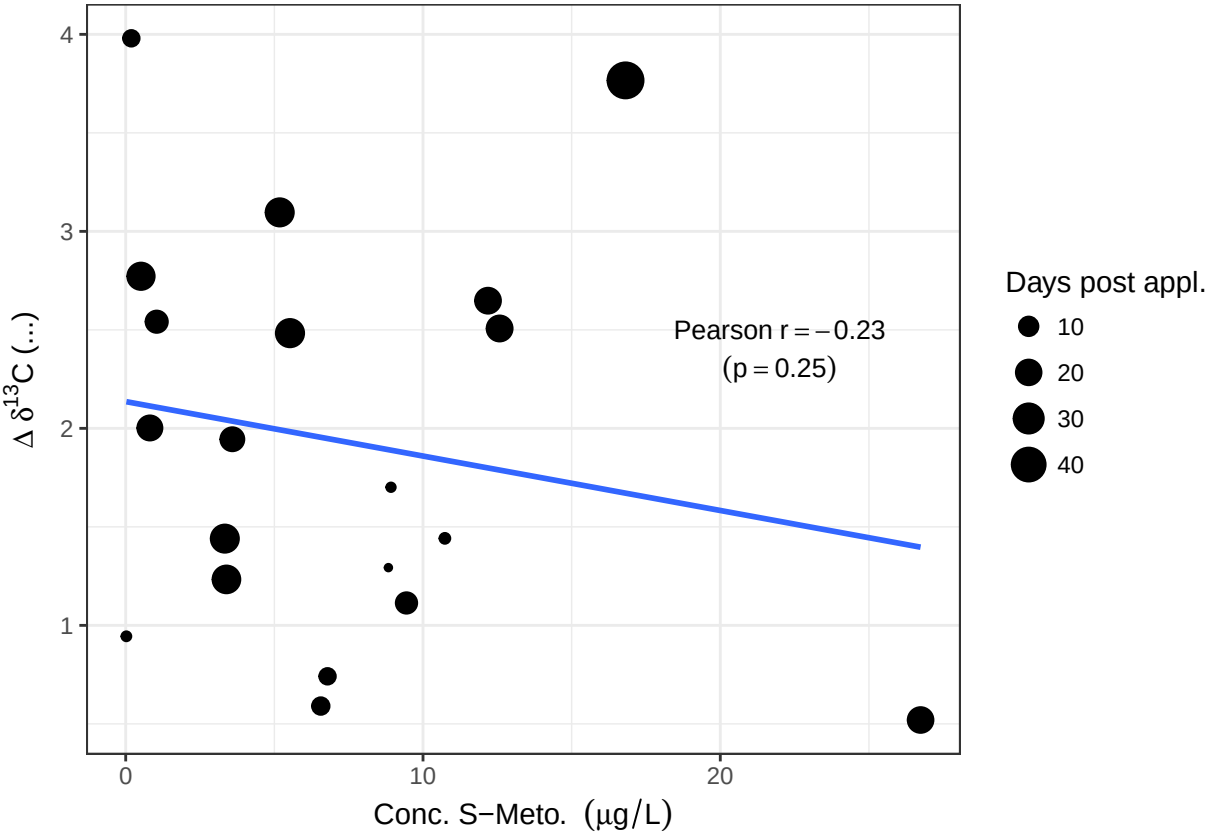
```
##  $ remainMedTheo_prc     : num  98.8 91 87.7 85.3 83.4 ...
##  $ remainMinTheo_prc     : num  99.3 94.2 92 90.5 89.2 ...
##  $ remainMaxTheo_prc     : num  97.2 79.7 72.8 68.1 64.4 ...
##  $ yRaleigh              : num  NA NA NA 0.000765 0.000609 ...
##  $ xRaleigh              : num  -4.69 -4.69 -2.03 -1.37 -1.4 ...
##  $ DIa                   : num  1.5 1.68 2.1 549.76 289.92 ...
```

```
ggplot(waterClean, aes(x=TotSMout.g, y=DD13C.diss))+
  geom_point(aes(group = Event, colour = Event))+
  theme_bw() +
  theme(legend.position="top"
        # axis.title.x = element_blank(),
        ) +
  guides(col = guide_legend(nrow =  3)) + #,
         # shape = guide_legend(nrow =  3)) +
  ylab(expression(paste({Delta~delta}^"13","C", ' (\u2030)'))) +
  # xlab(expression(paste("Conc. S-Meto.  ", {({mu}*g / L)}))) +
  geom_text_repel(aes(label=Events),
                  arrow = arrow(length = unit(0.005, 'npc'), type = "closed"),
                  force = 1,
                  point.padding = unit(1.0, 'lines'),
                  max.iter = 2e3,
                  nudge_x = .2)
```




```
# cor.test(waterClean$TotSMout.g, waterClean$DD13C.diss)

pearson_water_r <- cor.test(waterClean$Conc.mug.L, waterClean$DD13C.diss)[4]
water_r_label <- sprintf("Pearson~r == %0.2f", pearson_water_r)
water_p_value <- cor.test(waterClean$Conc.mug.L, waterClean$DD13C.diss)[3]
```

```
water_p_label <- sprintf("(p == %0.2f)", water_p_value)

waterIsoConc  <- ggplot(data = subset(waterClean, ngC.mean.diss > 5), aes(x=Conc.mug.L, y=DD13C.diss))+
  stat_smooth(data = subset(waterClean, ngC.mean.diss > 5),
              aes(x=Conc.mug.L, y=DD13C.diss), method = "lm", formula = y~x, se=F) +
  geom_point(aes(size = timeSinceApp)) +
  theme_bw() +
  scale_size_continuous(range = c(1, 6)) +
  labs(size="Days post appl.") +
  ylab(expression(paste({Delta~delta}^"13","C", ' (\u2030)'))) +
  xlab(expression(paste("Conc. S-Meto.  ", {({mu}*g / L)}))) +
  annotate("text", x = 22, y = 2.5, label = as.character(water_r_label), parse = T, size = 3.5) +
  annotate("text", x = 22, y = 2.3, label = water_p_label, parse = T, size = 3.5)

waterIsoConc
```




```
# ggsave(waterIsoConc , filename = "DDvsConc_water.png", width = 8, height = 5, units = "in", scale = 1
```

Correlations Waters

```
cor.test(waters$Conc.mug.L, waters$diss.d13C)
```

```
##
##  Pearson's product-moment correlation
##
## data:  waters$Conc.mug.L and waters$diss.d13C
```

```
## t = -1.1775, df = 25, p-value = 0.2501
## alternative hypothesis: true correlation is not equal to 0
## 95 percent confidence interval:
##  -0.5604226  0.1651756
## sample estimates:
##        cor
## -0.2292267
```

```
#cor.test(waters$TotSMout.g, waters$diss.d13C)

#esaoxa <- waters$MELsm.g-waters$TotSMout.g
# cor.test(esaoxa, waters$diss.d13C)
```

Merge Soil and Water data frames

Outlet Isotope Shifts (DD)

In the same plot consider this secondary axis, where the secondary axis is a formulat of the first:

ggplot(mpg, aes(displ, hwy)) + geom_point() + scale_y_continuous("mpg (US)", sec.axis = sec_axis(~ . * 1.20, name = "mpg (UK)"))

Or this: https://github.com/tidyverse/ggplot2/wiki/Align-two-plots-on-a-page

```
waterClean_ng <- subset(waterClean, ngC.mean.diss > 0)
WaterSoils <- merge(waterClean_ng, soils, by = "Date.ti", all = T)



str(WaterSoils)
```

```
## 'data.frame':    52 obs. of  112 variables:
##  $ Date.ti               : POSIXct, format: "2016-03-25 00:04:00" "2016-03-25 12:04:00" ...
##  $ WeekSubWeek           : Factor w/ 51 levels "W0-0x","W0-1",..: NA NA NA 4 5 NA 26 27 NA 29 ...
##  $ tf                    : Factor w/ 51 levels "2016-03-25 12:02:00",..: NA NA NA 4 5 NA 7 8 NA 10 .
##  $ iflux                 : num  NA NA NA 1.46 16.33 ...
##  $ fflux                 : num  NA NA NA 16.4 15.2 ...
##  $ changeflux            : num  NA NA NA 14.99 -1.15 ...
##  $ maxQ                  : num  NA NA NA 38.4 18.7 ...
##  $ minQ                  : num  NA NA NA 1.45 13.2 ...
##  $ dryHrs                : num  NA NA NA 66.13 1.65 ...
##  $ Duration.Hrs          : num  NA NA NA 27.3 23.1 ...
##  $ chExtreme             : num  NA NA NA 36.94 -3.13 ...
##  $ Peak                  : int  NA NA NA 1 NA NA 2 NA NA 3 ...
##  $ AveDischarge.m3.h     : num  NA NA NA 14.3 15.5 ...
##  $ Volume.m3             : num  NA NA NA 390 359 ...
##  $ Sampled.Hrs           : num  NA NA NA 27.3 23.1 ...
##  $ Sampled               : Factor w/ 2 levels "Not Sampled",..: NA NA NA 2 2 NA 2 2 NA 2 ...
##  $ Conc.mug.L            : num  NA NA NA 6.79 6.56 ...
##  $ Conc.SD               : num  NA NA NA 0.289 0.191 ...
##  $ OXA_mean              : num  NA NA NA 30.5 32.5 ...
##  $ OXA_SD                : num  NA NA NA 10.185 0.243 ...
##  $ ESA_mean              : num  NA NA NA 46 41.3 ...
##  $ ESA_SD                : num  NA NA NA 3.037 0.853 ...
```

```
##  $ diss.d13C.x           : num  NA NA NA -30.5 -30.6 ...
##  $ SD.d13C.x             : num  NA NA NA 0.106 0.151 ...
##  $ N_ngC.diss            : int  NA NA NA 3 3 NA 3 3 NA 3 ...
##  $ ngC.mean.diss         : num  NA NA NA 42.7 54.7 ...
##  $ ngC.SD.diss           : num  NA NA NA 1.92 2.54 ...
##  $ Conc.Solids.mug.gMES  : num  NA NA NA 0.126 0.436 ...
##  $ Conc.Solids.ug.gMES.SD: num  NA NA NA 0.0271 0.1232 ...
##  $ filt.d13C             : num  NA NA NA NA NA ...
##  $ filt.SD.d13C          : num  NA NA NA NA NA ...
##  $ N_ngC.fl              : int  NA NA NA NA NA NA 3 3 NA NA ...
##  $ ngC.mean.fl           : num  NA NA NA NA NA ...
##  $ ngC.SD.fl             : num  NA NA NA NA NA ...
##  $ DD13C.diss            : num  NA NA NA 0.741 0.59 ...
##  $ DD13C.filt            : num  NA NA NA NA NA ...
##  $ B.diss                : num  NA NA NA 35.4 29.4 ...
##  $ B.filt                : num  NA NA NA NA NA ...
##  $ NH4.mM                : num  NA NA NA 0.05 NA NA NA NA NA NA ...
##  $ TIC.ppm.filt          : num  NA NA NA 51.8 44.8 NA 66.7 52.1 NA 69.4 ...
##  $ Cl.mM                 : num  NA NA NA 1.48 1574 ...
##  $ NO3...mM              : num  NA NA NA 616 778 ...
##  $ PO4..mM               : int  NA NA NA NA NA NA NA NA NA NA ...
##  $ NPOC.ppm              : num  NA NA NA 4 4.4 NA 5.8 3.4 NA 9.1 ...
##  $ TIC.ppm.unfilt        : num  NA NA NA 44.8 26.4 NA 39 32.3 NA 54.8 ...
##  $ TOC.ppm.unfilt        : num  NA NA NA 4.7 5.4 NA 2.7 3.8 NA 3.9 ...
##  $ ExpMES.Kg             : num  NA NA NA 24.4 8.08 ...
##  $ Appl.Mass.g           : num  NA NA NA 0 0 ...
##  $ timeSinceApp.x        : num  NA NA NA 6.6 7.6 NA 12.6 14 NA 2.2 ...
##  $ CumAppMass.g.x        : num  NA NA NA 9498 9498 ...
##  $ DissSmeto.g           : num  NA NA NA 2.65 2.36 ...
##  $ DissSmeto.g.SD        : num  NA NA NA 0.113 0.0685 ...
##  $ DissOXA.g             : num  NA NA NA 11.9 11.7 ...
##  $ DissOXA.g.SD          : num  NA NA NA 3.976 0.0873 ...
##  $ DissESA.g             : num  NA NA NA 18 14.8 ...
##  $ DissESA.g.SD          : num  NA NA NA 1.186 0.307 ...
##  $ FiltSmeto.mg.SD       : num  NA NA NA 0.66 0.996 ...
##  $ FiltSmeto.g           : num  NA NA NA 0.00307 0.00352 ...
##  $ FiltSmeto.g.SD        : num  NA NA NA 0.00066 0.000996 ...
##  $ TotSMout.g            : num  NA NA NA 2.65 2.36 ...
##  $ TotSMout.g.SD         : num  NA NA NA 0.0799 0.0484 ...
##  $ MELsm.g               : num  NA NA NA 30.2 27 ...
##  $ MELsm.g.SD            : num  NA NA NA 2.406 0.163 ...
##  $ CumOutDiss.g          : num  NA NA NA 2.85 5.21 ...
##  $ CumOutFilt.g          : num  NA NA NA 0.0157 0.0192 ...
##  $ CumOutSmeto.g         : num  NA NA NA 2.86 5.22 ...
##  $ CumOutMELsm.g         : num  NA NA NA 35 62 ...
##  $ BalMassDisch.g        : num  NA NA NA 9463 9436 ...
##  $ prctMassOut           : num  NA NA NA 0.0189 0.0168 ...
##  $ FracDeltaOut          : num  NA NA NA -0.576 -0.515 ...
##  $ Events                : Factor w/ 51 levels "0-1","0-2","0-3",..: NA NA NA 4 5 NA 7 8 NA 10 ...
##  $ Weeks                 : Factor w/ 16 levels "W0","W1","W10",..: NA NA NA 2 2 NA 9 9 NA 10 ...
##  $ Event.x               : Factor w/ 19 levels "0","1","2","3",..: NA NA NA 2 2 NA 3 3 NA 4 ...
##  $ remainMedTheo_prc     : num  NA NA NA 85.3 83.4 ...
##  $ remainMinTheo_prc     : num  NA NA NA 90.5 89.2 ...
##  $ remainMaxTheo_prc     : num  NA NA NA 68.1 64.4 ...
```

```
##  $ yRaleigh              : num  NA NA NA 0.000765 0.000609 ...
##  $ xRaleigh              : num  NA NA NA -1.37 -1.4 ...
##  $ DIa                   : num  NA NA NA 550 290 ...
##  $ Event.y               : int  0 0 0 1 1 1 2 2 2 3 ...
##  $ timeSinceApp.y        : num  0.5 3.9 5.5 6.6 7.6 11.6 12.6 14 20.6 2.2 ...
##  $ diss.d13C.y           : num  NA NA NA -30.5 -30.6 ...
##  $ SD.d13C.y             : num  NA NA NA 0.106 0.151 ...
##  $ CumAppMass.g.y        : num  9498 9498 9498 9498 9498 ...
##  $ B.mean.comp.North     : num  NA NA NA NA NA ...
##  $ B.max.comp.North      : num  NA NA NA NA NA ...
##  $ B.min.comp.North      : num  NA NA NA NA NA ...
##  $ MassSoil.g.North      : num  12.4 NA NA 613.5 NA ...
##  $ comp.d13C.North       : num  NA NA NA NA NA ...
##  $ comp.d13C.SD.North    : num  NA NA NA NA NA ...
##  $ B.mean.comp.Talweg    : num  NA NA NA NA NA ...
##  $ B.max.comp.Talweg     : num  NA NA NA NA NA ...
##  $ B.min.comp.Talweg     : num  NA NA NA NA NA ...
##  $ MassSoil.g.Talweg     : num  4.33 NA NA 173.11 NA ...
##  $ comp.d13C.Talweg      : num  NA NA NA NA NA ...
##  $ comp.d13C.SD.Talweg   : num  NA NA NA NA NA ...
##  $ B.mean.comp.South     : num  NA NA NA NA NA ...
##  $ B.max.comp.South      : num  NA NA NA NA NA ...
##  $ B.min.comp.South      : num  NA NA NA NA NA ...
##   [list output truncated]
```

```
names(WaterSoils)
```

```
##   [1] "Date.ti"                "WeekSubWeek"
##   [3] "tf"                     "iflux"
##   [5] "fflux"                  "changeflux"
##   [7] "maxQ"                   "minQ"
##   [9] "dryHrs"                 "Duration.Hrs"
##  [11] "chExtreme"              "Peak"
##  [13] "AveDischarge.m3.h"      "Volume.m3"
##  [15] "Sampled.Hrs"            "Sampled"
##  [17] "Conc.mug.L"             "Conc.SD"
##  [19] "OXA_mean"               "OXA_SD"
##  [21] "ESA_mean"               "ESA_SD"
##  [23] "diss.d13C.x"            "SD.d13C.x"
##  [25] "N_ngC.diss"             "ngC.mean.diss"
##  [27] "ngC.SD.diss"            "Conc.Solids.mug.gMES"
##  [29] "Conc.Solids.ug.gMES.SD" "filt.d13C"
##  [31] "filt.SD.d13C"           "N_ngC.fl"
##  [33] "ngC.mean.fl"            "ngC.SD.fl"
##  [35] "DD13C.diss"             "DD13C.filt"
##  [37] "B.diss"                 "B.filt"
##  [39] "NH4.mM"                 "TIC.ppm.filt"
##  [41] "Cl.mM"                  "NO3...mM"
##  [43] "PO4..mM"                "NPOC.ppm"
##  [45] "TIC.ppm.unfilt"         "TOC.ppm.unfilt"
##  [47] "ExpMES.Kg"              "Appl.Mass.g"
##  [49] "timeSinceApp.x"         "CumAppMass.g.x"
##  [51] "DissSmeto.g"            "DissSmeto.g.SD"
##  [53] "DissOXA.g"              "DissOXA.g.SD"
##  [55] "DissESA.g"              "DissESA.g.SD"
```

```
##  [57] "FiltSmeto.mg.SD"       "FiltSmeto.g"
##  [59] "FiltSmeto.g.SD"        "TotSMout.g"
##  [61] "TotSMout.g.SD"         "MELsm.g"
##  [63] "MELsm.g.SD"            "CumOutDiss.g"
##  [65] "CumOutFilt.g"          "CumOutSmeto.g"
##  [67] "CumOutMELsm.g"         "BalMassDisch.g"
##  [69] "prctMassOut"           "FracDeltaOut"
##  [71] "Events"                "Weeks"
##  [73] "Event.x"               "remainMedTheo_prc"
##  [75] "remainMinTheo_prc"     "remainMaxTheo_prc"
##  [77] "yRaleigh"              "xRaleigh"
##  [79] "DIa"                   "Event.y"
##  [81] "timeSinceApp.y"        "diss.d13C.y"
##  [83] "SD.d13C.y"             "CumAppMass.g.y"
##  [85] "B.mean.comp.North"     "B.max.comp.North"
##  [87] "B.min.comp.North"      "MassSoil.g.North"
##  [89] "comp.d13C.North"       "comp.d13C.SD.North"
##  [91] "B.mean.comp.Talweg"    "B.max.comp.Talweg"
##  [93] "B.min.comp.Talweg"     "MassSoil.g.Talweg"
##  [95] "comp.d13C.Talweg"      "comp.d13C.SD.Talweg"
##  [97] "B.mean.comp.South"     "B.max.comp.South"
##  [99] "B.min.comp.South"      "MassSoil.g.South"
## [101] "comp.d13C.South"       "comp.d13C.SD.South"
## [103] "ID.S"                  "CatchMassSoil.g"
## [105] "BulkMass.g"            "BulkCatch.d13"
## [107] "BulkCatch.d13.SD"      "f.mean.bulk"
## [109] "B.mean.bulk"           "DD13C.North"
## [111] "DD13C.Talweg"          "DD13C.South"
```

```
keepWS <- c("Date.ti", "WeekSubWeek", "maxQ", "AveDischarge.m3.h",
            "DD13C.diss", "SD.d13C.x",
            "DD13C.filt", "filt.SD.d13C",
            "DD13C.Talweg", "comp.d13C.SD.Talweg",
            "DD13C.South", "comp.d13C.SD.South",
            "DD13C.North", "comp.d13C.SD.North",
            "Event.x", "BulkCatch.d13", "BulkCatch.d13.SD"
            #"timeSinceApp.x", "Event.x", "Events"
            )
wsSmall <- WaterSoils[ , (names(WaterSoils) %in% keepWS)]

wsSmall$DD13.Bulk <- wsSmall$BulkCatch.d13-initialDelta

names(wsSmall)
```

```
##  [1] "Date.ti"             "WeekSubWeek"         "maxQ"
##  [4] "AveDischarge.m3.h"   "SD.d13C.x"           "filt.SD.d13C"
##  [7] "DD13C.diss"          "DD13C.filt"          "Event.x"
## [10] "comp.d13C.SD.North"  "comp.d13C.SD.Talweg" "comp.d13C.SD.South"
## [13] "BulkCatch.d13"       "BulkCatch.d13.SD"    "DD13C.North"
## [16] "DD13C.Talweg"        "DD13C.South"         "DD13.Bulk"
```

```
wsSmall <- wsSmall[c("Date.ti", "Event.x", "WeekSubWeek", "maxQ", "AveDischarge.m3.h",
            "DD13C.diss", "SD.d13C.x",
            "DD13C.filt", "filt.SD.d13C" ,
            "DD13C.Talweg", "comp.d13C.SD.Talweg",
```

```
            "DD13C.South", "comp.d13C.SD.South",
            "DD13C.North", "comp.d13C.SD.North",
            "DD13.Bulk", "BulkCatch.d13.SD")]

names(wsSmall) <- c("Date", "Event", "Week", "Qmax", "Qmean",
            "diss.measure", "diss.SD",
            "filt.measure", "filt.SD",
            "Talweg.measure", "Talweg.SD",
            "South.measure", "South.SD",
            "North.measure", "North.SD",
            "BulkDD.measure", "BulkDD.SD"
            )
# Conventional way of melting won't work if we need SDs.
# ws <- melt(wsSmall, id=c("Date.ti", "timeSinceApp.x", "Events", "Event.x"))

# Need to rename the columns so that I can use separate and spread from the package tidyr
#names(wsSmall)[-1][seq(2, length(names(wsSmall)) - 1, 2)] <-
#  paste0(names(wsSmall)[-1][seq(1, length(names(wsSmall)) - 1, 2)], "-SD")
#names(wsSmall)[-1][seq(1, length(names(wsSmall)) - 1, 2)] <-
#  paste0(names(wsSmall)[-1][seq(1, length(names(wsSmall)) - 1, 2)], "-measure")

wstidier <- wsSmall %>%
  gather(measure, value, -Date, -Event, -Week, -Qmax, -Qmean) %>% # Melts data frame
  separate(measure, into = c("Location", "temporary_var")) %>% # parses the sep = "." into...
  spread(temporary_var, value)

wstidier$Type <- ifelse(wstidier$Location == "diss", "Dissolved",
                  ifelse(wstidier$Location == "filt", "Sediment",
                        "Top Soil"))

wstidier$Source <- ifelse(wstidier$Location == "diss", "Outlet",
                  ifelse(wstidier$Location == "filt", "Outlet",
                         ifelse(wstidier$Location == "South", "South",
                                ifelse(wstidier$Location == "Talweg", "Valley",
                                       ifelse(wstidier$Location == "BulkDD", "Bulk",
                                       "North"))) ))

wstidier$Source <- as.factor(wstidier$Source)
wstidier$Type <- as.factor(wstidier$Type)
wstidier$Event <- as.numeric(wstidier$Event)

# Copy all data
wstidierAll <- wstidier

levels(wstidier$Source)
```

```
## [1] "Bulk"   "North"  "Outlet" "South"  "Valley"
```

```
levels(wstidier$Type)
```

```
## [1] "Dissolved" "Sediment"  "Top Soil"
```

```
#wstidier$Source <- factor(wstidier$Source, levels = c("Bulk", "Plateau","Valley", "Outlet"))
wstidier$Source <- factor(wstidier$Source, levels = c("Bulk", "North", "Valley", "South", "Outlet"))
wstidier$Type <- factor(wstidier$Type, levels = c("Top Soil", "Dissolved", "Sediment" ))
```

```r
# epsilon
epsilon_field <- cof
initialDelta
```

```
## [1] -31.2144
```

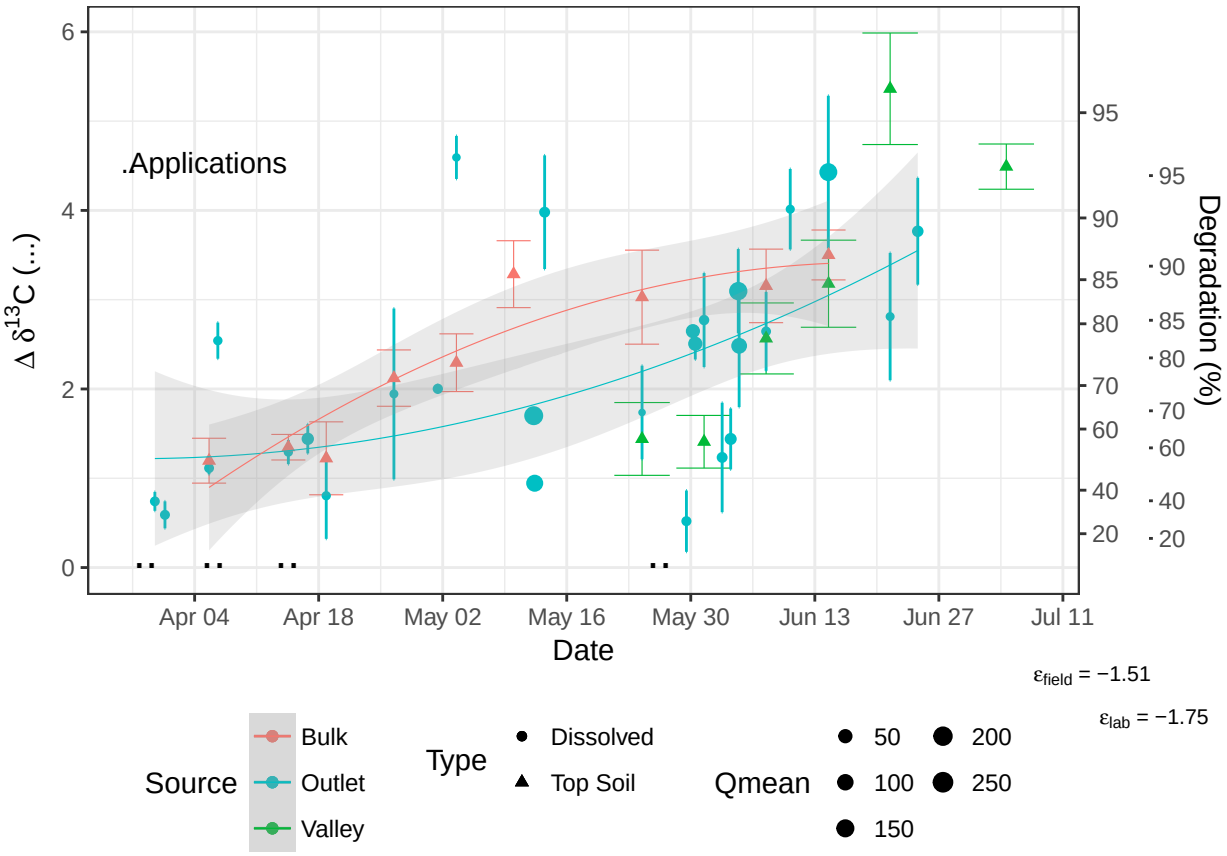
```r
wstidier$DegField <- (1-((1000 + d13Co + wstidier$measure)/(1000+d13Co))^(1000/epsilon_field))*100
wstidier$DegLab <- (1-((1000 + d13Co + wstidier$measure)/(1000+d13Co))^(1000/epsilon_lab))*100

wstidier$DegDiff <- (wstidier$DegField - wstidier$DegLab)

wstidier$Location <- as.factor(wstidier$Location)
#wstidier$Week <- as.factor(wstidier$Week)

#library(dplyr)
#detach("package:plyr")
sumary <- na.omit(wstidier) %>%
  group_by(Type) %>%
  summarise(mean = mean(DegDiff))

limits_DdC <- aes(ymin=measure-SD, ymax=measure+SD, colour = Source)



wstidier2 = subset(wstidier, SD <= 1 ) #& Source != "Bulk"  ) #& Date < as.POSIXct('2016-06-14 08:04:00
NoBASE <- subset(wstidier2, Week != "W6-1" )

pd <- position_dodge(width = 0.4)
wsALL_lab <- ggplot(data = wstidier2, aes(x = Date, y = measure, group = Source) )+
  geom_errorbar(data=subset(wstidier2, Source == 'Bulk'), limits_DdC, size=0.2) +
  geom_errorbar(data=subset(wstidier2, Source == 'Valley' &
                              Date > as.POSIXct('2016-05-14 08:04:00')), limits_DdC, size=0.2) +
  geom_errorbar(data=subset(wstidier2, Source == 'Outlet'), limits_DdC) +
  #geom_point(data=subset(wstidier2, Source == 'Outlet'), aes(shape = Type, colour = Source, size = Qma
  geom_point(data=subset(wstidier2, Source == 'Outlet'), aes(shape = Type, colour = Source, size = Qmea
  geom_point(data=subset(wstidier2, Source == 'Bulk'), aes(shape = Type, colour = Source)) +
  geom_point(data=subset(wstidier2, Source == 'Valley' &
                           Date > as.POSIXct('2016-05-14 08:04:00')), aes(shape = Type, colour = Source

  #stat_smooth(data=subset(wstidier,
  #                        (Source == "Valley" & Event > 8 )),
  #            method = "lm", formula = y ~ poly(x, 2), se = F, colour = 'darkgreen' , alpha = 0.1, siz
  #stat_smooth(data=subset(wstidier,
  #                        (Source != "Outlet" & Source != "Valley" & Event < 20 )),
  #            method = "lm", formula = y ~  poly(x, 2), se = F, alpha = 0.1, size=0.2) +

  # Water
  stat_smooth(data=subset(NoBASE,
                          (Source == "Outlet" & Event > 1 & Type == "Dissolved")),
              method = "lm", formula = y ~ poly(x, 2), se = T, aes(colour = 'Outlet'), alpha = 0.2, siz
  # North
  stat_smooth(data=subset(wstidier2,
                          (Source == "Bulk" )), #| Source == "South" )),
```

```
              method = "lm", formula = y ~ poly(x, 2), se = T, aes(colour = 'Bulk'), alpha = 0.2, size=0
  #stat_smooth(data=subset(wstidier2,
  #                         (Source == "South")),
  #            method = "lm", formula = y ~ poly(x, 2), se = T, aes(colour = 'South'), alpha = 0.2, siz
  theme_bw() +
  # Applics
  annotate("text", x = as.POSIXct('2016-03-28 08:04:00'), y = 0,
           label = as.character(expression(paste( "\u066D"))), parse = T, size = 6.0) +
  annotate("text", x = as.POSIXct('2016-04-05 00:04:00'), y = 0,
           label = as.character(expression(paste( "\u066D"))), parse = T, size = 6.0) +
  annotate("text", x = as.POSIXct('2016-04-13 08:04:00'), y = 0,
           label = as.character(expression(paste( "\u066D"))), parse = T, size = 6.0) +
  annotate("text", x = as.POSIXct('2016-05-25 08:04:00'), y = 0,
           label = as.character(expression(paste( "\u066D"))), parse = T, size = 6.0) +
  # Title applics
  annotate("text", x = as.POSIXct('2016-04-05 08:04:00'), y = 4.5,
           label = as.character(expression(paste( "\u066D", " Applications"))), parse = T, size = 4.0) +

  scale_x_datetime(breaks = date_breaks("2 weeks"), labels = date_format("%b %d")) +
  theme(legend.position="top"
        # axis.title.x = element_blank(),
        # axis.text.x=element_text(angle = 45, hjust = 1)
        ) +
  # geom_smooth(data=subset(ws, Source != "Outlet"), method = "lm", formula = y ~ poly(x, 2)) +
  xlab("Date") +
  #ylab(expression(paste({Delta~delta}^"13","C", ' (\u2030)'))) +
  scale_y_continuous(
    expression(paste({Delta~delta}^"13","C", ' (\u2030)')),
    sec.axis = sec_axis(trans = ~ (1-((1000 + d13Co + .)/(1000+d13Co))^(1000/epsilon_lab))*100 ,
                        name = element_blank(), breaks=c(20, 40, 60, 70, 80, 85, 90, 95) )# breaks=seq(
  )  +
  scale_color_manual(name= "Source",
                     values = c("#F8766D", "#00BFC4", "#00BA38", "#B79F00", "#619CFF", "#F564E3",
                                "#D55E00", "darkgreen", "dodgerblue")
                     ) +
  scale_size_continuous(range = c(1, 3)) # +
  # scale_shape_manual(name= )


wsALL_field <- ggplot(data = wstidier2, aes(x = Date, y = measure, group = Source) )+
  geom_errorbar(data=subset(wstidier2, Source == 'Bulk'), limits_DdC, size=0.2) +
  geom_errorbar(data=subset(wstidier2, Source == 'Valley' &
                              Date > as.POSIXct('2016-05-14 08:04:00')), limits_DdC, size=0.2) +
  geom_errorbar(data=subset(wstidier2, Source == 'Outlet'), limits_DdC) +
  #geom_point(data=subset(wstidier2, Source == 'Outlet'), aes(shape = Type, colour = Source, size = Qmas
  geom_point(data=subset(wstidier2, Source == 'Outlet'), aes(shape = Type, colour = Source, size = Qmean
  geom_point(data=subset(wstidier2, Source == 'Bulk'), aes(shape = Type, colour = Source)) +
  geom_point(data=subset(wstidier2, Source == 'Valley' &
                           Date > as.POSIXct('2016-05-14 08:04:00')), aes(shape = Type, colour = Source)

  #stat_smooth(data=subset(wstidier,
  #                         (Source == "Valley" & Event > 8 )),
  #            method = "lm", formula = y ~ poly(x, 2), se = F, colour = 'darkgreen' , alpha = 0.1, siz
```

```
#stat_smooth(data=subset(wstidier,
#                         (Source != "Outlet" & Source != "Valley" & Event < 20 )),
#            method = "lm", formula = y ~  poly(x, 2), se = F, alpha = 0.1, size=0.2) +

# Water
stat_smooth(data=subset(wstidier2, #NoBASE,
                        (Source == "Outlet" & Event > 1 & Type == "Dissolved")),
            method = "lm", formula = y ~ poly(x, 2), se = T, aes(colour = 'Outlet'), alpha = 0.2, size
# North
stat_smooth(data=subset(wstidier2,
                        (Source == "Bulk" )), #| Source == "South" )),
            method = "lm", formula = y ~ poly(x, 2), se = T, aes(colour = 'Bulk'), alpha = 0.2, size=0
#stat_smooth(data=subset(wstidier2,
#                         (Source == "South")),
#            method = "lm", formula = y ~ poly(x, 2), se = T, aes(colour = 'South'), alpha = 0.2, siz
theme_bw() +
# Applics
annotate("text", x = as.POSIXct('2016-03-28 08:04:00'), y = 0,
         label = as.character(expression(paste( "\u066D"))), parse = T, size = 6.0) +
annotate("text", x = as.POSIXct('2016-04-05 00:04:00'), y = 0,
         label = as.character(expression(paste( "\u066D"))), parse = T, size = 6.0) +
annotate("text", x = as.POSIXct('2016-04-13 08:04:00'), y = 0,
         label = as.character(expression(paste( "\u066D"))), parse = T, size = 6.0) +
annotate("text", x = as.POSIXct('2016-05-25 08:04:00'), y = 0,
         label = as.character(expression(paste( "\u066D"))), parse = T, size = 6.0) +
# Title applics
annotate("text", x = as.POSIXct('2016-04-05 08:04:00'), y = 4.5,
         label = as.character(expression(paste( "\u066D", " Applications"))), parse = T, size = 4.0) +

scale_x_datetime(breaks = date_breaks("1 month"), labels = date_format("%b %d")) +
theme(legend.position="top"
      # axis.title.x = element_blank()
      # axis.text.x=element_text(angle = 45, hjust = 1)
      ) +
# geom_smooth(data=subset(ws, Source != "Outlet"), method = "lm", formula = y ~ poly(x, 2)) +
xlab("Date") +
#ylab(expression(paste({Delta~delta}^"13","C", ' (\u2030)'))) +
scale_y_continuous(
  expression(paste({Delta~delta}^"13","C", ' (\u2030)')),
  sec.axis = sec_axis(trans = ~ (1-((1000 + d13Co + .)/(1000+d13Co))^(1000/epsilon_field))*100 ,
                      name = "Degradation (%)", breaks=c(20, 40, 60, 70, 80, 85, 90, 95) )# breaks=se
)  +
scale_color_manual(name= "Source",
                   values = c("#F8766D", "#00BFC4", "#00BA38", "#B79F00", "#619CFF", "#F564E3",
                              "#D55E00", "darkgreen", "dodgerblue")
                  ) +
scale_size_continuous(range = c(1, 3)) +
guides(col = guide_legend(nrow =  3), shape=guide_legend(nrow=2), size = guide_legend(nrow=3))# +
# scale_shape_manual(name= )
```

Join all figures

```
#wsALL_lab
#wsALL_field
#wsPlot
# ggsave(wsALL, filename = "WaterSoilvsTime.png", width = 8, height = 5, units = "in", scale = 1)
# ggsave(wsALL, filename = "WaterBulkvsTime.png", width = 8, height = 5, units = "in", scale = 1)

wsALL_field_noLeg <- wsALL_field + theme(legend.position='none')
wsALL_lab_noLeg <- wsALL_lab + theme(legend.position='none')
wsAll_field_Leg  <- get_legend(wsALL_field)



label <- substitute(paste(epsilon, " = ", epsilon_f, ", Field", epsilon, " = " , epsilon_l),
                    list(epsilon_f = signif(epsilon_field, 2), epsilon_l = signif(epsilon_lab, 2) ))

label2 <- substitute(paste(epsilon ["field"] , " = ", epsilon_f),
                     list(epsilon_f = signif(epsilon_field, 3)))

label3 <- substitute(paste(epsilon ["lab"] , " = ", epsilon_l),
                     list(epsilon_l = signif(epsilon_lab, 3)))
# adding label via ggdraw, in the ggdraw coordinates


wsALL <- ggdraw() +
  draw_plot(wsALL_field_noLeg, x=0, y=.2, width = 1, height = .8) +
  draw_plot(wsALL_lab_noLeg, x=0, y = 0.2, width = 0.935, height = 0.8) +
  draw_label(label2, x= .89, y = .2, size = 8) +
  draw_label(label3, x= .94, y = .15, size = 8) +
  draw_plot(wsAll_field_Leg, x=0.2, y=0.0, width = 0.55, height = 0.15)

wsALL
```

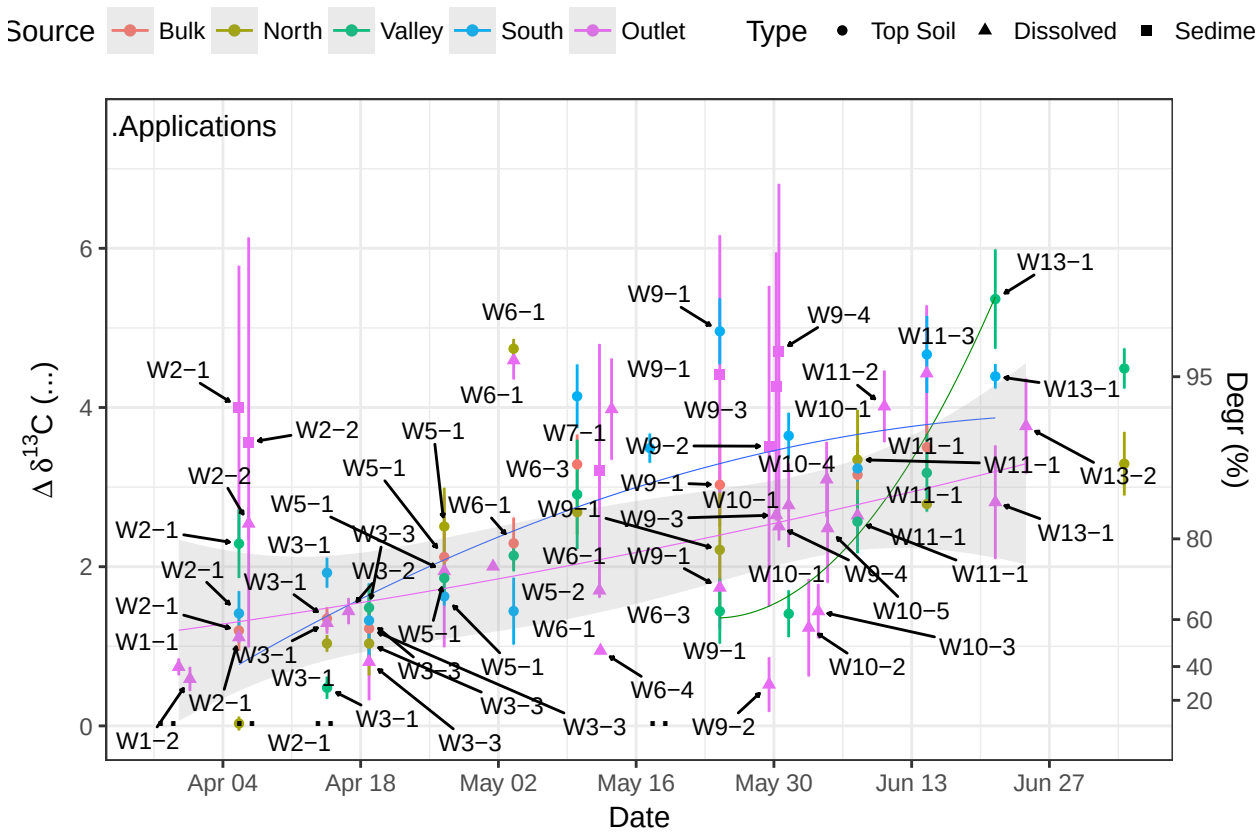



```
#ggsave(wsALL, filename = "WaterSoilvsTime.png", width = 8, height = 5, units = "in", scale = 1)
```

Soils and Water with labels (inspection)

```
# Data without the Plateau
#wsNoPlat <- subset(wstidierAll, Source != "Plateau")
wsNoPlat <- subset(wstidier, SD < 4)
#wsNoPlat$Source <- factor(wsNoPlat$Source, levels = c("Bulk", "Valley", "Outlet"))
#levels(wsNoPlat$Source)

# Subset the data to values with SD < 1
#wsNoPlat2 = subset(wsNoPlat, SD < 1.50)


limits_DdC <- aes(ymin=measure-SD, ymax=measure+SD, colour = Source)

wsPlot <- ggplot(data = wsNoPlat, aes(x = Date, y = measure)) +
  geom_errorbar(limits_DdC) +
  geom_jitter(aes(shape = Type, colour = Source)) +
  stat_smooth(data=subset(wsNoPlat,
                          (Source == "Valley" & Event > 8 )),
              method = "lm", formula = y ~ poly(x, 2), se = F, colour = 'green4' , alpha = 0.1, size=0.
  stat_smooth(data=subset(wsNoPlat,
                          (Source != "Outlet" & Source != "Valley" & Event < 20 )),
```

```
              method = "lm", formula = y ~  poly(x, 2), se = F, alpha = 0.1, size=0.2) +
  stat_smooth(data=subset(wsNoPlat,
                          (Source == "Outlet" & Event > 1 & Type == "Dissolved")),
              method = "lm", formula = y ~ poly(x, 2), se = T, aes(colour = 'Outlet'), alpha = 0.2, size
  #stat_smooth(data=subset(wsNoPlat,
  #                        (Source == "Bulk")),
  #            method = "lm", formula = y ~ poly(x, 2), se = T, aes(colour = 'Bulk'), alpha = 0.2, size
  theme_bw() +
  # Applics
  annotate("text", x = as.POSIXct('2016-03-28 08:04:00'), y = 0,
           label = as.character(expression(paste( "\u066D"))), parse = T, size = 6.0) +
  annotate("text", x = as.POSIXct('2016-04-05 08:04:00'), y = 0,
           label = as.character(expression(paste( "\u066D"))), parse = T, size = 6.0) +
  annotate("text", x = as.POSIXct('2016-04-13 08:04:00'), y = 0,
           label = as.character(expression(paste( "\u066D"))), parse = T, size = 6.0) +
  annotate("text", x = as.POSIXct('2016-05-17 08:04:00'), y = 0,
           label = as.character(expression(paste( "\u066D"))), parse = T, size = 6.0) +
  # Title applics
  annotate("text", x = as.POSIXct('2016-04-01 08:04:00'), y = 7.5,
           label = as.character(expression(paste( "\u066D", " Applications"))), parse = T, size = 4.0) +

  scale_x_datetime(breaks = date_breaks("2 weeks"), labels = date_format("%b %d")) +
  theme(legend.position="top"
        # axis.title.x = element_blank(),
        # axis.text.x=element_text(angle = 45, hjust = 1)
        ) +
  # geom_smooth(data=subset(ws, Source != "Outlet"), method = "lm", formula = y ~ poly(x, 2)) +
  xlab("Date") +
  #ylab(expression(paste({Delta~delta}^"13","C", ' (\u2030)'))) +
  scale_y_continuous(
    expression(paste({Delta~delta}^"13","C", ' (\u2030)')),
    sec.axis = sec_axis(trans = ~ (1-((1000 + d13Co + .)/(1000+d13Co))^(1000/epsilon_field))*100 ,
                        name = "Degr (%)", breaks=c(20, 40, 60, 80, 95) )# breaks=seq(20, 120, 15))
  ) +
  geom_text_repel(aes(label=as.factor(Week)),
                  size = 3,
                   arrow = arrow(length = unit(0.005, 'npc'), type = "closed"),
                   force = 0.5,
                   point.padding = unit(0.5, 'lines'),
                  max.iter = 2e3,
                 nudge_x = .05)

# +
  #scale_color_manual(name= "Source",
  #                    values = c("black", "dodgerblue", "green", "red")
  #                   ) +
  # scale_shape_manual(name= )

wsPlot
```



Testing difference in $\Delta\delta$ between groups

Based on ANOVA tests, there is:

- No significant difference between soils and water

```
names(WaterSoils)
```

```
##   [1] "Date.ti"                  "WeekSubWeek"
##   [3] "tf"                       "iflux"
##   [5] "fflux"                    "changeflux"
##   [7] "maxQ"                     "minQ"
##   [9] "dryHrs"                   "Duration.Hrs"
##  [11] "chExtreme"                "Peak"
##  [13] "AveDischarge.m3.h"        "Volume.m3"
##  [15] "Sampled.Hrs"              "Sampled"
##  [17] "Conc.mug.L"               "Conc.SD"
##  [19] "OXA_mean"                 "OXA_SD"
##  [21] "ESA_mean"                 "ESA_SD"
##  [23] "diss.d13C.x"              "SD.d13C.x"
##  [25] "N_ngC.diss"               "ngC.mean.diss"
##  [27] "ngC.SD.diss"              "Conc.Solids.mug.gMES"
##  [29] "Conc.Solids.ug.gMES.SD"   "filt.d13C"
##  [31] "filt.SD.d13C"             "N_ngC.fl"
##  [33] "ngC.mean.fl"              "ngC.SD.fl"
##  [35] "DD13C.diss"               "DD13C.filt"
##  [37] "B.diss"                   "B.filt"
```

```
##  [39] "NH4.mM"                "TIC.ppm.filt"
##  [41] "Cl.mM"                 "NO3...mM"
##  [43] "PO4..mM"               "NPOC.ppm"
##  [45] "TIC.ppm.unfilt"        "TOC.ppm.unfilt"
##  [47] "ExpMES.Kg"             "Appl.Mass.g"
##  [49] "timeSinceApp.x"        "CumAppMass.g.x"
##  [51] "DissSmeto.g"           "DissSmeto.g.SD"
##  [53] "DissOXA.g"             "DissOXA.g.SD"
##  [55] "DissESA.g"             "DissESA.g.SD"
##  [57] "FiltSmeto.mg.SD"       "FiltSmeto.g"
##  [59] "FiltSmeto.g.SD"        "TotSMout.g"
##  [61] "TotSMout.g.SD"         "MELsm.g"
##  [63] "MELsm.g.SD"            "CumOutDiss.g"
##  [65] "CumOutFilt.g"          "CumOutSmeto.g"
##  [67] "CumOutMELsm.g"         "BalMassDisch.g"
##  [69] "prctMassOut"           "FracDeltaOut"
##  [71] "Events"                "Weeks"
##  [73] "Event.x"               "remainMedTheo_prc"
##  [75] "remainMinTheo_prc"     "remainMaxTheo_prc"
##  [77] "yRaleigh"              "xRaleigh"
##  [79] "DIa"                   "Event.y"
##  [81] "timeSinceApp.y"        "diss.d13C.y"
##  [83] "SD.d13C.y"             "CumAppMass.g.y"
##  [85] "B.mean.comp.North"     "B.max.comp.North"
##  [87] "B.min.comp.North"      "MassSoil.g.North"
##  [89] "comp.d13C.North"       "comp.d13C.SD.North"
##  [91] "B.mean.comp.Talweg"    "B.max.comp.Talweg"
##  [93] "B.min.comp.Talweg"     "MassSoil.g.Talweg"
##  [95] "comp.d13C.Talweg"      "comp.d13C.SD.Talweg"
##  [97] "B.mean.comp.South"     "B.max.comp.South"
##  [99] "B.min.comp.South"      "MassSoil.g.South"
## [101] "comp.d13C.South"       "comp.d13C.SD.South"
## [103] "ID.S"                  "CatchMassSoil.g"
## [105] "BulkMass.g"            "BulkCatch.d13"
## [107] "BulkCatch.d13.SD"      "f.mean.bulk"
## [109] "B.mean.bulk"           "DD13C.North"
## [111] "DD13C.Talweg"          "DD13C.South"
```

```
keepDDtest <- c(
  "Date.ti",
  "diss.d13C.x", # "DD13C.diss",
  "comp.d13C.North", "comp.d13C.Talweg", "comp.d13C.South" #,
  #"DD13C.North", "DD13C.Talweg", "DD13C.South"
)

wsStatTest <- WaterSoils[, colnames(WaterSoils) %in% keepDDtest]

mwsStatTest <- melt(wsStatTest, id="Date.ti")
mwsStatTest$Group1 <- ifelse(mwsStatTest$variable == "diss.d13C.x", "Outlet", "Soil")
mwsStatTest$Group2 <- ifelse(mwsStatTest$variable == "diss.d13C.x", "Outlet",
                             ifelse(mwsStatTest$variable == "comp.d13C.Talweg", "Valley", "Plateau"))
mwsStatTest$Group3 <- ifelse(mwsStatTest$variable == "diss.d13C.x" &
                               mwsStatTest$Date.ti > as.POSIXct('2016-06-05 00:06:00', tz = 'EST'), "Ou
                       ifelse(mwsStatTest$variable == "diss.d13C.x" &
```

```
                              mwsStatTest$Date.ti <= as.POSIXct('2016-06-05 00:06:00', tz = 'EST'), "Ou
                      ifelse(mwsStatTest$variable == "comp.d13C.Talweg" &
                              mwsStatTest$Date.ti > as.POSIXct('2016-06-05 00:06:00', tz = 'EST'), "Val
                      ifelse(mwsStatTest$variable == "comp.d13C.Talweg" &
                              mwsStatTest$Date.ti <= as.POSIXct('2016-06-05 00:06:00', tz = 'EST'), "Va
                      ifelse( (mwsStatTest$variable == "comp.d13C.North" | mwsStatTest$variable == "comp
                              mwsStatTest$Date.ti <= as.POSIXct('2016-06-05 00:06:00', tz = 'EST'), "Pl
                      ifelse( (mwsStatTest$variable == "comp.d13C.North" | mwsStatTest$variable == "comp
                              mwsStatTest$Date.ti > as.POSIXct('2016-06-05 00:06:00', tz = 'EST'), "Pla
                             ))))))

Gr1 <- na.omit(mwsStatTest[, colnames(mwsStatTest) %in% c("value", "Group1")])
Gr2 <- na.omit(mwsStatTest[, colnames(mwsStatTest) %in% c("value", "Group2")])
Gr3 <- na.omit(mwsStatTest[, colnames(mwsStatTest) %in% c("value", "Group3")])


# Test for homogeneity of variance
# Large p-value means no confirmation of homogeneity of variance
bartlett.test(value ~ as.factor(Group3), data = Gr3)
```

```
##
##  Bartlett test of homogeneity of variances
##
## data:  value by as.factor(Group3)
## Bartlett's K-squared = 6.27, df = 5, p-value = 0.2808
```

```
# Non-parameteric
# Reject Ho that pop. means are the same if low p-value
res.krs.Grp3 <- kruskal.test(value ~ as.factor(Group3), data = Gr3)
res.krs.Grp3
```

```
##
##  Kruskal-Wallis rank sum test
##
## data:  value by as.factor(Group3)
## Kruskal-Wallis chi-squared = 26.435, df = 5, p-value = 7.346e-05
```

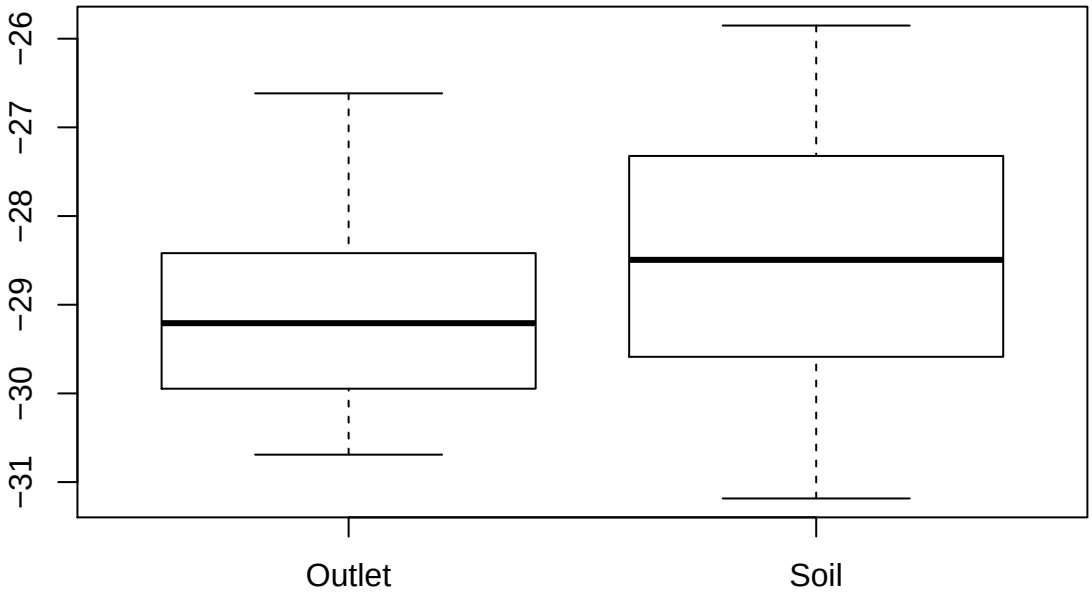
```
# Want a TukeyHSD function, but this only works with
# parametric data. So, will pass the ranks of the data instead of the actual values
Gr3.ranks <- rank( Gr3$value )
Gr3.groups <- Gr3$Group3
group3.aov <- aov(Gr3.ranks ~ Gr3.groups)
res.grp3 <- TukeyHSD(group3.aov, ordered = T)
aov.res.grp3.df <- as.data.frame(res.grp3$Gr3.groups)
aov.res.grp3.df$P <- round(aov.res.grp3.df$`p adj`, 3)
# High p-value indicates no significant difference
write.csv(aov.res.grp3.df, "aovResISOs_ranked.csv", row.names = T)
```

ANOVA and ANOSIM

Not actually used, as Grouping 3 does not have homegenity of variance

```
# Simple ANOVA tests
# (high p-value indicates lack of difference)
```

```r
# Big P-value no significant difference
boxplot(Gr1$value ~ Gr1$Group1)
```



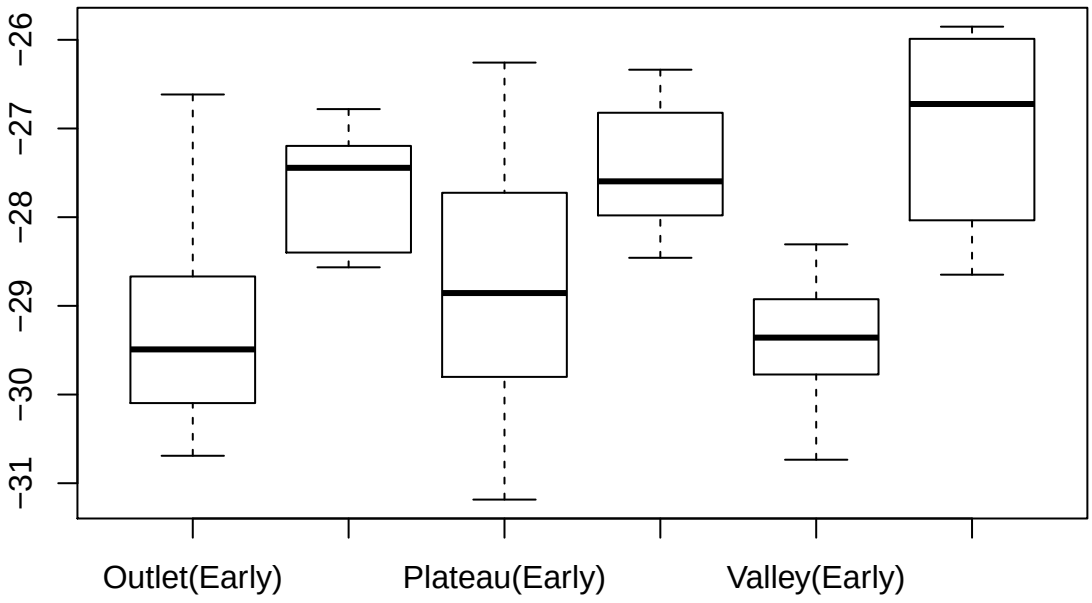

```r
summary(aov(Gr1$value ~ Gr1$Group1))
```

```
##             Df Sum Sq Mean Sq F value Pr(>F)
## Gr1$Group1   1   5.99   5.995   3.549 0.0639 .
## Residuals   67 113.18   1.689
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```r
TukeyHSD(aov(Gr1$value ~ Gr1$Group1))
```

```
##   Tukey multiple comparisons of means
##     95% family-wise confidence level
##
## Fit: aov(formula = Gr1$value ~ Gr1$Group1)
##
## $`Gr1$Group1`
##                 diff         lwr     upr     p adj
## Soil-Outlet 0.603957 -0.03596571 1.24388 0.0639287
```

```r
boxplot(Gr3$value ~ Gr3$Group3)
```




```
group3.aov <- aov(Gr3$value ~ Gr3$Group3)
summary(group3.aov)
```

```
##              Df Sum Sq Mean Sq F value   Pr(>F)
## Gr3$Group3    5  44.94   8.988   7.627 1.18e-05 ***
## Residuals    63  74.24   1.178
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
# Transform data and compute dissimilarity
Gr1.hell <- decostand(Gr1[ , 1], "hellinger", na.rm=T, MARGIN = 2) # Transform/Standardize
Gr1.hell.daisy = daisy(Gr1.hell, "euclidean") # Dissimilarity
attach(Gr1)
anosim.group1 <- anosim(Gr1.hell.daisy, grouping = Group1)
summary(anosim.group1)
```

```
##
## Call:
## anosim(dat = Gr1.hell.daisy, grouping = Group1)
## Dissimilarity:
##
## ANOSIM statistic R: -0.002349
##       Significance: 0.462
##
## Permutation: free
## Number of permutations: 999
##
## Upper quantiles of permutations (null model):
##    90%    95%  97.5%    99%
## 0.0406 0.0566 0.0793 0.1083
##
## Dissimilarity ranks between and within classes:
##         0%    25%    50%     75% 100%    N
## Between  4 581.25 1163.5 1780.75 2342 1134
## Outlet   2 540.00 1076.0 1623.50 2297  351
## Soil     1 619.00 1217.0 1787.00 2346  861
```

```r
Gr2.hell <- decostand(Gr2[ , 1], "hellinger", na.rm=T, MARGIN = 2) # Transform/Standardize
Gr2.hell.daisy = daisy(Gr2.hell, "euclidean") # Dissimilarity
attach(Gr2)
anosim.group2 <- anosim(Gr2.hell.daisy, grouping = Group2)
summary(anosim.group2)
```

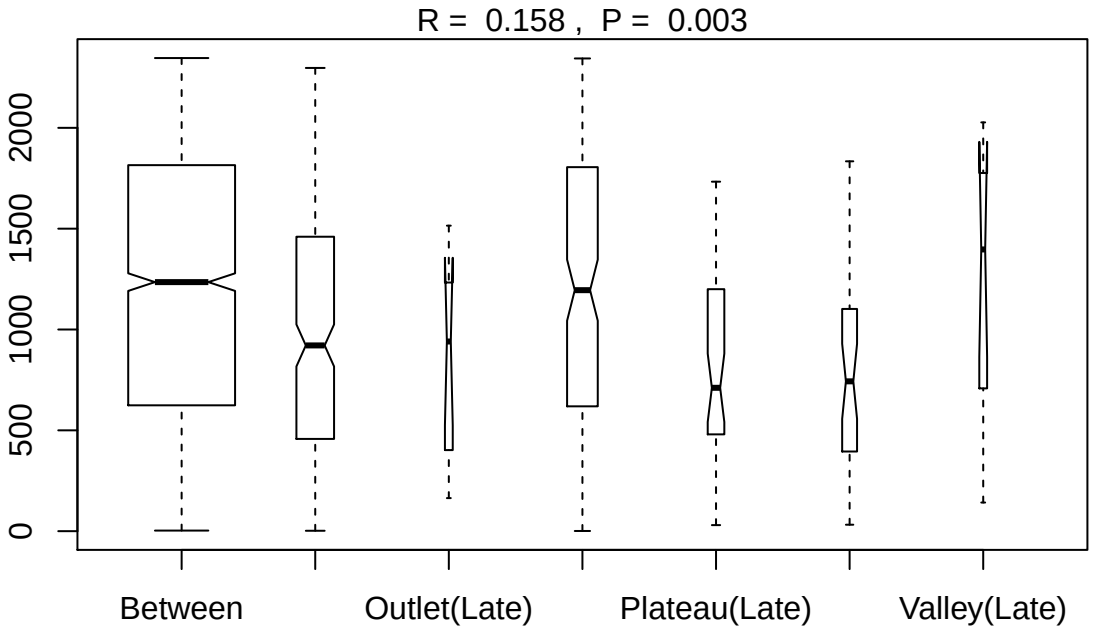
```
##
## Call:
## anosim(dat = Gr2.hell.daisy, grouping = Group2)
## Dissimilarity:
##
## ANOSIM statistic R: 0.01931
##       Significance: 0.208
##
## Permutation: free
## Number of permutations: 999
##
## Upper quantiles of permutations (null model):
##    90%    95%  97.5%    99%
## 0.0391 0.0543 0.0694 0.0861
##
## Dissimilarity ranks between and within classes:
##         0%    25%    50%     75% 100%    N
## Between  3 592.25 1179.5 1782.75 2346 1526
## Outlet   2 540.00 1076.0 1623.50 2297  351
## Plateau  1 629.50 1221.0 1766.75 2344  378
## Valley  32 653.00 1183.0 1943.00 2343   91
```

```r
Gr3.hell <- decostand(Gr3[ , 1], "hellinger", na.rm=T, MARGIN = 2) # Transform/Standardize
Gr3.hell.daisy = daisy(Gr3.hell, "euclidean") # Dissimilarity
attach(Gr3)
anosim.group3 <- anosim(Gr3.hell.daisy, grouping = Group3)
summary(anosim.group3)
```

```
##
## Call:
## anosim(dat = Gr3.hell.daisy, grouping = Group3)
## Dissimilarity:
##
## ANOSIM statistic R: 0.1577
##       Significance: 0.003
##
## Permutation: free
## Number of permutations: 999
##
## Upper quantiles of permutations (null model):
##    90%    95%  97.5%    99%
## 0.0484 0.0707 0.0898 0.1143
##
## Dissimilarity ranks between and within classes:
##                   0%   25%    50%     75% 100%    N
## Between            3 624.0 1235.0 1815.00 2346 1861
## Outlet(Early)      2 457.5  921.0 1460.00 2297  231
## Outlet(Late)     164 460.0  940.5 1192.00 1515   10
```

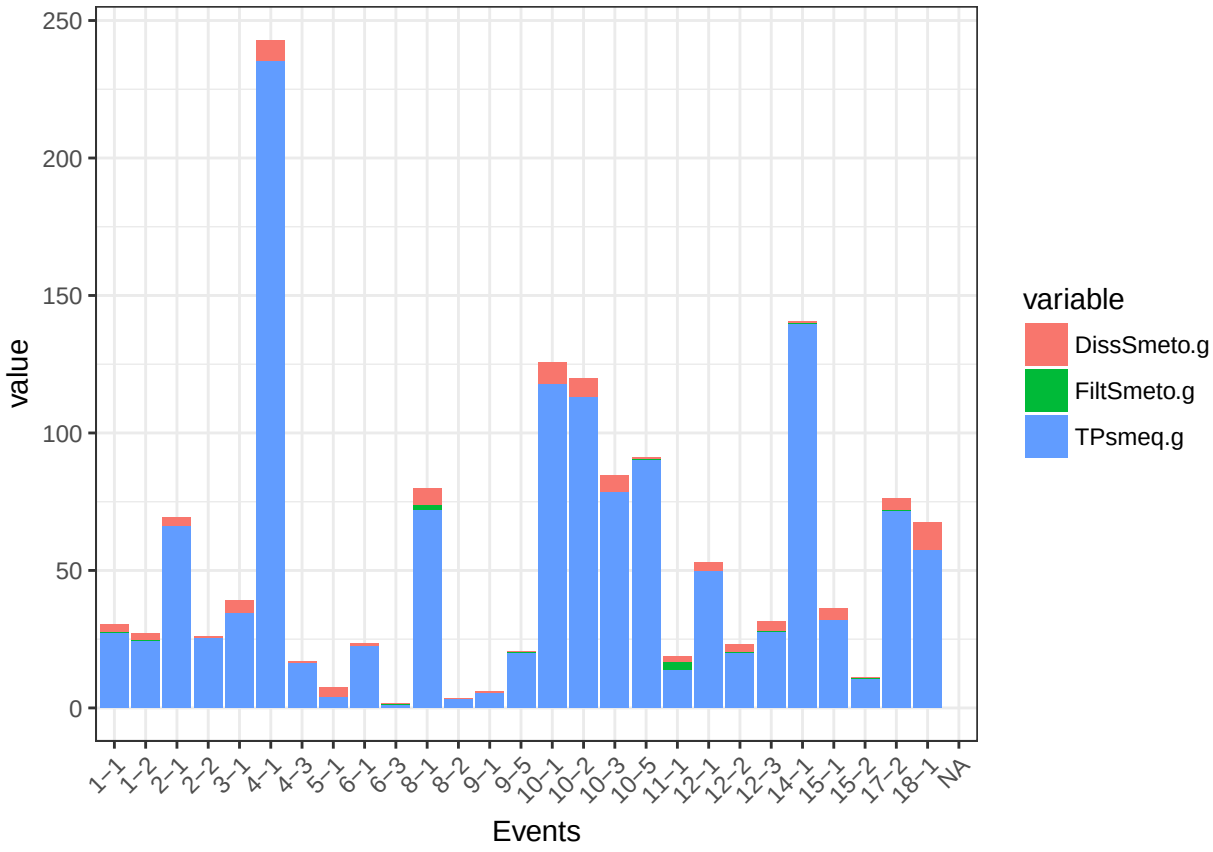
```
## Plateau(Early)   1 619.0 1195.0 1805.00 2344  153
## Plateau(Late)   30 480.0  711.0 1200.00 1733   45
## Valley(Early)   32 400.0  743.0 1093.00 1834   36
## Valley(Late)   142 740.0 1397.0 1755.75 2027   10
```

```
plot(anosim.group3)
```

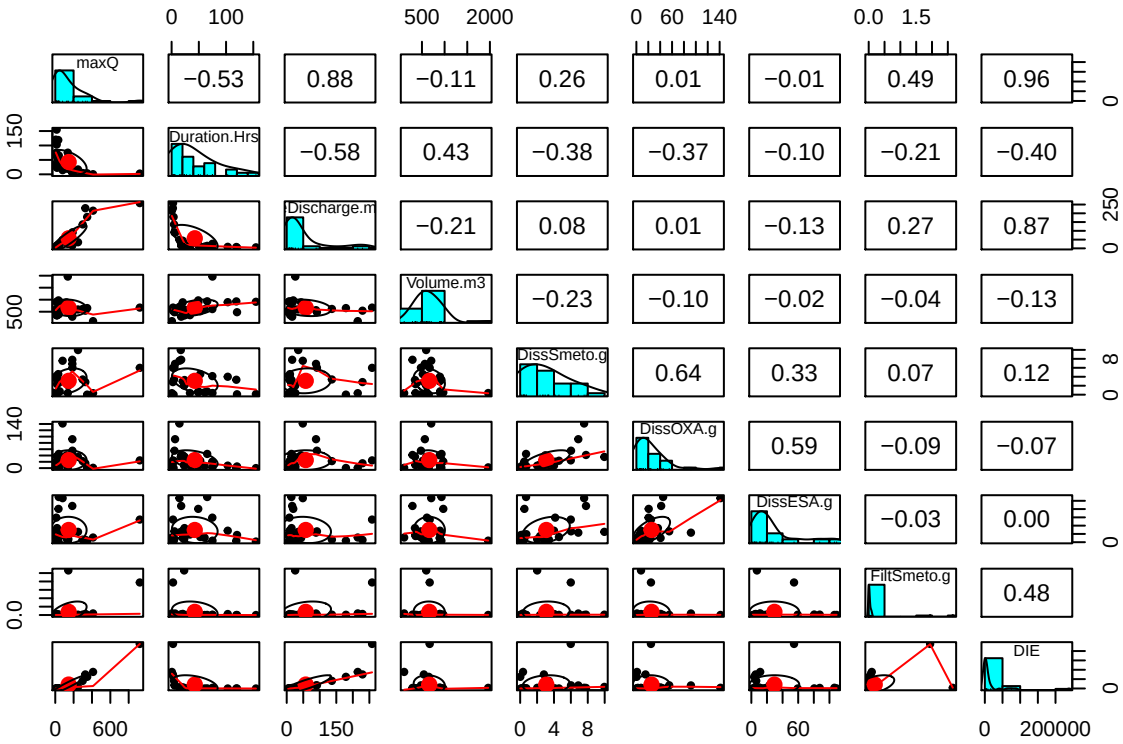


Loadings

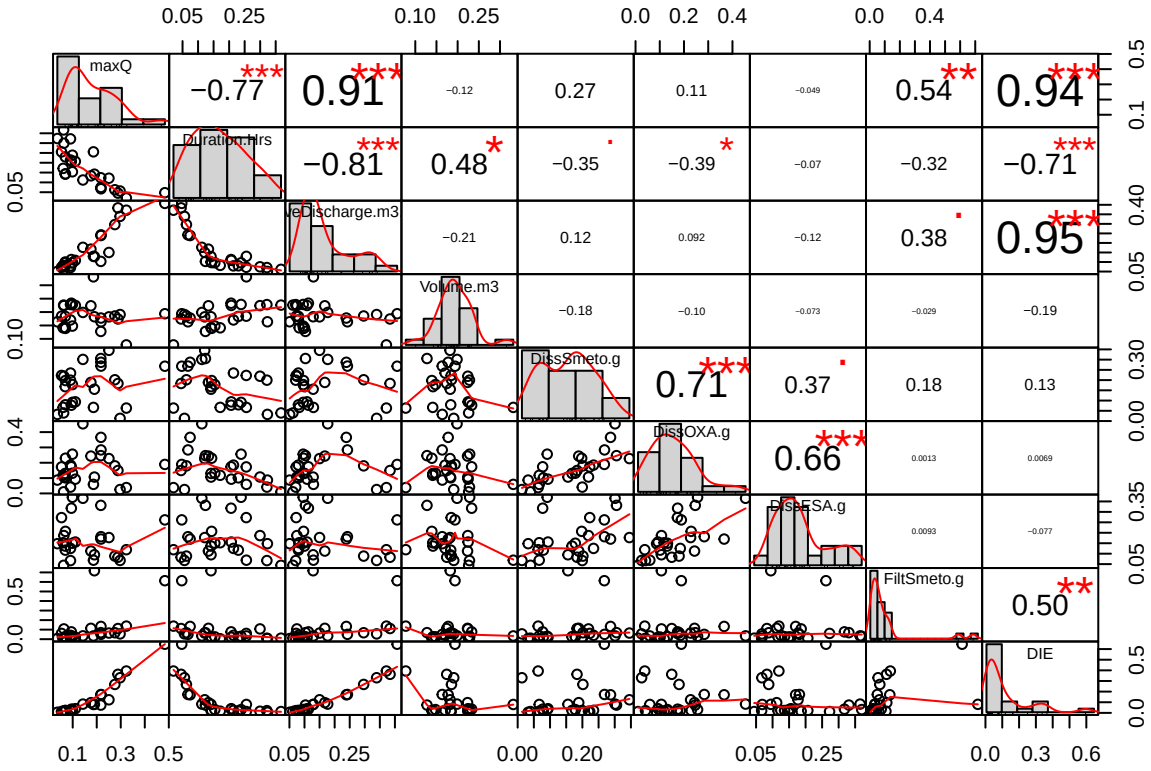
```
keepLoads <- c("Date.ti",
               "DissOXA.g", "DissESA.g", "DissSmeto.g", "FiltSmeto.g",
               "Event.x", "Events")
wsLoads <- WaterSoils[ , (names(WaterSoils) %in% keepLoads)]

mw.SM <- 283.796 # g/mol
mw.MOXA <- 279.33 # g/ml
mw.MESA <- 329.1 # g/mol
wsLoads$TPsmeq.g <-
  wsLoads$DissOXA.g * (mw.SM/mw.MOXA) +
  wsLoads$DissESA.g * (mw.SM/mw.MESA)

wsLoads <- wsLoads[ , !(names(wsLoads) %in% c("DissOXA.g", "DissESA.g"))]

loads <- melt(wsLoads, id=c("Date.ti", "Events", "Event.x"))

ggplot(data = loads , aes(x=Events, y=value, fill = variable))+
  theme_bw() +
  geom_bar(stat = "identity") +
  theme(# legend.position="top"
        # axis.title.x = element_blank(),
        axis.text.x=element_text(angle = 45, hjust = 1)
        )
```




```
  # geom_bar(stat = "identity", position = position_dodge())

WaterSoils$DIE <- WaterSoils$maxQ*WaterSoils$Volume.m3/WaterSoils$Duration.Hrs

keepCor <- c("maxQ", "Duration.Hrs", "AveDischarge.m3.h", "Volume.m3", "DIE",
             "DissOXA.g", "DissESA.g", "DissSmeto.g", "FiltSmeto.g" #,
             #"NH4.mM", "TIC.ppm.filt", "Cl.mM", "NO3..mM", "PO4..mM", "NPOC.ppm",
             #"TIC.ppm.unfilt", "TOC.ppm.unfilt"
             )

corData <- WaterSoils[ , (names(WaterSoils) %in% keepCor)]

# Transform / normalize
corData.hell <- decostand(corData, "hellinger", na.rm=T, MARGIN = 2)

library(psych)
pairs.panels(corData)
```




```
library(PerformanceAnalytics)
chart.Correlation(corData.hell)
```




```
keepLoads <- c("Date.ti",
               "DissOXA.g", "DissESA.g", "DissSmeto.g", "FiltSmeto.g",
               "Event.x", "Events")
```

```
wsLoads <- WaterSoils[ , (names(WaterSoils) %in% keepLoads)]
```

Outliers

```
# Test function
g_param = 1.5
# g_param = 2.2  #  (Hoaglin et al.,1986; Hoaglin & Iglewicz, 1987)
is_outlier <- function(x) {
  return(x < quantile(x, 0.25) - g_param * IQR(x) | x > quantile(x, 0.75) + g_param * IQR(x))
}
```

Soil concentrations

Correlation will be made after variable transformation. Options tested:

a) Z-scoring transformation by translation and expansion is done to create unit-free variables with means of zero and standard deviations of one. Standardised values differ from one another in units of standard deviation. The mean of each variable is subtracted from the original values and the difference divided by the variable's standard deviation and is given by:

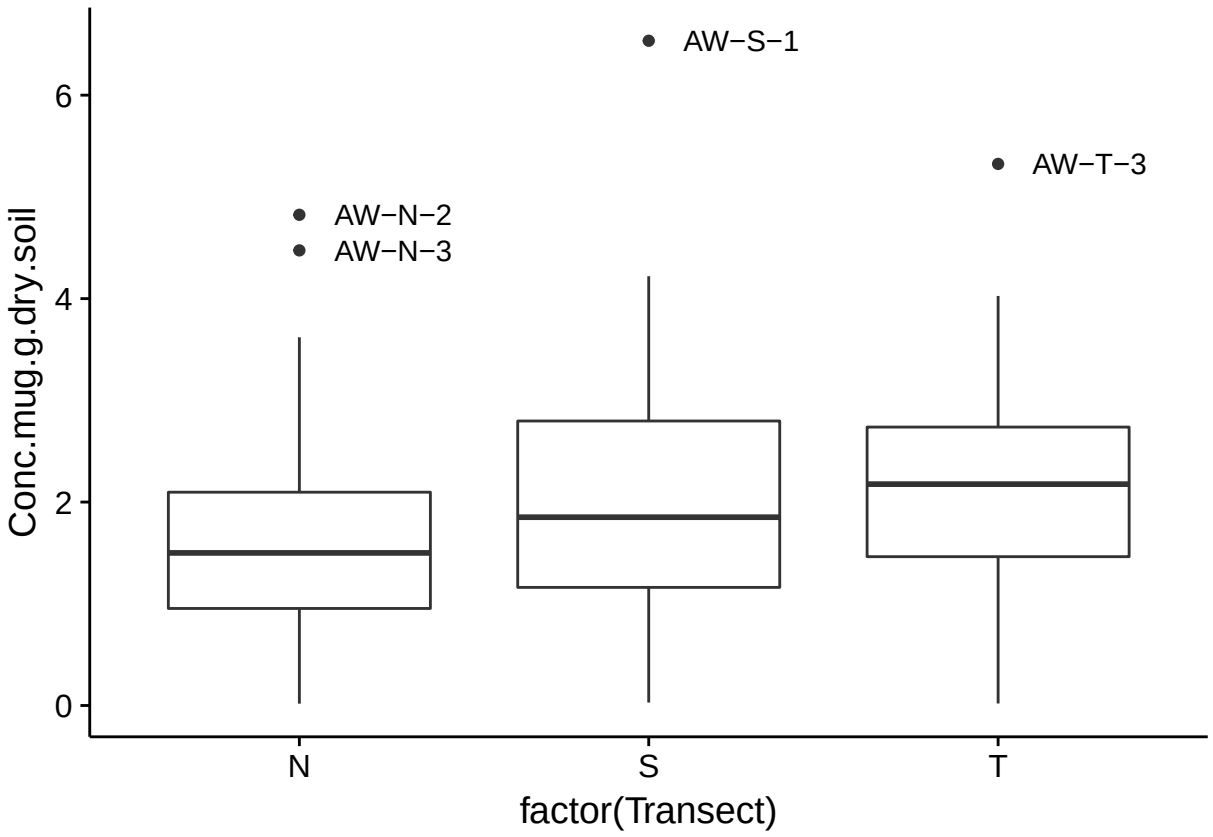
$$z_i = \frac{y_i - \bar{y}}{s_y}$$

Z-scoring did not change correlation results, nor outlier reduction.

b) Scaling by expansion where all values are divided by the maximum observation.

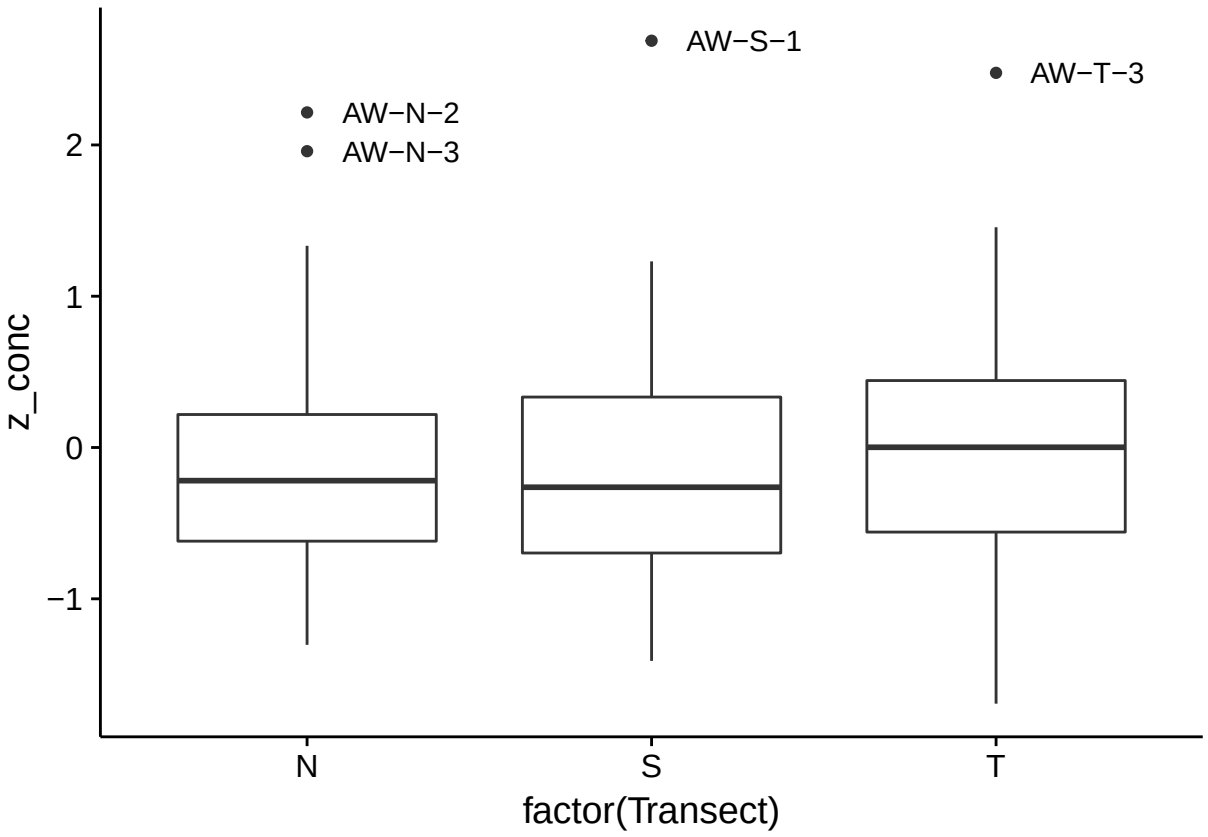
Outliers before transformation

```
# Concentrations
soilGroups %>%
  group_by(Transect) %>%
  mutate(outlier = ifelse(is_outlier(Conc.mug.g.dry.soil), as.character(ID), NA)) %>%
  ggplot(., aes(x = factor(Transect), y = Conc.mug.g.dry.soil)) +
    geom_boxplot() +
    geom_text(aes(label = outlier), na.rm = TRUE, hjust = -0.3)
```



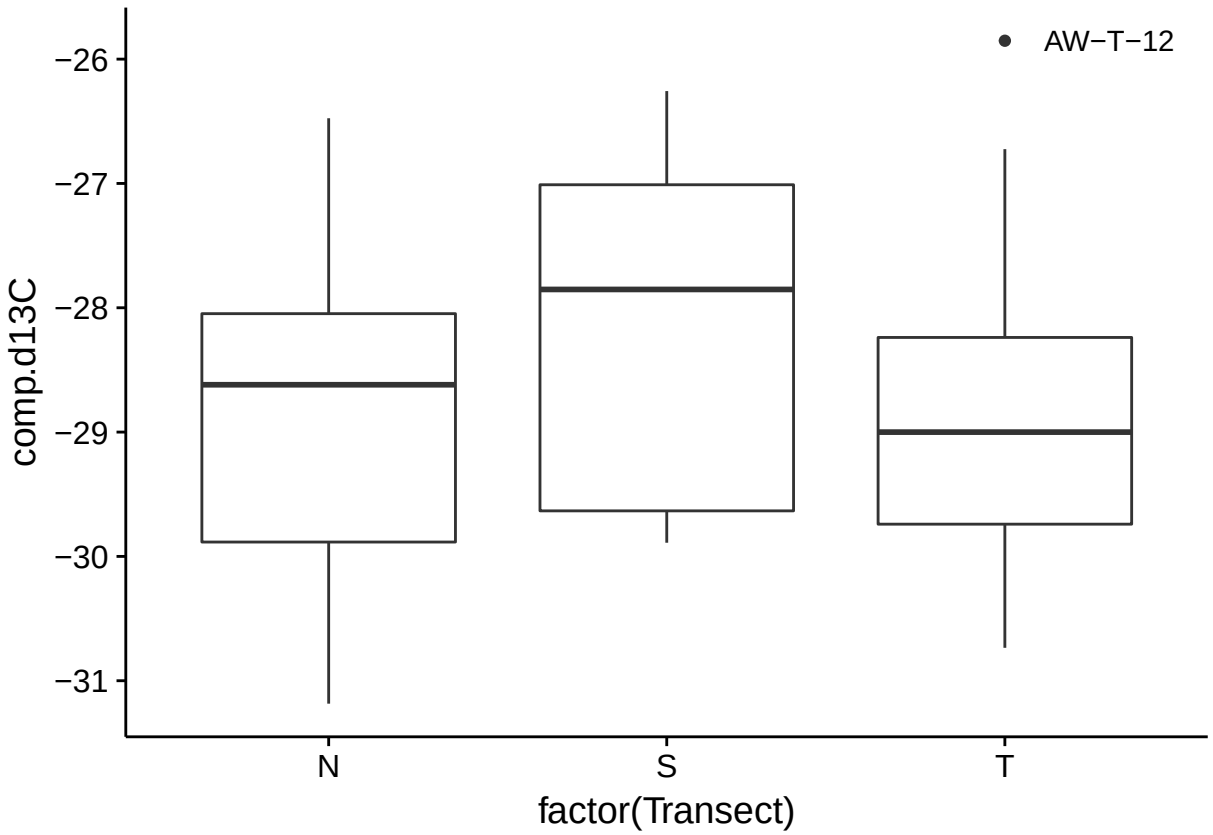
Outliers after transformation

```
soilGroups <- soilGroups %>%
  group_by(Transect) %>%
  mutate(z_conc = (Conc.mug.g.dry.soil-mean(Conc.mug.g.dry.soil))/sd(Conc.mug.g.dry.soil))


soilGroups %>%
  group_by(Transect) %>%
  mutate(outlier = ifelse(is_outlier(z_conc), as.character(ID), NA)) %>%
  ggplot(., aes(x = factor(Transect), y = z_conc)) +
    geom_boxplot() +
    geom_text(aes(label = outlier), na.rm = TRUE, hjust = -0.3)
```



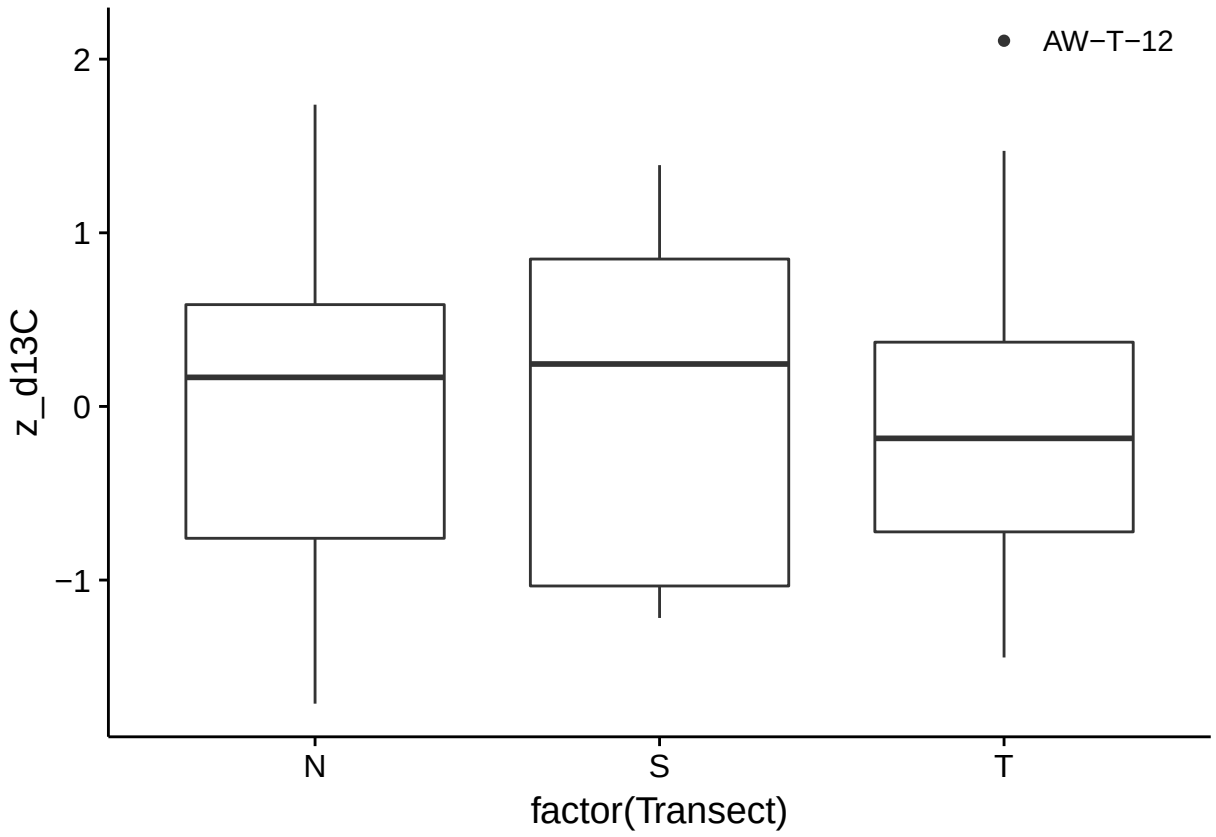
Soil Isotopes

```
# Isotopes

temp <- na.omit(soilGroups)

temp %>%
  group_by(Transect) %>%
  mutate(outlier = ifelse(is_outlier(comp.d13C), as.character(ID), NA)) %>%
  ggplot(., aes(x = factor(Transect), y = comp.d13C)) +
    geom_boxplot() +
    geom_text(aes(label = outlier), na.rm = TRUE, hjust = -0.3)
```



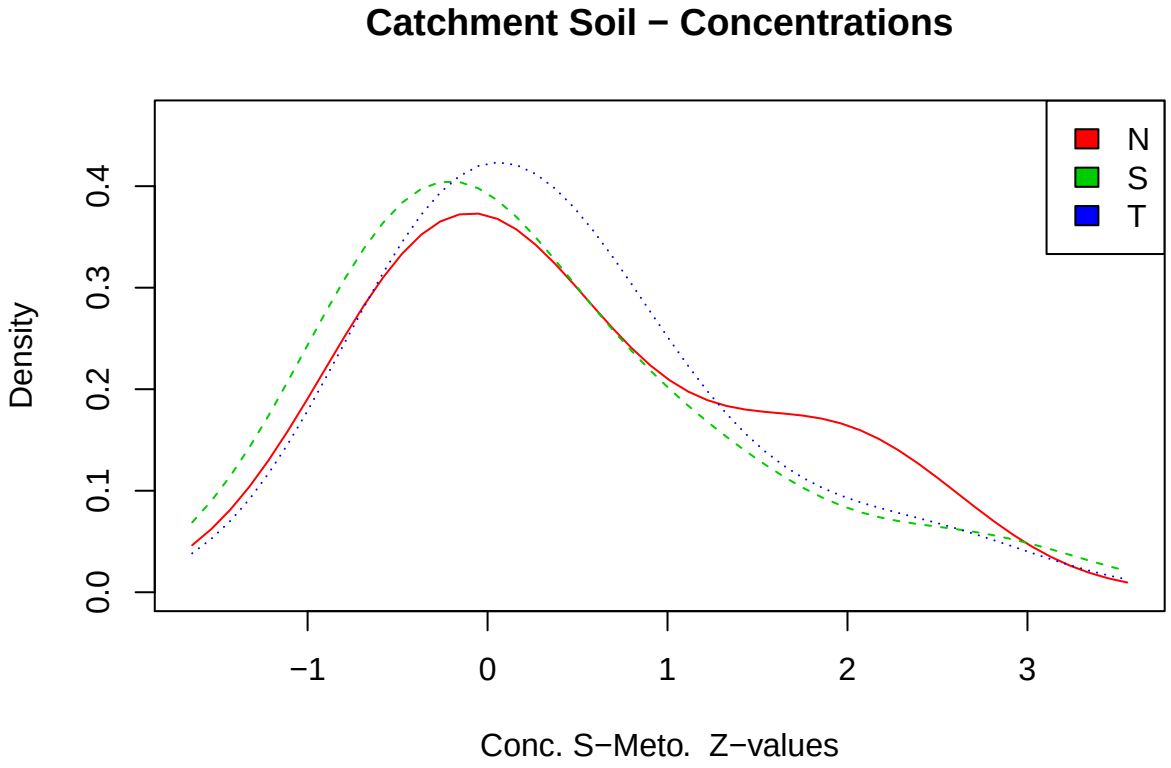
Looks like 7 potential outliers in concentrations and 1 for isotopes. Removing NA's for isotopes and re-computing outliers, reduces the number of outliers to 2 in concentrations and 1 for isotopes.

```
temp <- temp %>%
  group_by(Transect) %>%
  mutate(z_d13C = (comp.d13C-mean(comp.d13C))/sd(comp.d13C))

temp %>%
  group_by(Transect) %>%
  mutate(outlier = ifelse(is_outlier(z_d13C), as.character(ID), NA)) %>%
  ggplot(., aes(x = factor(Transect), y = z_d13C)) +
    geom_boxplot() +
    geom_text(aes(label = outlier), na.rm = TRUE, hjust = -0.3)
```



Distribution of z values (same as non-transformed)

```
# plot densities
#sm.density.compare(temp$z_conc, temp$Transect, xlab=expression(paste("Conc. S-Meto.  ", {({mu}*g / g.s
sm.density.compare(temp$z_conc, temp$Transect, xlab=expression(paste("Conc. S-Meto.  Z-values")))
title(main="Catchment Soil - Concentrations")
legend("topright", levels( soilGroups$Transect), fill=2+(0:nlevels(soilGroups$Transect)))
```

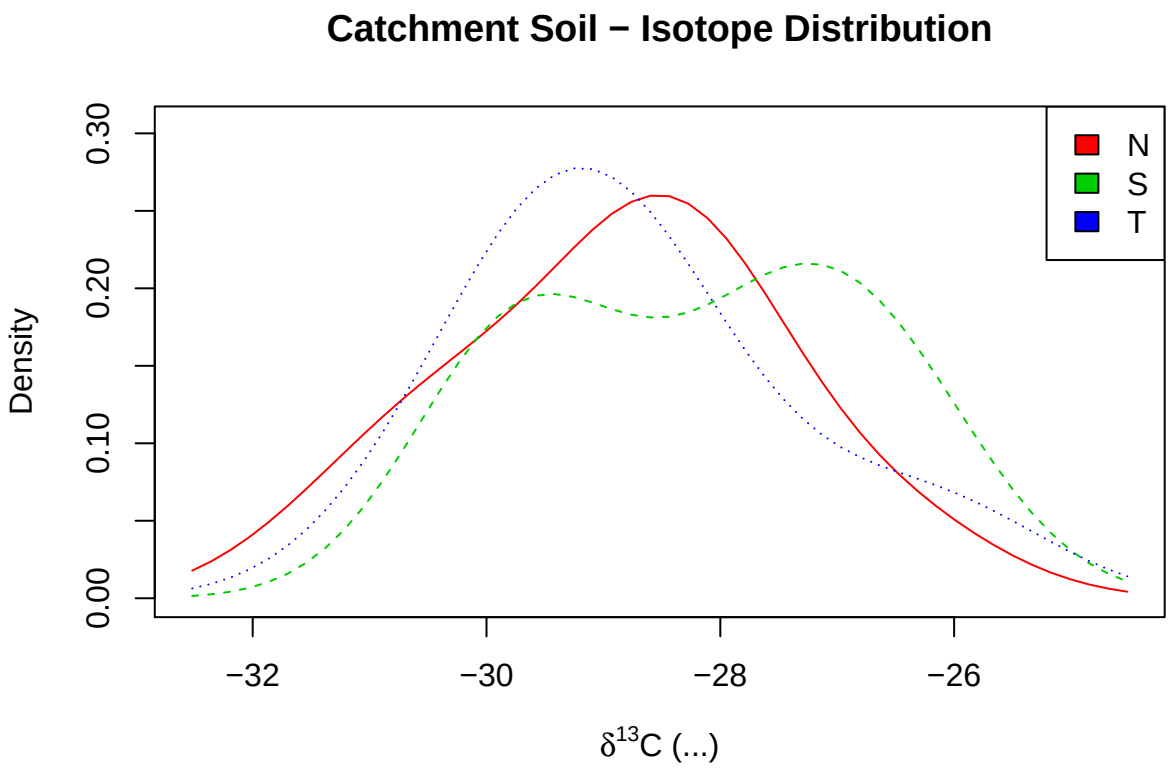



```
#vioplot(soilGroups$Conc.mug.g.dry.soil,  names = "Catchment")
#title(expression(paste("Conc. S-Meto.  ", {({mu}*g / g.soil.dry)})))
```

Soil Isotopes

```
#vioplot(na.omit(soilGroups$comp.d13C),  names = "Catchment")
#title(expression(paste({delta}^"13","C", ' (\u2030)')))
```

```
temp <- na.omit(soilGroups)
sm.density.compare(temp$comp.d13C, temp$Transect,
                   xlab=expression(paste({delta}^"13","C", ' (\u2030)')))
title(main="Catchment Soil - Isotope Distribution")
legend("topright", levels( soilGroups$Transect), fill=2+(0:nlevels(soilGroups$Transect)))
```


Catchment Soil − Isotope Distribution
Density
0.00
0.10
0.20
0.30
−32
−30
−28
−26
δ13C (...)
N
S
T