Data importation

Time point objects

Gentoypic layout

1. endpoint

Comparisons between raw and cleaned data

2. S_timeseries

Raw data

- 1. Detection of outliers for single observations
- 2. Correction for spatial trends
- 3. Outlier detection for series of observations
- 4. With the cleaned data, re-do the spatial correction

UCPH Data Analysis Timepoints

Elise

2024-06-09

Set the right working directory.

```
rm(list = ls())
setwd("C:/Users/elise/Documents/Mémoire/Main/Data/Templates/UCPH")
platform <- "UCPH"</pre>
```

Data importation

Reimport the data sets extracted from the Data Preparation and Data Analysis R Markdown.

```
list.files()
```

```
plant_info <- read.table("plant_info.txt", header = TRUE, sep = "\t")</pre>
endpoint <- read.table("endpoint.txt", header = TRUE, sep = "\t")</pre>
S_timeseries <- read.table("S_timeseries.txt", header = TRUE, sep = "\t")</pre>
# plant info
plant_info <- lapply(plant_info, factor)</pre>
# endpoint
matching_cols <- intersect(names(endpoint), names(plant_info))</pre>
endpoint[, matching_cols] <- lapply(endpoint[, matching_cols], factor)</pre>
endpoint$Date <- date(endpoint$Date)</pre>
endpoint$Timestamp <- NA
# timeseries
# No data for UCPH
# S_timeseries
matching_cols <- intersect(names(S_timeseries), names(plant_info))</pre>
S_timeseries[, matching_cols] <- lapply(S_timeseries[, matching_cols], factor)</pre>
S_timeseries$Timestamp <- as.POSIXct(S_timeseries$Timestamp, format = "%Y-%m-%d %H:%M:%</pre>
S")
S_timeseries$Date <- date(S_timeseries$Date)</pre>
# T_timeseries
# No data
platform <- "UCPH"
# endpoint
df <- endpoint[,colSums(is.na(endpoint))<nrow(endpoint)]</pre>
genotype_index <- which(colnames(df) == "Genotype")</pre>
variables <- colnames(df[, c(3:(genotype_index - 1))]) # We remove the two first column
s that are "Unit.ID" and "Date"
# timeseries
# no data
# S timeseries
df_S_timeseries <- S_timeseries[,colSums(is.na(S_timeseries))<nrow(S_timeseries)]</pre>
genotype_index <- which(colnames(df_S_timeseries) == "Genotype")</pre>
variables_S <- "S_Height_cm"</pre>
# T_timeseries
# no data
print(paste(platform, ": The variables for endpoint are", paste(variables, collapse =
", "), sep = " "))
```

```
## [1] "UCPH : The variables for endpoint are DW_shoot_g, DW_root_g"
```

```
print(paste(platform, ": The variables for S_timeseries are", paste(variables_S, collap
se = ", "), sep = " "))
```

```
## [1] "UCPH : The variables for S_timeseries are S_Height_cm"
```

```
endpoint$Plant_type <- substr(endpoint$Genotype, nchar(as.character(endpoint$Genotyp
e)), nchar(as.character(endpoint$Genotype)))
S_timeseries$Plant_type <- substr(S_timeseries$Genotype, nchar(as.character(S_timeseries$Genotype)))</pre>
```

Get the cleaned endpoint data

Time point objects

Generation of the timePoints objects using the function "createTimePoints".

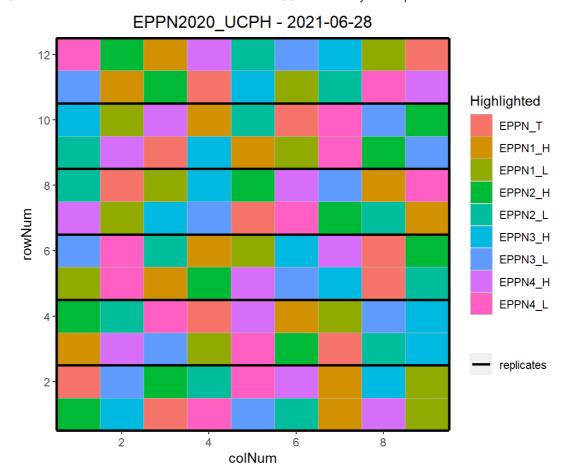
```
timePoint_endpoint <- createTimePoints(dat = endpoint,</pre>
                                        experimentName = "EPPN2020_UCPH",
                                        genotype = "Genotype",
                                        timePoint = "Date",
                                        plotId = "Unit.ID",
                                        rowNum = "Row",
                                        colNum = "Column",
                                        repId = "Replication")
timePoint_endpoint_clean <- createTimePoints(dat = endpoint_clean,</pre>
                                       experimentName = "EPPN2020_UCPH",
                                        genotype = "Genotype",
                                       timePoint = "Date",
                                        plotId = "Unit.ID",
                                        rowNum = "Row",
                                        colNum = "Column",
                                        repId = "Replication")
S_timeseries <- S_timeseries %>%
  group_by(Date, Unit.ID) %>%
  slice(1) %>% # Keep the first line of every duplicate
  ungroup()
timePoint_S <- createTimePoints(dat = S_timeseries,</pre>
                               experimentName = "EPPN2020_UCPH",
                               genotype = "Genotype",
                               timePoint = "Date",
                               plotId = "Unit.ID",
                               rowNum = "Row",
                               colNum = "Column",
                               repId = "Replication",
                               addCheck = TRUE,
                               checkGenotypes = "EPPN_T")
```

Gentoypic layout

Check the layout of the platforms' genotypes.

```
genotypes_list <- as.character(unique(endpoint$Genotype))

plot(timePoint_endpoint,
    plotType = "layout",
    highlight = genotypes_list,
    showGeno = FALSE)</pre>
```



1. endpoint

Comparisons between raw and cleaned data

View timePoint object.

```
summary(timePoint_endpoint)

## timePoint_endpoint contains data for experiment EPPN2020_UCPH.
##
## It contains 1 time points.
## First time point: 2021-06-28
## Last time point: 2021-06-28
##
## No check genotypes are defined.

getTimePoints(timePoint_endpoint)

## timeNumber timePoint
## 1 1 2021-06-28
```

Count the number of observations per trait.

```
for (trait_name in traits) {
  print(paste("How many data observations for", trait_name))
  num_observations <- countValid(timePoint_endpoint, trait_name)
  print(num_observations)
}</pre>
```

```
## [1] "How many data observations for DW_shoot_g"
## 2021-06-28
## 107
## [1] "How many data observations for DW_root_g"
## 2021-06-28
## 108
```

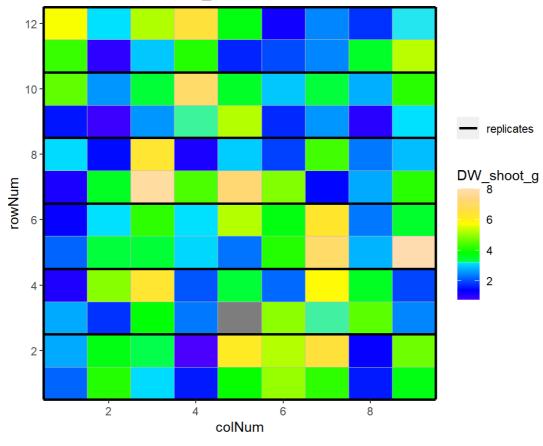
```
for (trait_name in traits) {
  print(paste("How many cleaned data observations for", trait_name))
  num_observations <- countValid(timePoint_endpoint_clean, trait_name)
  print(num_observations)
}</pre>
```

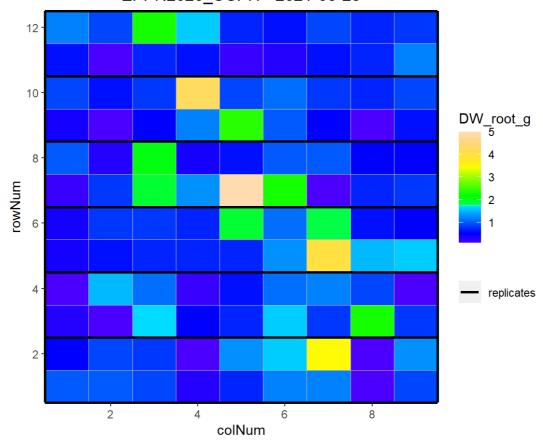
```
## [1] "How many cleaned data observations for DW_shoot_g"
## 2021-06-28
## 101
## [1] "How many cleaned data observations for DW_root_g"
## 2021-06-28
## 104
```

Check the heatmap of the data at harvest

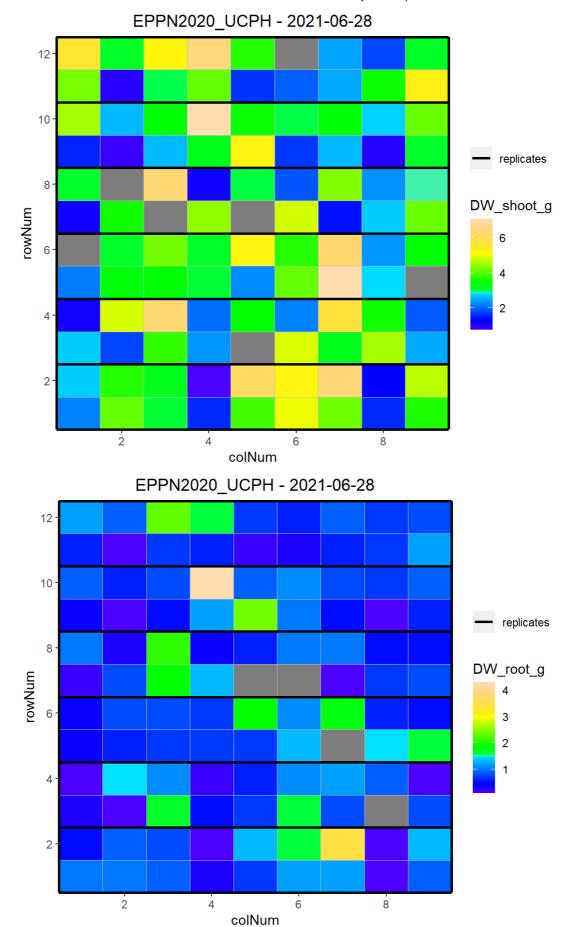
```
for (trait_name in traits) {
  plot(timePoint_endpoint,
    plotType = "layout",
    timePoints = 1,
    traits = trait_name)
}
```







```
for (trait_name in traits) {
  plot(timePoint_endpoint_clean,
     plotType = "layout",
     timePoints = 1,
     traits = trait_name)
}
```



2. S_timeseries

Raw data

View timePoint object

```
summary(timePoint_S)
```

```
## timePoint_S contains data for experiment EPPN2020_UCPH.
##
## It contains 17 time points.
## First time point: 2021-06-13
## Last time point: 2021-06-29
##
## The following genotypes are defined as check genotypes: EPPN_T.
```

```
getTimePoints(timePoint_S)
```

```
##
      timeNumber timePoint
              1 2021-06-13
## 1
## 2
               2 2021-06-14
## 3
               3 2021-06-15
## 4
               4 2021-06-16
## 5
               5 2021-06-17
## 6
               6 2021-06-18
## 7
              7 2021-06-19
## 8
              8 2021-06-20
## 9
              9 2021-06-21
              10 2021-06-22
## 10
              11 2021-06-23
## 11
## 12
              12 2021-06-24
## 13
              13 2021-06-25
## 14
              14 2021-06-26
## 15
              15 2021-06-27
## 16
              16 2021-06-28
## 17
              17 2021-06-29
```

```
num_timepoints <- getTimePoints(timePoint_S)</pre>
```

Count the number of observations per trait and time point

We focus on the Height [cm] and Leaf area, because these are the two most common among the platforms.

Height is computed for 6 platforms out of 9 and area for 4 out of 9.

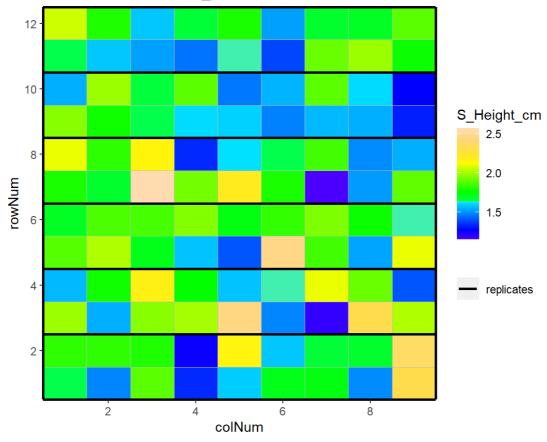
```
var_voulues <- c(variables_S[1])
traits <- var_voulues

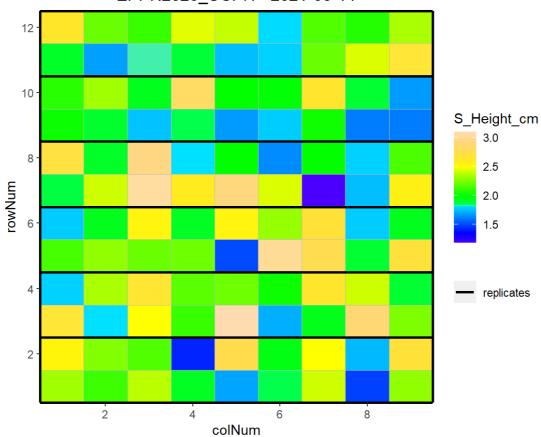
for (trait_name in traits) {
  print(paste("How many observations for", trait_name))
  valid_count <- countValid(timePoint_S, trait_name)
  print(valid_count)
}</pre>
```

```
## [1] "How many observations for S_Height_cm"
## 2021-06-13 2021-06-14 2021-06-15 2021-06-16 2021-06-17 2021-06-18 2021-06-19
                    108
                               108
                                          108
                                                     108
                                                                108
## 2021-06-20 2021-06-21 2021-06-22 2021-06-23 2021-06-24 2021-06-25 2021-06-26
                    108
         108
                               108
                                          108
                                                     108
                                                                108
                                                                           108
## 2021-06-27 2021-06-28 2021-06-29
           66
                    108
```

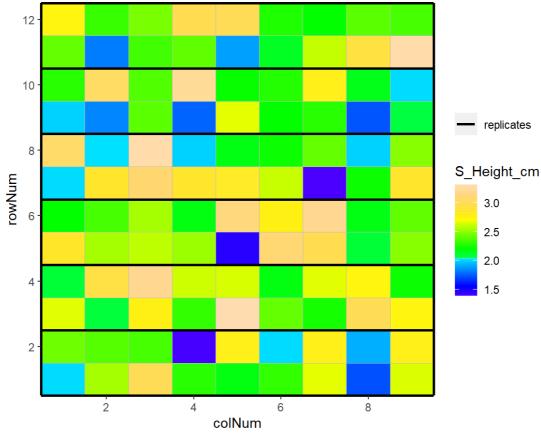
Check the heatmap of the raw data per time point

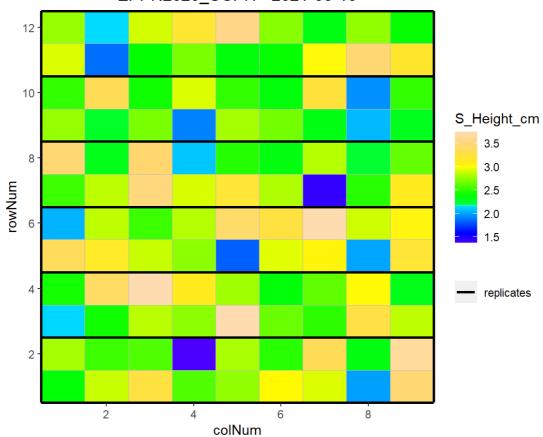




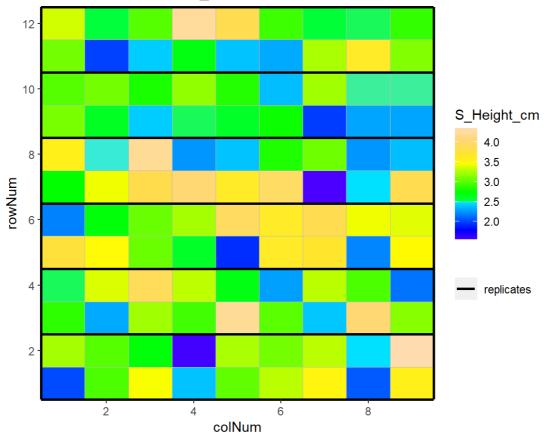


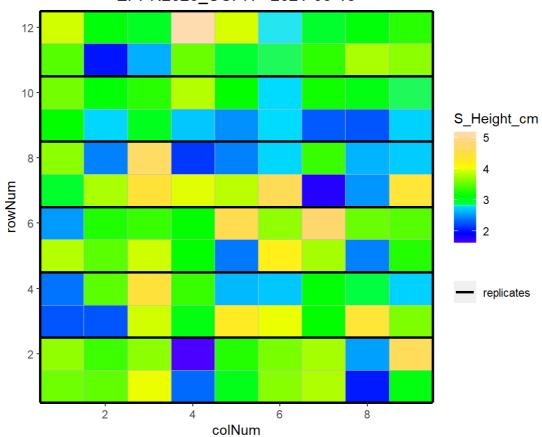




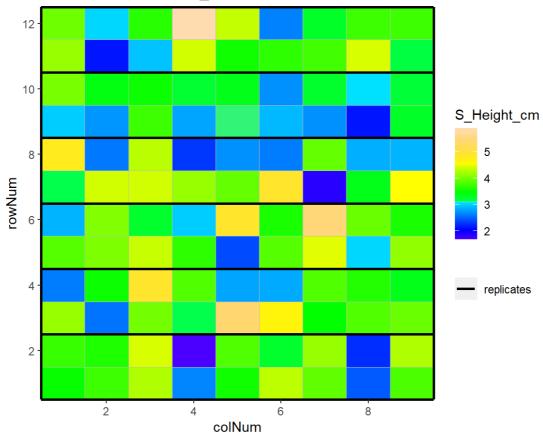


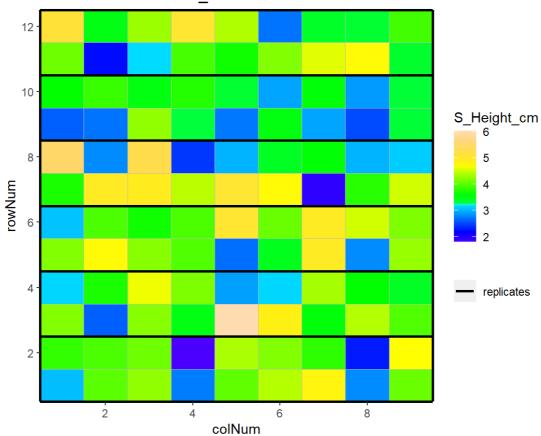




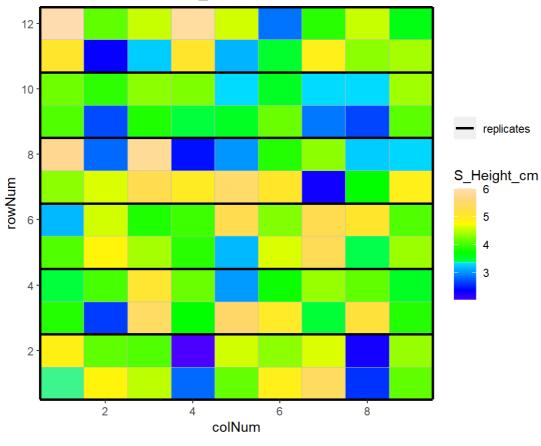


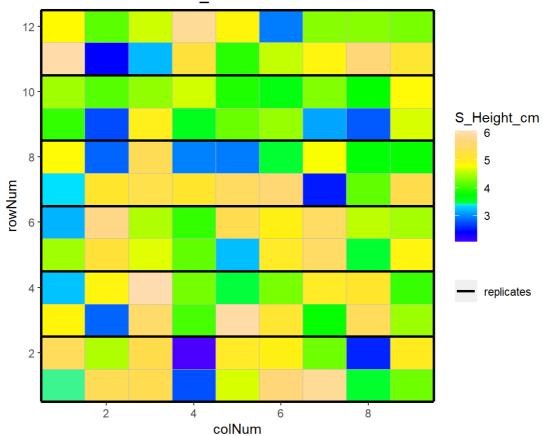




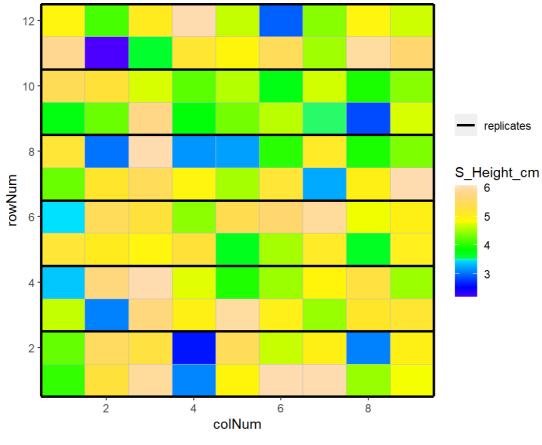


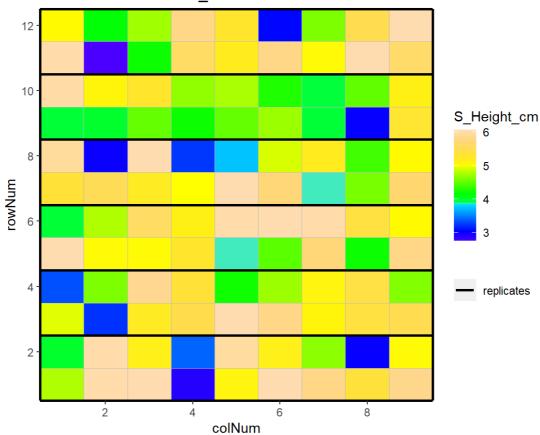




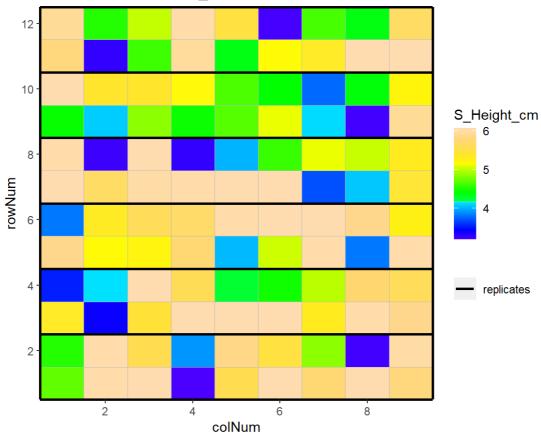


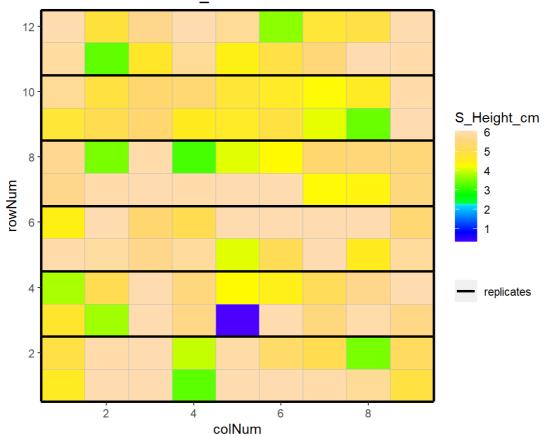


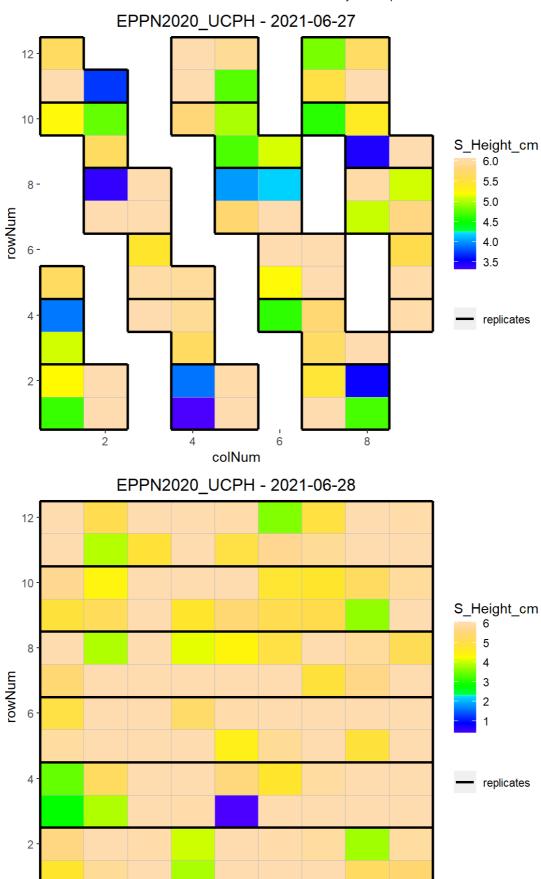












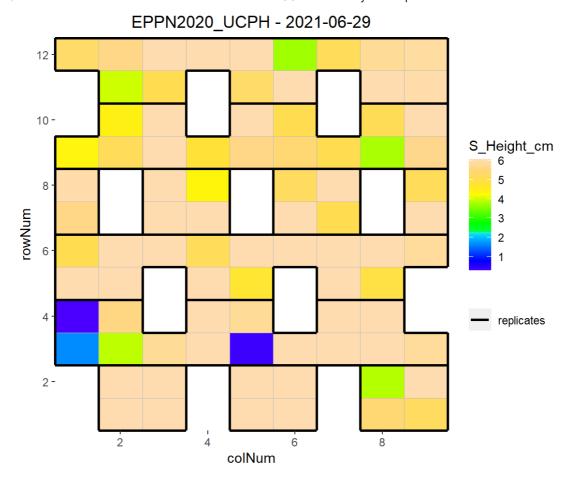
4

colNum

6

8

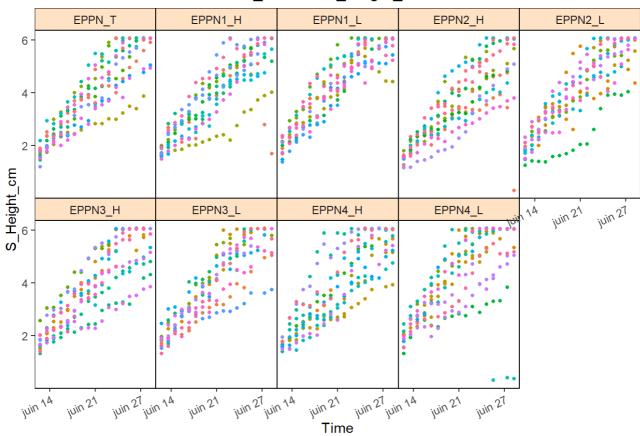
2



Check time course of raw data per time point

```
for (trait_name in traits) {
  plot(timePoint_S,
        traits = trait_name,
        plotType = "raw")
}
```

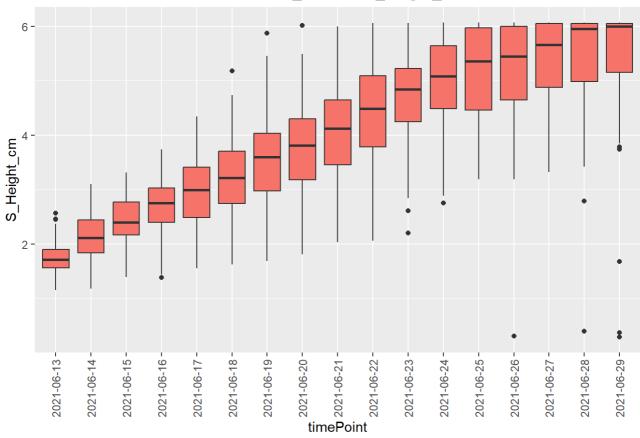
EPPN2020_UCPH - S_Height_cm - raw data



Check the boxplots of raw data per time point

```
for (trait_name in traits) {
  plot(timePoint_S,
    plotType = "box",
    traits = trait_name)
}
```

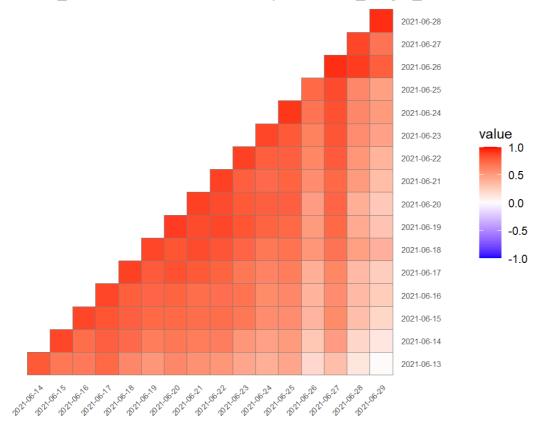
EPPN2020_UCPH - S_Height_cm



Check the correlation plots of raw data per time point

```
for (trait_name in traits) {
  plot(timePoint_S,
     plotType = "cor",
     traits = trait_name)
}
```

EPPN2020_UCPH - Correlations of timepoints for S_Height_cm



1. Detection of outliers for single observations

Using the SingleOut detect and single functions. We select a subset of plants to adjust the settings for the confIntSize and nnLocfit.

```
plantSel<- c(1,2,3,4,5,6,7,8,9,10)

ci <- 5 # confidence interval

nn <- 0.8 # nearest neighbor

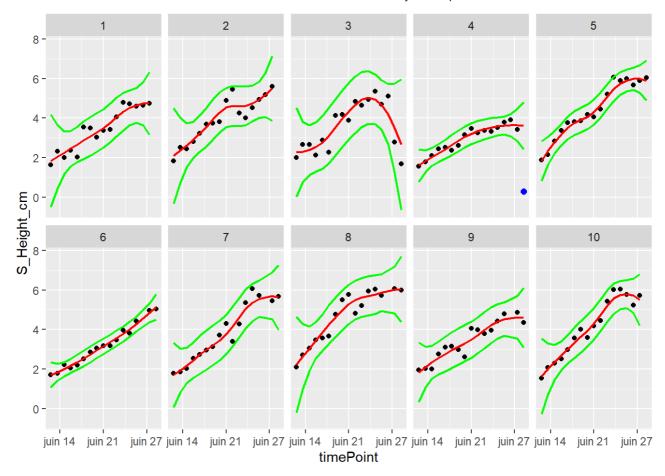
ce <- FALSE
```

```
for (trait_name in traits) {
   variable_name <- paste0("Single_test_", trait_name)

single_test <- detectSingleOut(
   TP = timePoint_S,
    trait = trait_name,
   plotIds = plantSel,
   confIntSize = ci,
   nnLocfit = nn,
   checkEdges = TRUE # check for outlier values in start and end of experiment
)

assign(variable_name, single_test)

plot(single_test, outOnly = FALSE)
}</pre>
```



We can then run on all plants of the data set.

```
for (trait_name in traits) {
    single_test_object_name <- paste0("Single_test_", trait_name)
    Single_test <- get(single_test_object_name)
    if (any(Single_test$outlier == 1)) {
        outliers_count <- with(Single_test[Single_test$outlier == 1,], table(timePoint))
        print(trait_name)
        print(outliers_count)

    Single_outliers <- removeSingleOut(timePoint_S, Single_test)
        assign(paste0("Single_outliers_", trait_name), Single_outliers)

    readr::write_tsv(Single_test, sprintf("%s/single_outliers_%s.tsv", datadir, trait_name))
    } else {
        cat("No outlier for", trait_name, "\n")
    }
}</pre>
```

```
## [1] "S_Height_cm"

## timePoint

## 2021-06-29

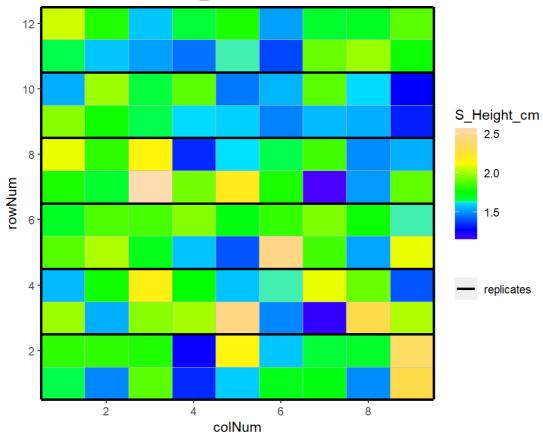
## 1
```

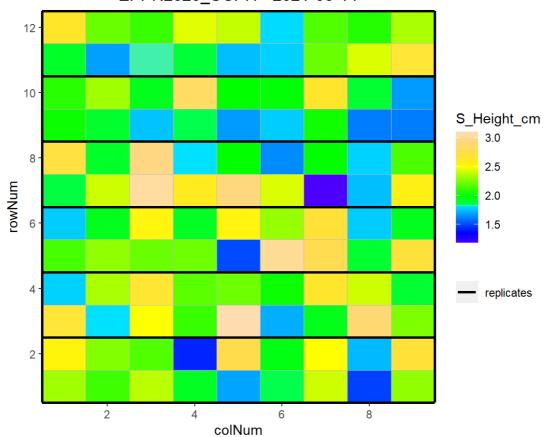
Data visualisation after single observations outliers removal

Heatmap of data

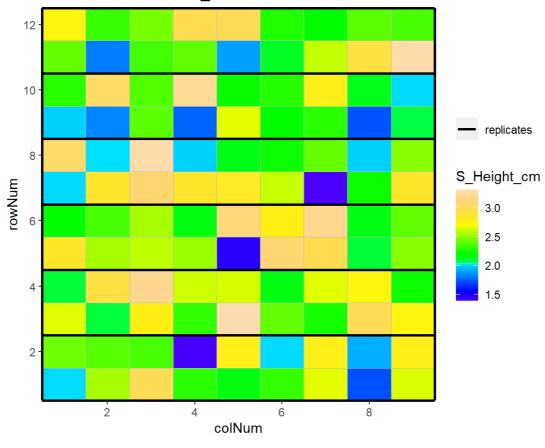
Check the heatmap of the data with outliers detection at all the time points.

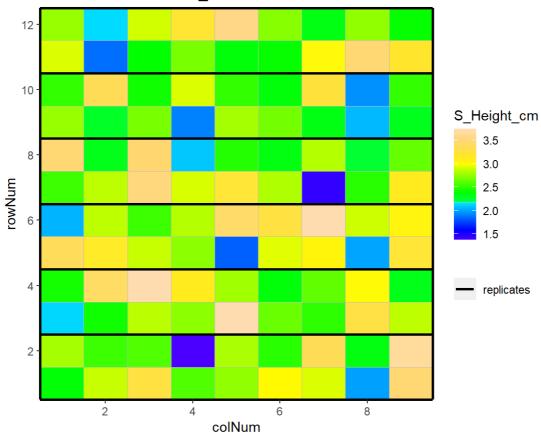




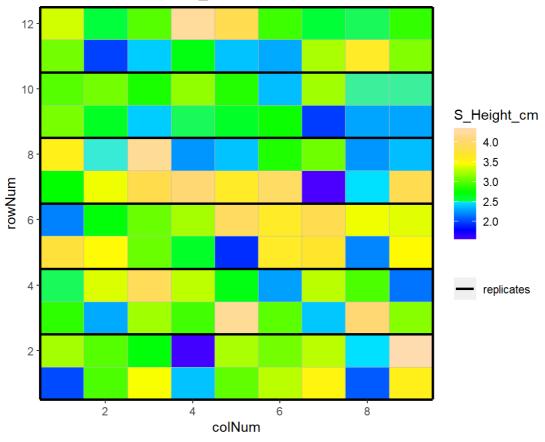


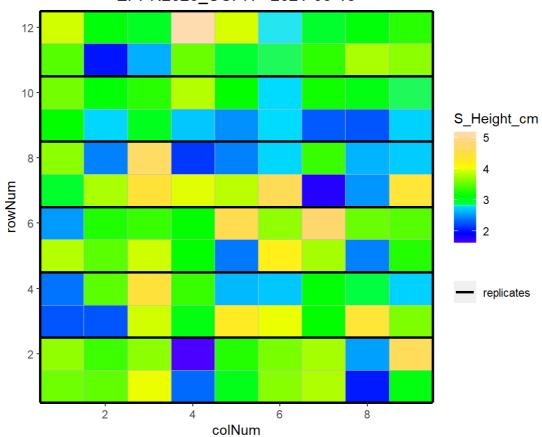




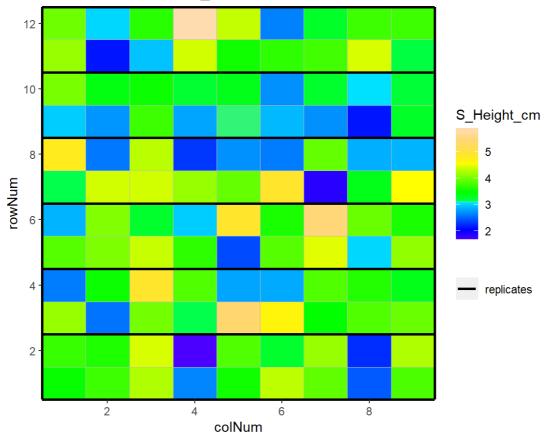


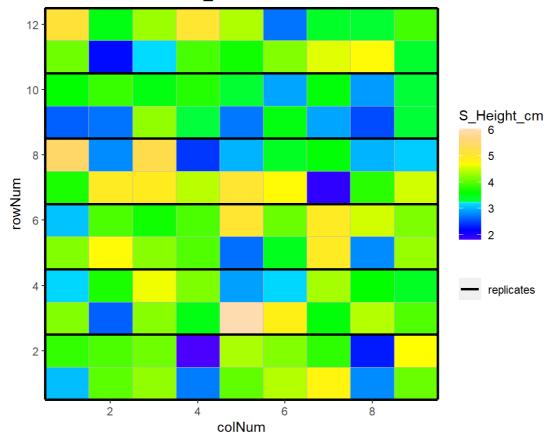




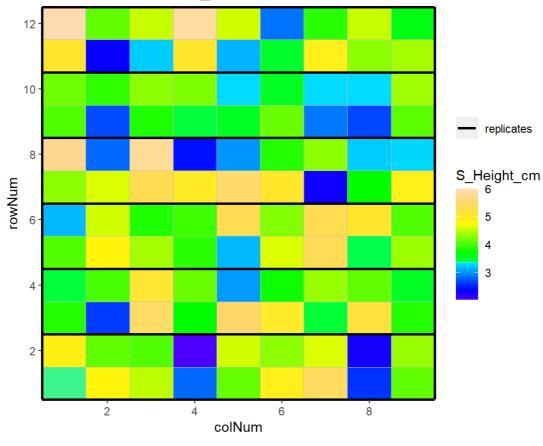


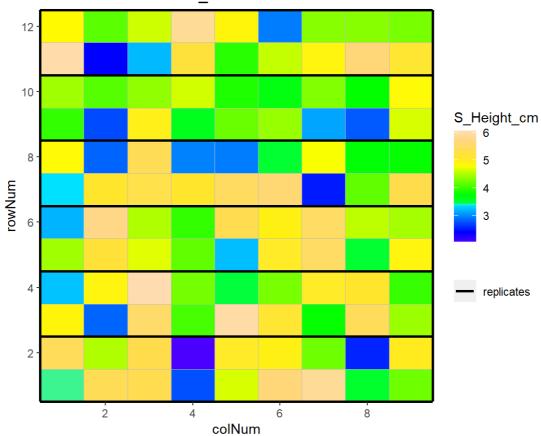




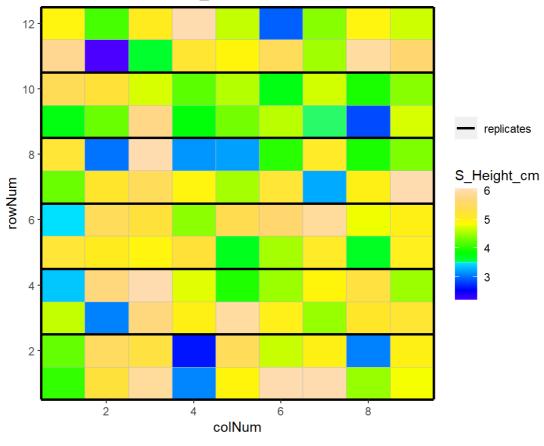


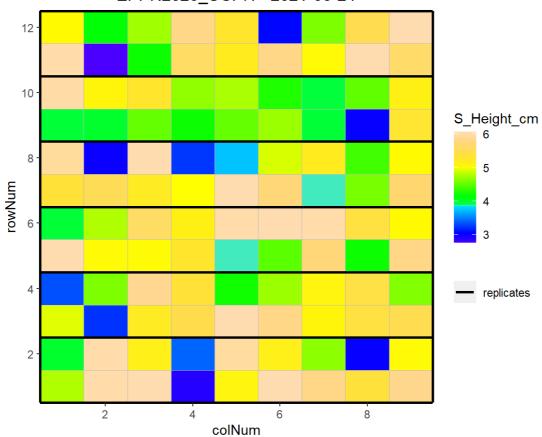




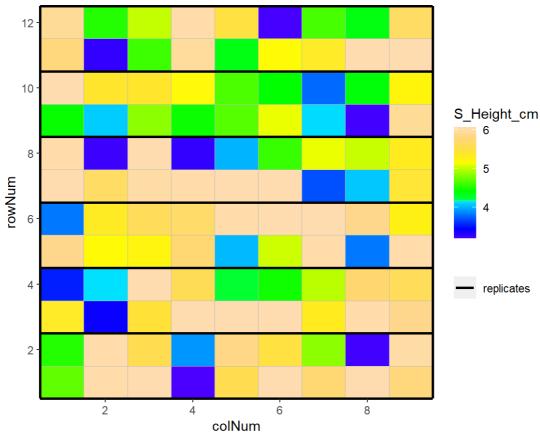


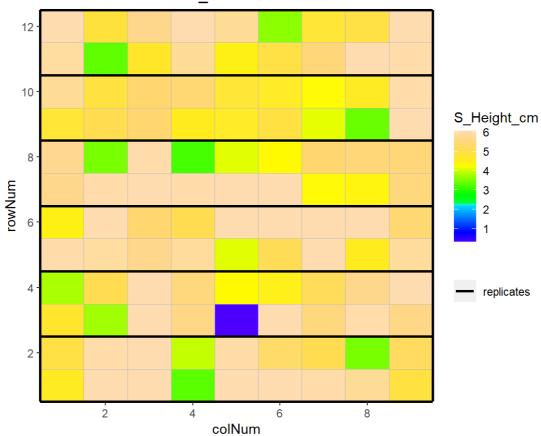


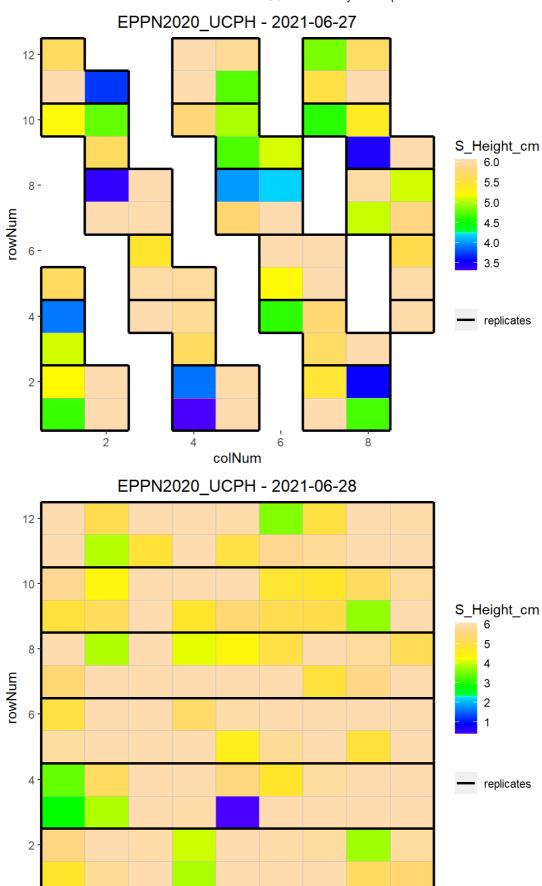












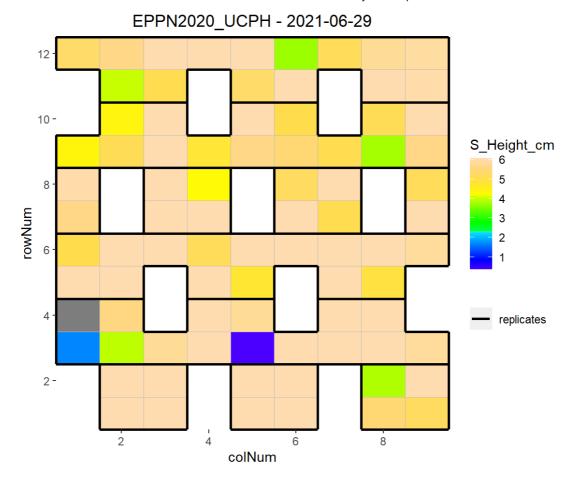
4

colNum

6

8

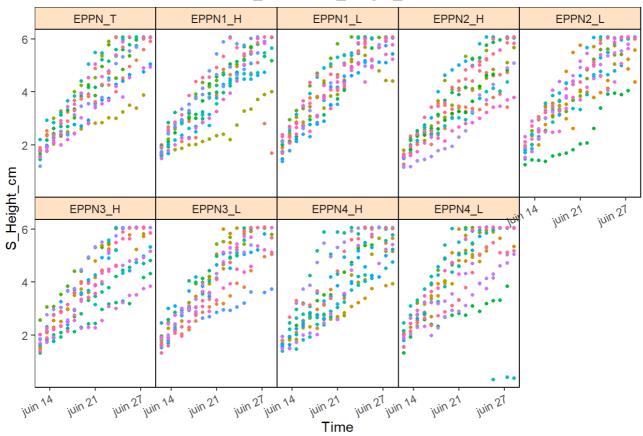
2



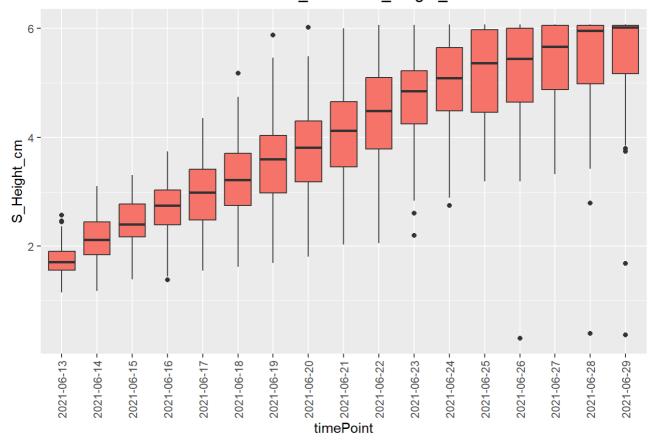
Time course, boxplots and correlation plots of data

```
for (trait_name in traits) {
  single_outliers_name <- paste0("Single_outliers_", trait_name)</pre>
  if (exists(single_outliers_name)) {
    Single_outliers <- get(single_outliers_name)</pre>
    plot(Single_outliers,
         traits = trait_name,
         plotType = "raw")
    plot(Single_outliers,
         plotType = "box",
         traits = trait_name)
    plot(Single_outliers,
         plotType = "cor",
         traits = trait_name)
  } else {
    cat("No Single_outliers object found for trait", trait_name, "\n")
  }
}
```

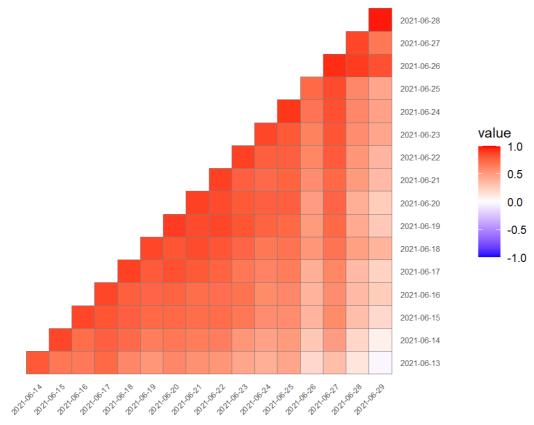
EPPN2020_UCPH - S_Height_cm - raw data



EPPN2020_UCPH - S_Height_cm



EPPN2020_UCPH - Correlations of timepoints for S_Height_cm



2. Correction for spatial trends

Fit a model for all time points with no extra fixed effects.

```
## 2021-06-13
```

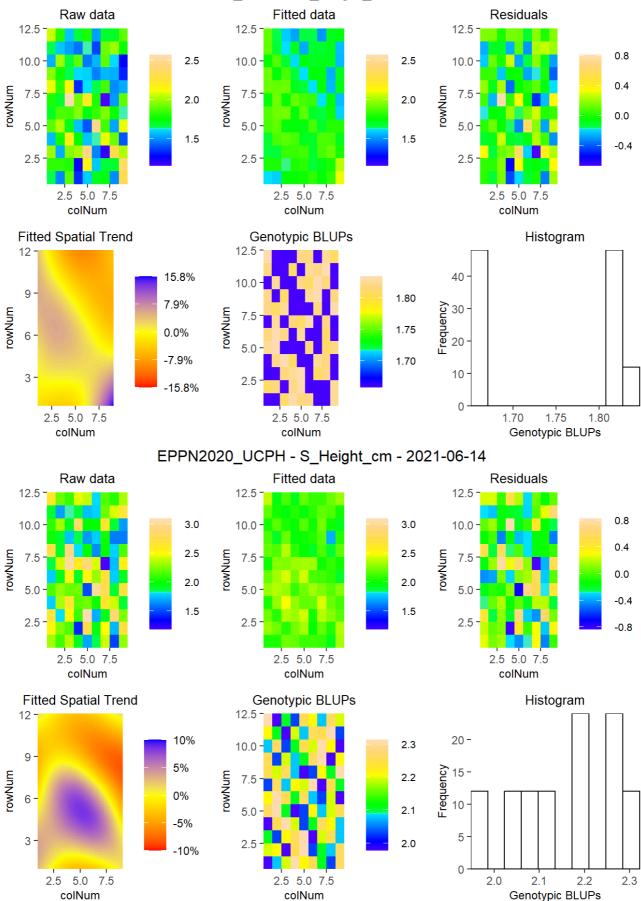
```
## 2021-06-14
```

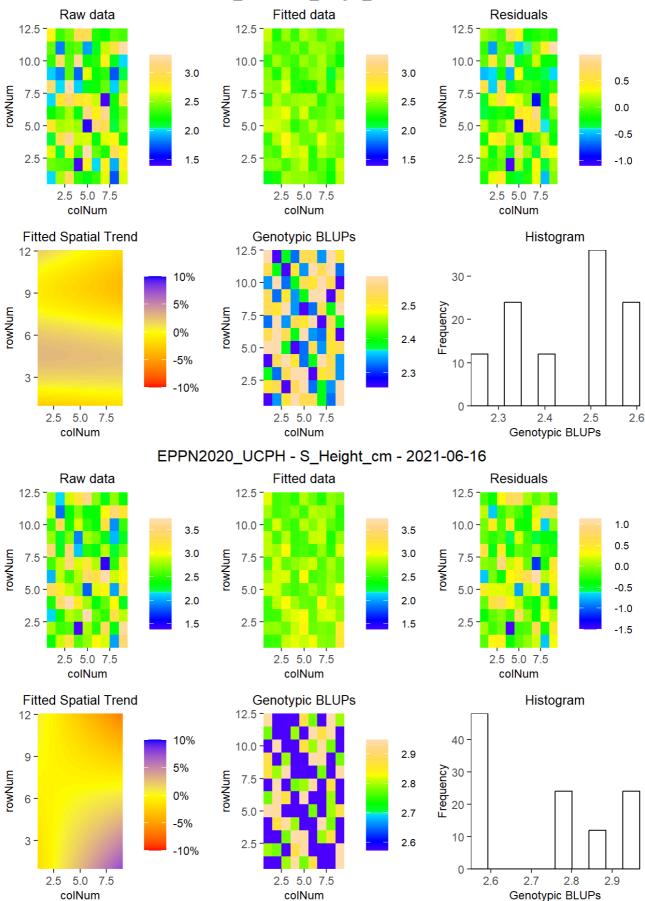
```
## 2021-06-15
```

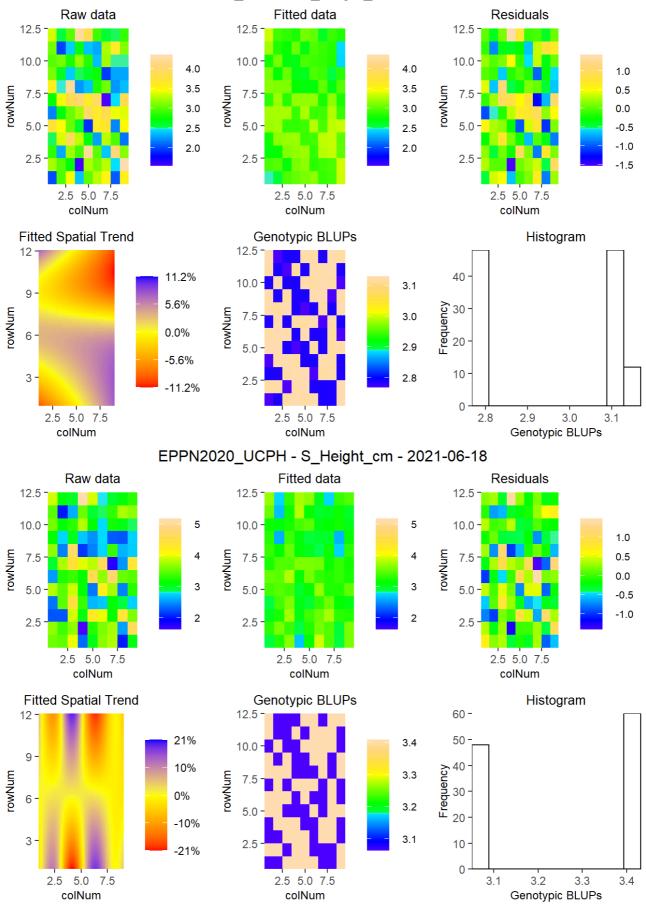
00/2024 17:49	OCI 11 Data Arialysis Timepoints
## 2021-06-16	
## 2021-06-17	
## 2021-06-18	
## 2021-06-19	
## 2021-06-20	
## 2021-06-21	
## 2021-06-22	
## 2021-06-23	
## 2021-06-24	
## 2021-06-25	
## 2021-06-26	
## 2021-06-27	
## 2021-06-28	
## 2021-06-29	

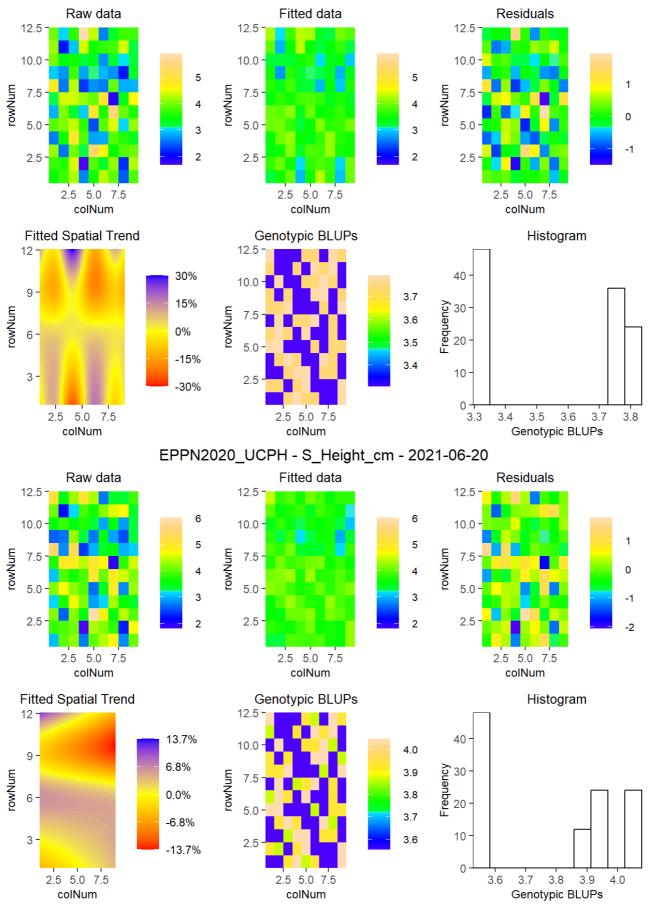
Model visualisation

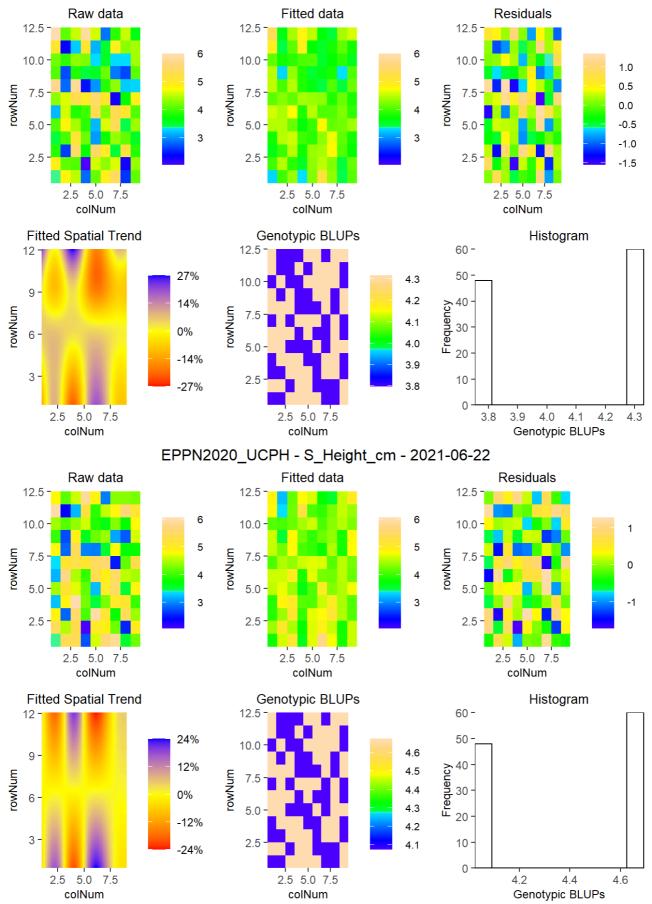
```
for (trait_name in traits) {
  mod_name <- paste0("modTP_", trait_name)</pre>
  if (exists(mod_name)) {
    mod <- get(mod_name)</pre>
    for (tp in 1:length(num_timepoints$timeNumber)) {
      plot(mod,
           timePoints = tp,
           plotType = "spatial",
           spaTrend = "percentage")
    }
    gif_file <- sprintf("%s/%s_mod.gif", datadir, trait_name)</pre>
    plot(mod,
         plotType = "timeLapse",
         spaTrend = "percentage",
         outFile = gif_file)
  } else {
    cat("No model found for", trait_name, "\n")
  }
}
```

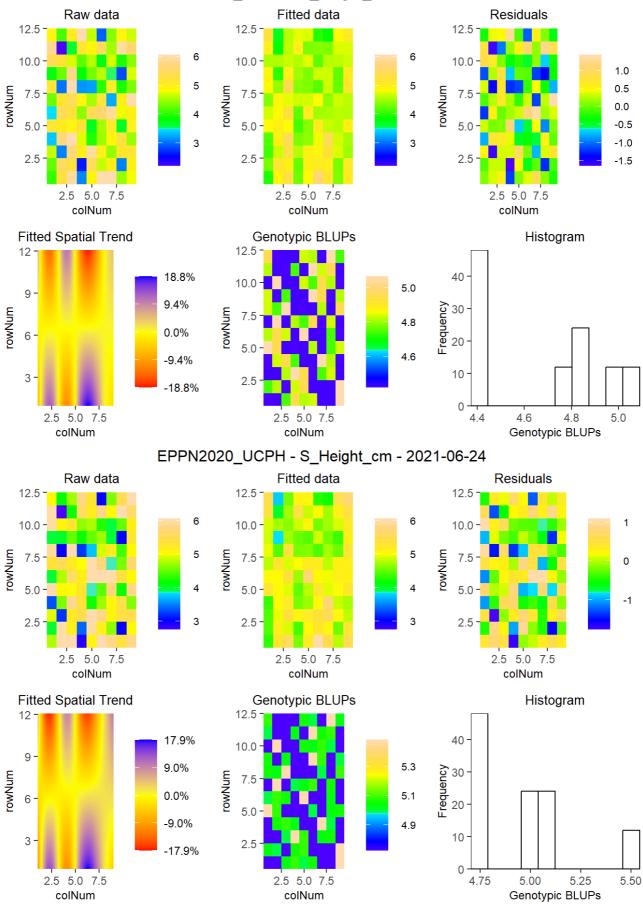


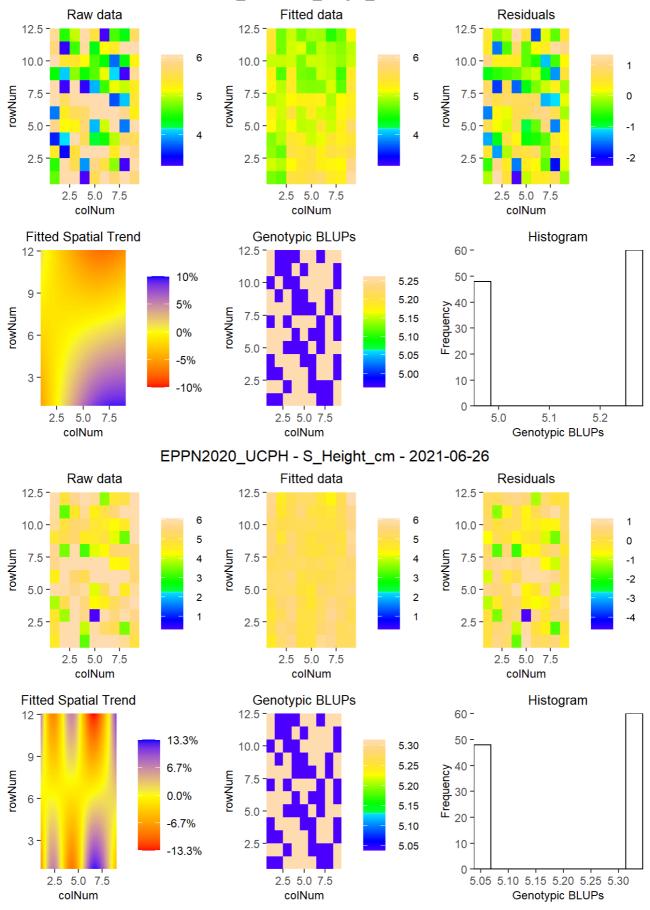


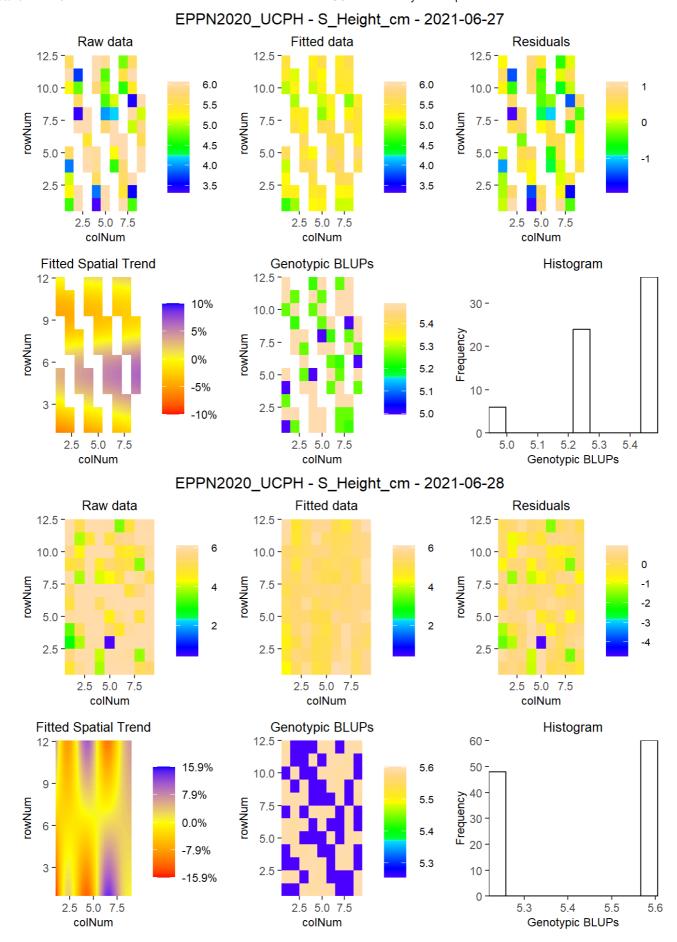




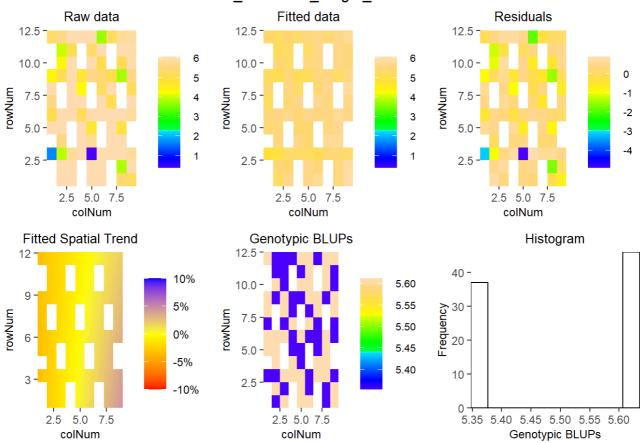






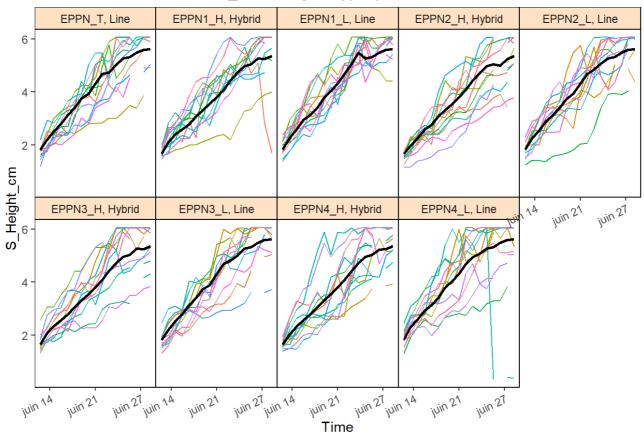


Output at: C:/Users/elise/Documents/Mémoire/Main/Data/Extracted/S_Height_cm_mod.gif

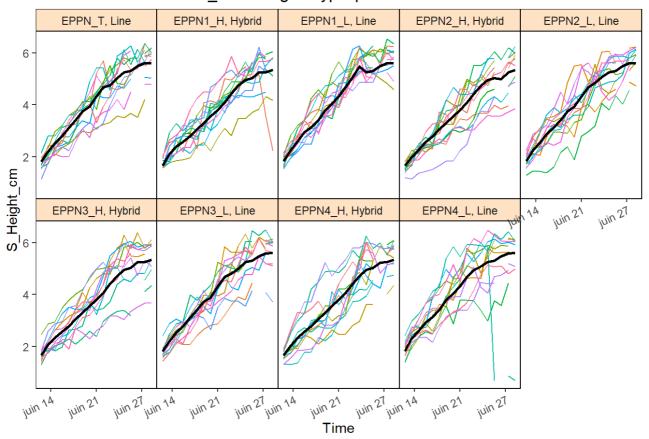


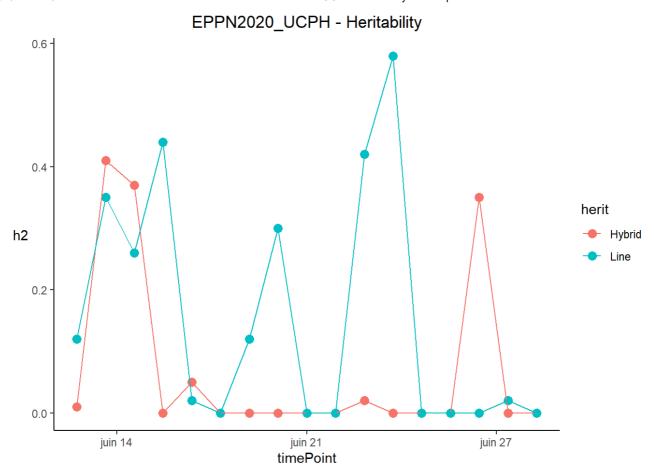
```
for (trait_name in traits) {
 mod_name <- paste0("modTP_", trait_name)</pre>
    if (exists(mod_name)) {
    mod <- get(mod_name)</pre>
    plot(mod,
         plotType = "rawPred",
         plotLine = TRUE)
    plot(mod,
         plotType = "corrPred",
         plotLine = TRUE)
    plot(mod,
         plotType = "herit",
         yLim = c(0, 0.5))
    plot(mod,
         plotType = "effDim",
         EDType = "ratio",
         yLim = c(0, 1))
    plot(mod,
         plotType = "corrPred")
    cat("No model found for the trait", trait_name, "\n")
  }
}
```

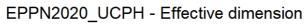
EPPN2020_UCPH - genotypic prediction + raw data

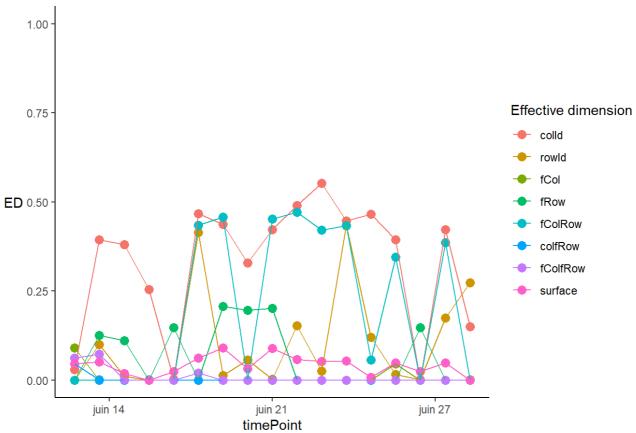


EPPN2020_UCPH - genotypic prediction + corrected data

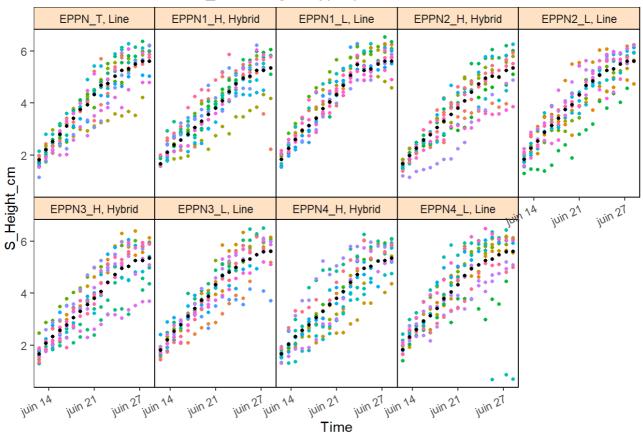








EPPN2020_UCPH - genotypic prediction + corrected data



3. Outlier detection for series of observations

By using the splines.

fitModels

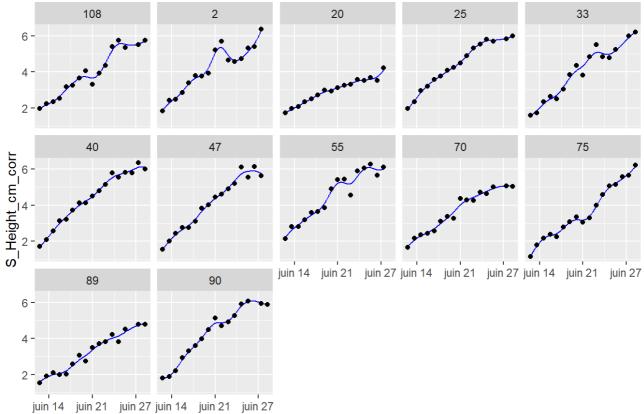
```
for (trait_name in traits) {
   Spatial_Corrected_name <- paste0("Spatial_Corrected_", trait_name)
   modTP_name <- paste0("modTP_", trait_name)
}</pre>
```

```
knots \leftarrow c(30)
mintimepoints <- c(9) # Minimal number of observations
for (trait name in traits) {
 # Nom de la variable pour les données corrigées
 Spatial_Corrected_name <- paste0("Spatial_Corrected_", trait_name)</pre>
 modTP_name <- paste0("modTP_", trait_name)</pre>
 # Vérifier si le modèle existe
 if (exists(modTP_name)) {
    modTP <- get(modTP_name)</pre>
    Spatial_Corrected <- getCorrected(modTP)</pre>
    assign(Spatial_Corrected_name, Spatial_Corrected)
    # Ajuster les splines pour les données corrigées
    fit.spline <- fitSpline(inDat = Spatial_Corrected,</pre>
                             trait = paste0(trait_name, "_corr"),
                              knots = knots,
                             minNoTP = mintimepoints)
    # Extraire les tables de valeurs prédites et coefficients de splines
    predDat_name <- paste0("predDat_", trait_name)</pre>
    coefDat_name <- paste0("coefDat_", trait_name)</pre>
    assign(predDat_name, fit.spline$predDat)
    assign(coefDat_name, fit.spline$coefDat)
 } else {
    cat("No model found for", trait_name, "\n")
  }
}
```

Plot the splines for a plant selection

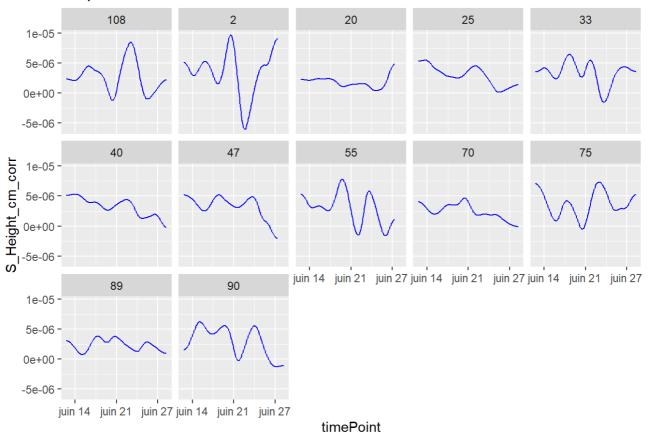
```
for (trait_name in traits) {
 plantSel <- S_timeseries[grepl('EPPN_T', S_timeseries$Genotype), "Unit.ID", drop = TR</pre>
 plantSel <- as.character(plantSel)</pre>
 plot(fit.spline,
       plotIds = plantSel,
       plotType = "predictions",
       main = paste("Predictions for", trait_name))
 plot(fit.spline,
       plotIds = plantSel,
       plotType = "derivatives",
       main = paste("Derivatives for", trait_name))
 plot(fit.spline,
       plotIds = plantSel,
       plotType = "derivatives2",
       main = paste("Second Derivatives for", trait_name))
}
```

Corrected data and P-spline prediction

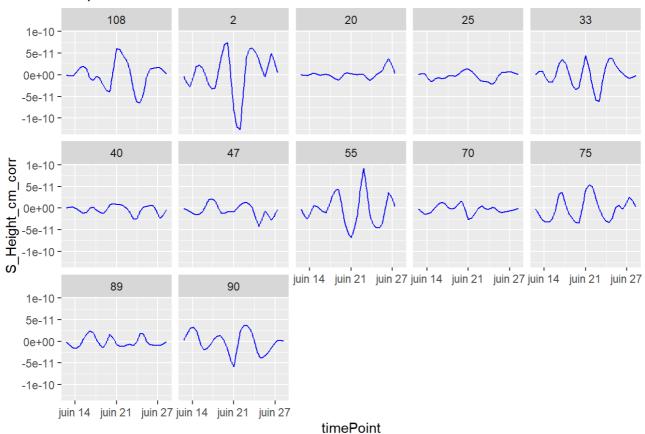


timePoint

P-spline first derivatives

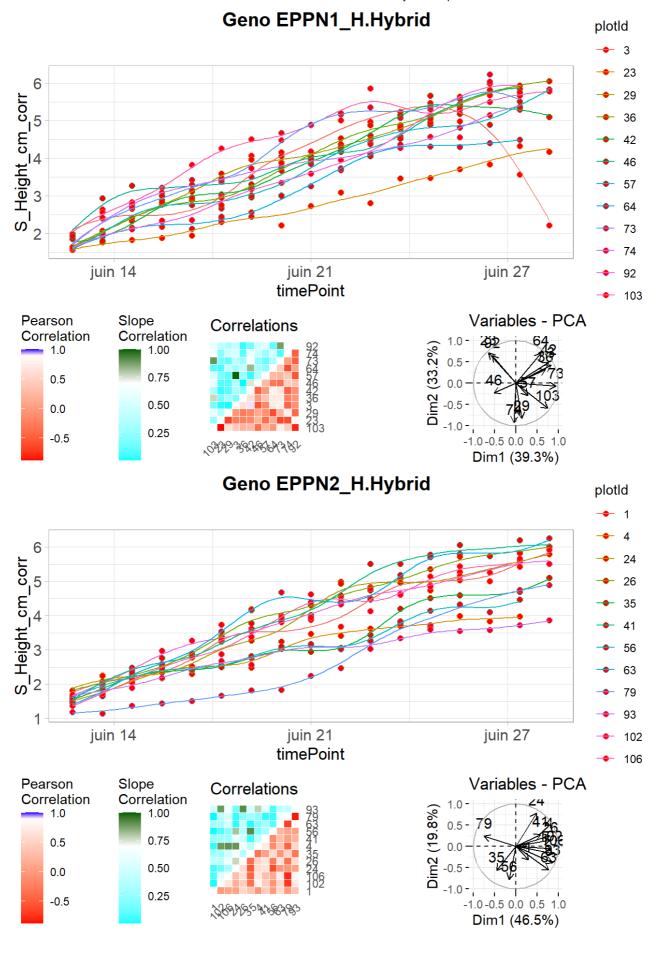


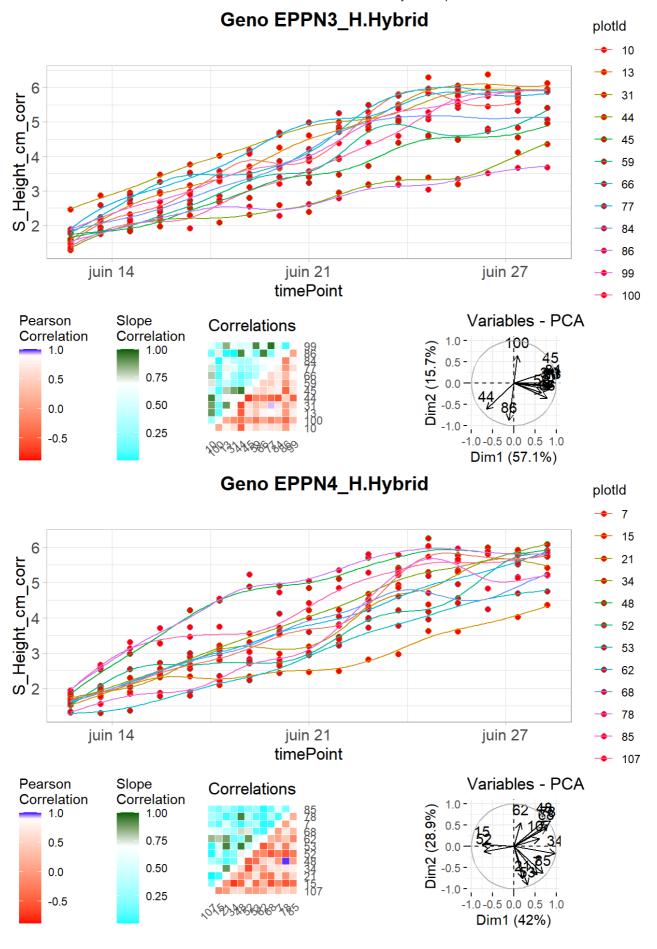
P-spline second derivatives

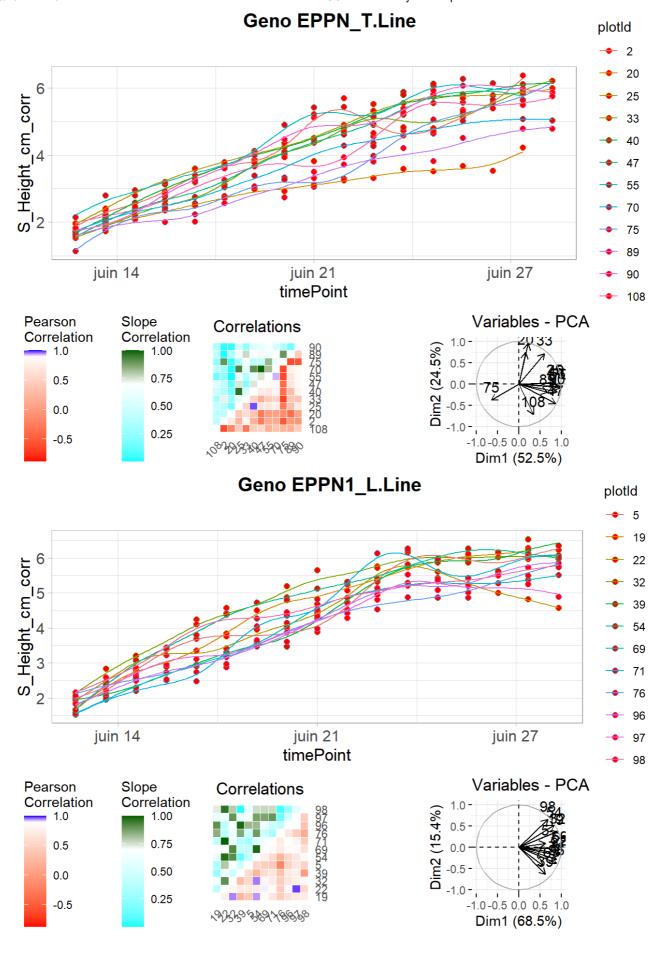


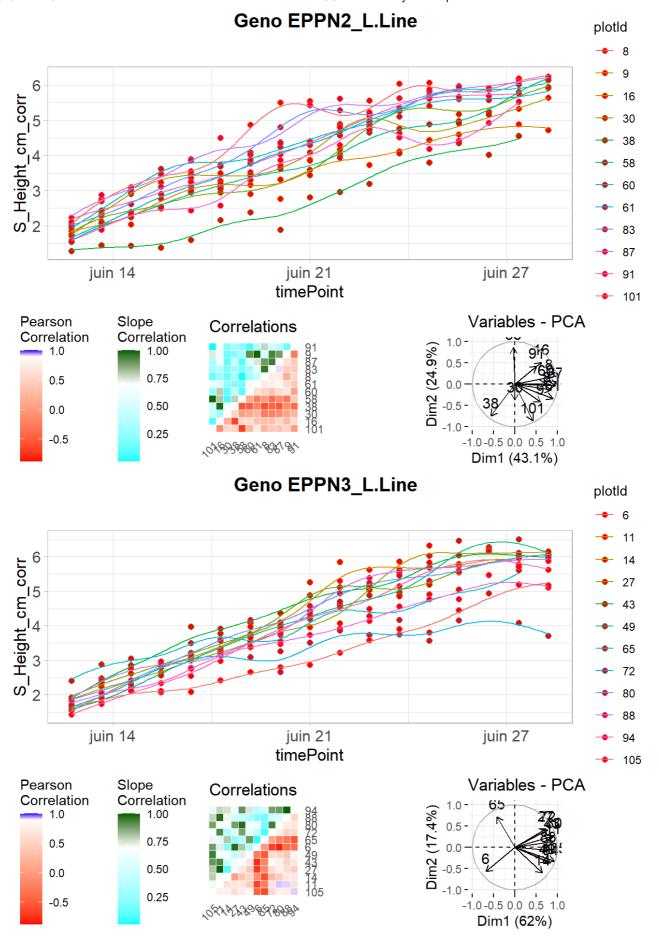
detectSerieOut

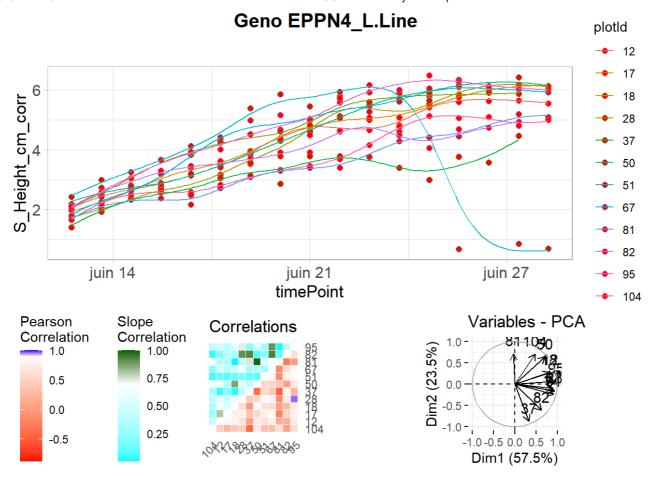
```
thrCor <- c(0.9) # correlation threshold
thrPca <- c(30) # pca angle threshold
thrSlope <- c(0.7) # slope threshold
for (trait name in traits) {
  Spatial_Corrected_name <- paste0("Spatial_Corrected_", trait_name)</pre>
  predDat_name <- paste0("predDat_", trait_name)</pre>
  coefDat_name <- paste0("coefDat_", trait_name)</pre>
  if (exists(Spatial_Corrected_name) && exists(predDat_name) && exists(coefDat_name)) {
    Spatial_Corrected <- get(Spatial_Corrected_name)</pre>
    predDat <- get(predDat_name)</pre>
    coefDat <- get(coefDat_name)</pre>
    Series_test <- detectSerieOut(corrDat = Spatial_Corrected,</pre>
                                   predDat = predDat,
                                   coefDat = coefDat,
                                   trait = paste0(trait_name, "_corr"),
                                   thrCor = thrCor,
                                   thrPca = thrPca,
                                   thrSlope = thrSlope,
                                   geno.decomp = "geno.decomp")
    plot(Series_test, genotypes = levels(factor(Series_test$genotype)))
    assign(paste0("Series_test_", trait_name), Series_test)
    assign(paste0("Spatial_Corrected_Out_", trait_name), Spatial_Corrected)
  } else {
    cat("No corrected data or prediction data found for", trait_name, "\n")
}
```











removeSerieOut

```
for (trait_name in traits) {
  # Nom de la variable pour les données corrigées
  Spatial_Corrected_name <- paste0("Spatial_Corrected_", trait_name)</pre>
  Series_test_name <- paste0("Series_test_", trait_name)</pre>
  # Extraire les données corrigées et les résultats des séries
  if (exists(Spatial_Corrected_name) && exists(Series_test_name)) {
    Spatial_Corrected <- get(Spatial_Corrected_name)</pre>
    Series_test <- get(Series_test_name)</pre>
    # Supprimer les outliers de la série
    Spatial_Corrected_Out <- removeSerieOut(dat = Spatial_Corrected, serieOut = Series_</pre>
test)
    # Assigner le résultat à une nouvelle variable
    assign(paste0("Spatial_Corrected_Out_", trait_name), Spatial_Corrected_Out)
    cat("No corrected data or series test data found for", trait_name, "\n")
  }
}
```

```
for (trait_name in traits) {
    Spatial_Corrected_Out_name <- paste0("Spatial_Corrected_Out_", trait_name)

if (exists(Spatial_Corrected_Out_name)) {
    Spatial_Corrected_Out <- get(Spatial_Corrected_Out_name)
    output_file <- sprintf("%s/timeSeriesOutliers_%s.tsv", datadir, trait_name)
    readr::write_tsv(Spatial_Corrected_Out, output_file)

    cat("Data written to:", output_file, "\n")
} else {
    cat("No corrected data found for", trait_name, "\n")
}</pre>
```

Data written to: C:/Users/elise/Documents/Mémoire/Main/Data/Extracted/timeSeriesOutl
iers_S_Height_cm.tsv

4. With the cleaned data, re-do the spatial correction

This is used to compare the values before and after.

Need to write a for loop for all the variables.

For S_Height_cm

```
## 2021-06-13
```

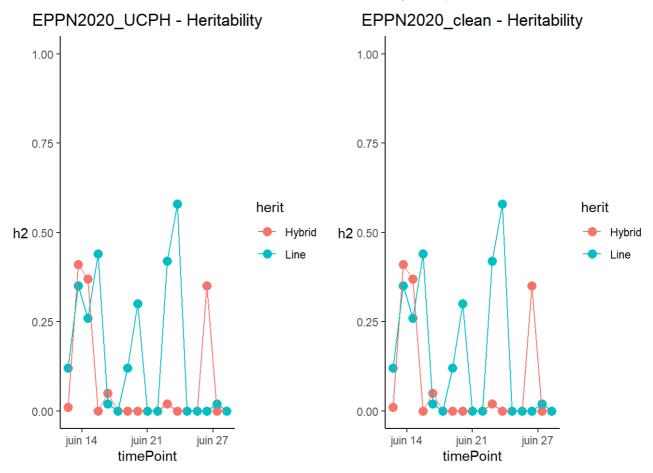
```
## 2021-06-14
```

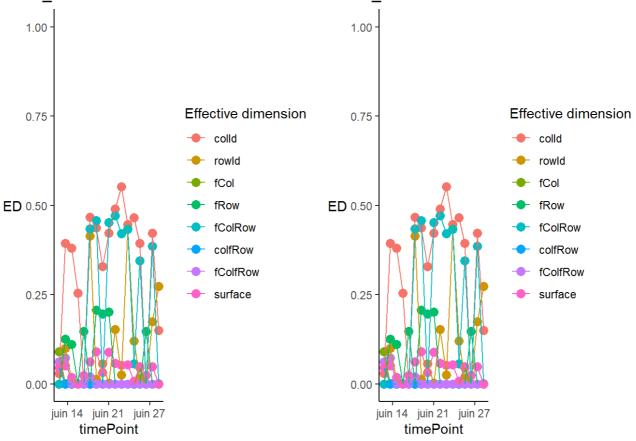
```
## 2021-06-15
```

```
## 2021-06-16
```

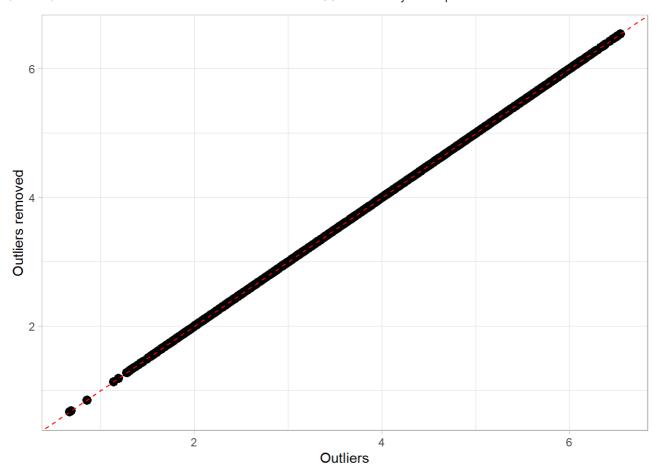
```
## 2021-06-17
```

```
## 2021-06-18
## 2021-06-19
## 2021-06-20
## 2021-06-21
## 2021-06-22
## 2021-06-23
## 2021-06-24
## 2021-06-25
## 2021-06-26
## 2021-06-27
## 2021-06-28
## 2021-06-29
## Extract corrected values
Spatial_Corrected_2 <- getCorrected(modTP_2)</pre>
#Check the values before and after:
h21<-plot(modTP, output = FALSE,
          plotType = "herit",
          yLim = c(0.4,1)
h22<-plot(modTP_2, output = FALSE,
          plotType = "herit",
          yLim = c(0.4,1)
grid.arrange(h21, h22, nrow = 1)
```





Warning: Removed 1 rows containing missing values (`geom_point()`).



Estimation of parameter from time series

```
##
     genotype geno.decomp plotId max_derivatives max_timeNumber
## 1
       EPPN_T
                      Line
                              108
                                     8.427168e-06
                                                           892800
## 2
       EPPN T
                      Line
                                2
                                     9.671293e-06
                                                           652800
       EPPN T
                      Line
                               20
                                     4.874353e-06
## 3
                                                          1296000
       EPPN_T
                               25
## 4
                      Line
                                     5.491787e-06
                                                            96000
## 5
       EPPN_T
                      Line
                               33
                                     6.457257e-06
                                                           470400
## 6
       EPPN_T
                      Line
                               40
                                     5.298470e-06
                                                           115200
##
           max_timePoint
## 1 2021-06-23 08:00:00
## 2 2021-06-20 13:20:00
## 3 2021-06-28 00:00:00
## 4 2021-06-14 02:40:00
## 5 2021-06-18 10:40:00
## 6 2021-06-14 08:00:00
```

