Spectra-trait PLSR example using leaf-level spectra and leaf mass per area (LMA) data from CONUS NEON sites

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Overview

This is an R Markdown Notebook to illustrate how to retrieve a dataset from the EcoSIS spectral database, choose the "optimal" number of plsr components, and fit a plsr model for leaf-mass area (LMA)

Getting Started

Installation

```
### Install and load required R packages
list.of.packages <- c("devtools","readr","RCurl","httr","pls","dplyr","reshape2","here",
                      "ggplot2","gridExtra")  # packages needed for script
# check for dependencies and install if needed
new.packages <- list.of.packages[!(list.of.packages %in% installed.packages()[,"Package"])]
if(length(new.packages)) install.packages(new.packages)

# Load libraries
invisible(lapply(list.of.packages, library, character.only = TRUE))
```

```
## Loading required package: usethis
```

```
##
## Attaching package: 'pls'
```

```
## The following object is masked from 'package:stats':
##
##     loadings
```

```
##
## Attaching package: 'dplyr'
```

```
## The following objects are masked from 'package:stats':
##
##     filter, lag
```

```
## The following objects are masked from 'package:base':
##
##     intersect, setdiff, setequal, union
```

```
## here() starts at /Users/sserbin/Data/GitHub/PLSR_for_plant_trait_prediction
```

```
##
## Attaching package: 'gridExtra'
```

```
## The following object is masked from 'package:dplyr':
##
##     combine
```

Setup other functions and options

```
### Setup other functions and options
github_dir <- file.path(here::here(),"R_Scripts")
source_from_gh <- FALSE
if (source_from_gh) {
  # Source helper functions from GitHub
  devtools::source_url("https://raw.githubusercontent.com/TESTgroup-BNL/PLSR_for_plant_trait_prediction/
} else {
  functions <- file.path(github_dir,"functions.R")
  source(functions)
}

# not in
`%notin%` <- Negate(`%in%`)

# Script options
pls::pls.options(plsralg = "oscorespls")
pls::pls.options("plsralg")
```

```
## $plsralg
## [1] "oscorespls"
```

```
# Default par options
opar <- par(no.readonly = T)

# What is the target variable?
inVar <- "LMA_gDW_m2"

# What is the source dataset from EcoSIS?
ecosis_id <- "5617da17-c925-49fb-b395-45a51291bd2d"
```

Set working directory (scratch space)

```
## [1] "Output directory: /private/var/folders/xp/h3k9vf3n2jx181ts786_yjrn9c2gjq/T/RtmpfflMVP"
```

Grab data from EcoSIS

```
print(paste0("Output directory: ",getwd()))  # check wd
```

URL: https://ecosis.org/package/fresh-leaf-spectra-to-estimate-lma-over-neon-domains-in-eastern-united-states

```
## [1] "Output directory: /Users/sserbin/Data/GitHub/PLSR_for_plant_trait_prediction/vignettes"
```

```
### Get source dataset from EcoSIS
dat_raw <- get_ecosis_data(ecosis_id = ecosis_id)
```

```
## [1] "**** Downloading Ecosis data ****"
```

```
## Downloading data...
```

```
## Parsed with column specification:
## cols(
##   .default = col_double(),
##   Affiliation = col_character(),
##   `Common Name` = col_character(),
##   Domain = col_character(),
##   Functional_type = col_character(),
##   `Latin Genus` = col_character(),
##   `Latin Species` = col_character(),
##   PI = col_character(),
##   Project = col_character(),
##   Sample_ID = col_character(),
##   `USDA Symbol` = col_character()
## )
```

```
## See spec(...) for full column specifications.
```

```
## Download complete!
```

```
head(dat_raw)
```

```
## # A tibble: 6 x 2,162
##   Affiliation `Common Name` Domain Functional_type   LMA `Latin Genus`
##   <chr>       <chr>         <chr>  <chr>           <dbl> <chr>
## 1 University~ black walnut  D02    broadleaf        72.9 Juglans
## 2 University~ black walnut  D02    broadleaf        72.9 Juglans
## 3 University~ black walnut  D02    broadleaf        60.8 Juglans
## 4 University~ black walnut  D02    broadleaf        60.8 Juglans
## 5 University~ black walnut  D02    broadleaf        85.9 Juglans
## 6 University~ black walnut  D02    broadleaf        85.9 Juglans
## # ... with 2,156 more variables: `Latin Species` <chr>, PI <chr>,
## #   Project <chr>, Sample_ID <chr>, `USDA Symbol` <chr>, `350` <dbl>,
## #   `351` <dbl>, `352` <dbl>, `353` <dbl>, `354` <dbl>, `355` <dbl>,
## #   `356` <dbl>, `357` <dbl>, `358` <dbl>, `359` <dbl>, `360` <dbl>,
## #   `361` <dbl>, `362` <dbl>, `363` <dbl>, `364` <dbl>, `365` <dbl>,
## #   `366` <dbl>, `367` <dbl>, `368` <dbl>, `369` <dbl>, `370` <dbl>,
## #   `371` <dbl>, `372` <dbl>, `373` <dbl>, `374` <dbl>, `375` <dbl>,
## #   `376` <dbl>, `377` <dbl>, `378` <dbl>, `379` <dbl>, `380` <dbl>,
## #   `381` <dbl>, `382` <dbl>, `383` <dbl>, `384` <dbl>, `385` <dbl>,
## #   `386` <dbl>, `387` <dbl>, `388` <dbl>, `389` <dbl>, `390` <dbl>,
## #   `391` <dbl>, `392` <dbl>, `393` <dbl>, `394` <dbl>, `395` <dbl>,
## #   `396` <dbl>, `397` <dbl>, `398` <dbl>, `399` <dbl>, `400` <dbl>,
## #   `401` <dbl>, `402` <dbl>, `403` <dbl>, `404` <dbl>, `405` <dbl>,
## #   `406` <dbl>, `407` <dbl>, `408` <dbl>, `409` <dbl>, `410` <dbl>,
## #   `411` <dbl>, `412` <dbl>, `413` <dbl>, `414` <dbl>, `415` <dbl>,
## #   `416` <dbl>, `417` <dbl>, `418` <dbl>, `419` <dbl>, `420` <dbl>,
## #   `421` <dbl>, `422` <dbl>, `423` <dbl>, `424` <dbl>, `425` <dbl>,
## #   `426` <dbl>, `427` <dbl>, `428` <dbl>, `429` <dbl>, `430` <dbl>,
## #   `431` <dbl>, `432` <dbl>, `433` <dbl>, `434` <dbl>, `435` <dbl>,
## #   `436` <dbl>, `437` <dbl>, `438` <dbl>, `439` <dbl>, `440` <dbl>,
## #   `441` <dbl>, `442` <dbl>, `443` <dbl>, `444` <dbl>, ...
```

```
names(dat_raw)[1:40]
```

```
##  [1] "Affiliation"     "Common Name"     "Domain"          "Functional_type"
```

```
##  [5] "LMA"             "Latin Genus"     "Latin Species"   "PI"
##  [9] "Project"         "Sample_ID"       "USDA Symbol"     "350"
## [13] "351"             "352"             "353"             "354"
## [17] "355"             "356"             "357"             "358"
## [21] "359"             "360"             "361"             "362"
## [25] "363"             "364"             "365"             "366"
## [29] "367"             "368"             "369"             "370"
## [33] "371"             "372"             "373"             "374"
## [37] "375"             "376"             "377"             "378"
```

Create full plsr dataset

```
### Create plsr dataset
Start.wave <- 500
End.wave <- 2400
wv <- seq(Start.wave,End.wave,1)
Spectra <- as.matrix(dat_raw[,names(dat_raw) %in% wv])
colnames(Spectra) <- c(paste0("Wave_",wv))
sample_info <- dat_raw[,names(dat_raw) %notin% seq(350,2500,1)]
head(sample_info)
```

```
## # A tibble: 6 x 11
##   Affiliation `Common Name` Domain Functional_type   LMA `Latin Genus`
##   <chr>       <chr>         <chr>  <chr>           <dbl> <chr>
## 1 University~ black walnut  D02    broadleaf        72.9 Juglans
## 2 University~ black walnut  D02    broadleaf        72.9 Juglans
## 3 University~ black walnut  D02    broadleaf        60.8 Juglans
## 4 University~ black walnut  D02    broadleaf        60.8 Juglans
## 5 University~ black walnut  D02    broadleaf        85.9 Juglans
## 6 University~ black walnut  D02    broadleaf        85.9 Juglans
## # ... with 5 more variables: `Latin Species` <chr>, PI <chr>, Project <chr>,
## #   Sample_ID <chr>, `USDA Symbol` <chr>
```

```
sample_info2 <- sample_info %>%
  select(Domain,Functional_type,Sample_ID,USDA_Species_Code=`USDA Symbol`,LMA_gDW_m2=LMA)
head(sample_info2)
```

```
## # A tibble: 6 x 5
##   Domain Functional_type Sample_ID USDA_Species_Code LMA_gDW_m2
##   <chr>  <chr>           <chr>     <chr>                  <dbl>
## 1 D02    broadleaf       P0001     JUNI                    72.9
## 2 D02    broadleaf       L0001     JUNI                    72.9
## 3 D02    broadleaf       P0002     JUNI                    60.8
## 4 D02    broadleaf       L0002     JUNI                    60.8
## 5 D02    broadleaf       P0003     JUNI                    85.9
## 6 D02    broadleaf       L0003     JUNI                    85.9
```

```
plsr_data <- data.frame(sample_info2,Spectra)
rm(sample_info,sample_info2,Spectra)
```

Create cal/val datasets

```
### Create cal/val datasets
## Make a stratified random sampling in the strata USDA_Species_Code and Domain

method <- "dplyr" #base/dplyr
# base R - a bit slow
# dplyr - much faster
split_data <- create_data_split(approach=method, split_seed=2356812, prop=0.8,
                                group_variables=c("USDA_Species_Code","Domain"))
names(split_data)
```

```
## [1] "cal_data" "val_data"
```

```
cal.plsr.data <- split_data$cal_data
head(cal.plsr.data)[1:8]
```

```
##   Domain Functional_type Sample_ID USDA_Species_Code LMA_gDW_m2   Wave_500
## 1    D08       broadleaf     L2644              ACBA      44.18 0.04170800
## 2    D08       broadleaf     L2646              ACBA      41.71 0.05067800
## 3    D08       broadleaf     L2645              ACBA      40.66 0.04701700
## 4    D08       broadleaf     P2639              ACBA      44.18 0.04125300
## 5    D03       broadleaf     P0614              ACFL      52.91 0.03895800
## 6    D03       broadleaf     L0609              ACFL      81.67 0.04186169
##     Wave_501   Wave_502
## 1 0.04208700 0.04283700
## 2 0.05087600 0.05153500
## 3 0.04718200 0.04766500
## 4 0.04150300 0.04247100
## 5 0.03915100 0.03956200
## 6 0.04217802 0.04258768
```

```
val.plsr.data <- split_data$val_data
head(val.plsr.data)[1:8]
```

```
##      Domain Functional_type Sample_ID USDA_Species_Code LMA_gDW_m2 Wave_500
## 4923    D08       broadleaf     P2462              <NA>      21.10 0.044964
## 4924    D08       broadleaf     L2462              SANI     100.72 0.068921
## 4925    D08       broadleaf     P2463              <NA>      29.59 0.036254
## 4926    D08       broadleaf     L2463              SANI      96.48 0.051810
## 4927    D08       broadleaf     P2464              <NA>      31.08 0.056587
## 4928    D08       broadleaf     L2464              SANI      61.40 0.037310
##      Wave_501 Wave_502
## 4923 0.045854 0.046911
## 4924 0.069633 0.070254
## 4925 0.036999 0.037671
## 4926 0.052113 0.052896
## 4927 0.057006 0.057734
## 4928 0.037223 0.037671
```

```
rm(split_data)

# Datasets:
print(paste("Cal observations: ",dim(cal.plsr.data)[1],sep=""))
```

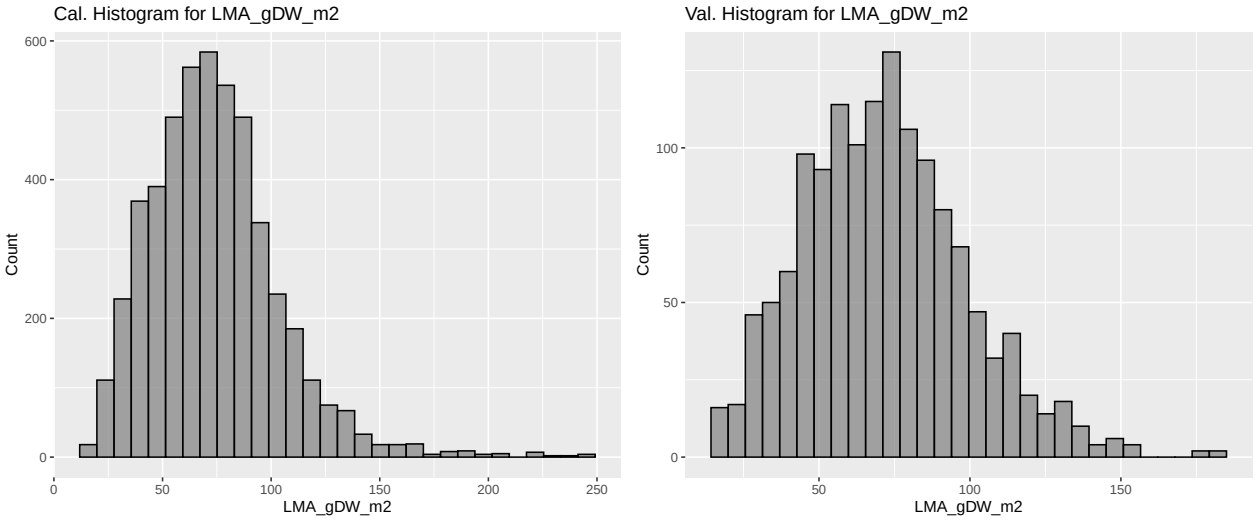
```
## [1] "Cal observations: 4922"
```

```
print(paste("Val observations: ",dim(val.plsr.data)[1],sep=""))
```

```
## [1] "Val observations: 1390"
```

```
cal_hist_plot <- qplot(cal.plsr.data[,paste0(inVar)],geom="histogram",
                       main = paste0("Cal. Histogram for ",inVar),
                       xlab = paste0(inVar),ylab = "Count",fill=I("grey50"),
                       col=I("black"),alpha=I(.7))
val_hist_plot <- qplot(val.plsr.data[,paste0(inVar)],geom="histogram",
                       main = paste0("Val. Histogram for ",inVar),
                       xlab = paste0(inVar),ylab = "Count",fill=I("grey50"),
                       col=I("black"),alpha=I(.7))
grid.arrange(cal_hist_plot, val_hist_plot, ncol=2)
```

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



Create calibration and validation PLSR datasets

```
### Format PLSR data for model fitting
cal_spec <- as.matrix(cal.plsr.data[, which(names(cal.plsr.data) %in% paste0("Wave_",wv))])
cal.plsr.data <- data.frame(cal.plsr.data[, which(names(cal.plsr.data) %notin% paste0("Wave_",wv))],
                            Spectra=I(cal_spec))
head(cal.plsr.data)[1:5]
```

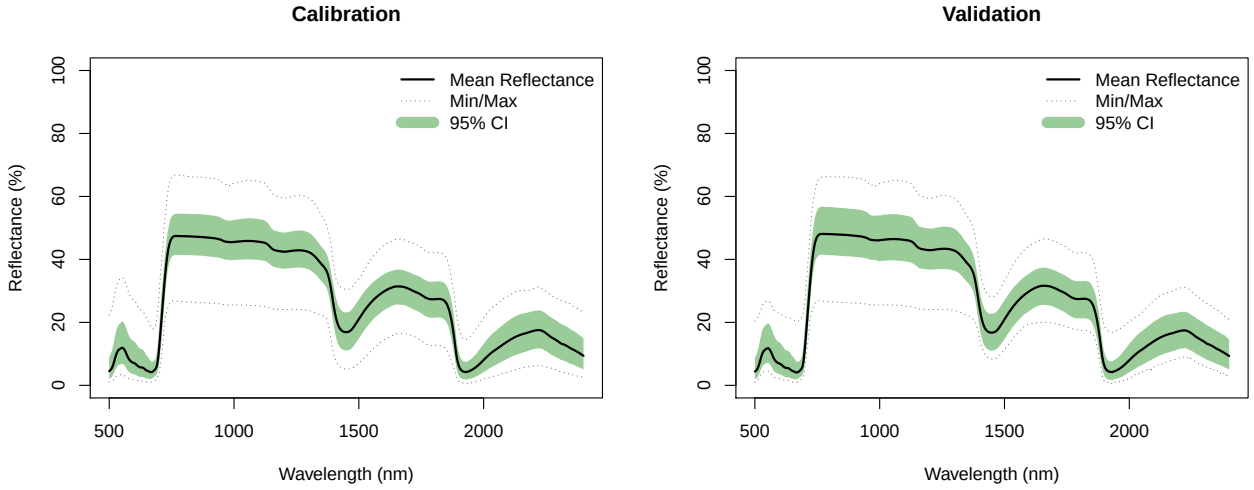
```
##   Domain Functional_type Sample_ID USDA_Species_Code LMA_gDW_m2
## 1    D08       broadleaf     L2644              ACBA      44.18
## 2    D08       broadleaf     L2646              ACBA      41.71
## 3    D08       broadleaf     L2645              ACBA      40.66
## 4    D08       broadleaf     P2639              ACBA      44.18
## 5    D03       broadleaf     P0614              ACFL      52.91
## 6    D03       broadleaf     L0609              ACFL      81.67
```

```
val_spec <- as.matrix(val.plsr.data[, which(names(val.plsr.data) %in% paste0("Wave_",wv))])
val.plsr.data <- data.frame(val.plsr.data[, which(names(val.plsr.data) %notin% paste0("Wave_",wv))],
                            Spectra=I(val_spec))
head(val.plsr.data)[1:5]
```

```
##      Domain Functional_type Sample_ID USDA_Species_Code LMA_gDW_m2
## 4923    D08       broadleaf     P2462              <NA>      21.10
## 4924    D08       broadleaf     L2462              SANI     100.72
## 4925    D08       broadleaf     P2463              <NA>      29.59
## 4926    D08       broadleaf     L2463              SANI      96.48
## 4927    D08       broadleaf     P2464              <NA>      31.08
## 4928    D08       broadleaf     L2464              SANI      61.40
```

plot cal and val spectra

```
par(mfrow=c(1,2)) # B, L, T, R
f.plot.spec(Z=cal.plsr.data$Spectra,wv=seq(Start.wave,End.wave,1),plot_label="Calibration")
f.plot.spec(Z=val.plsr.data$Spectra,wv=seq(Start.wave,End.wave,1),plot_label="Validation")
```



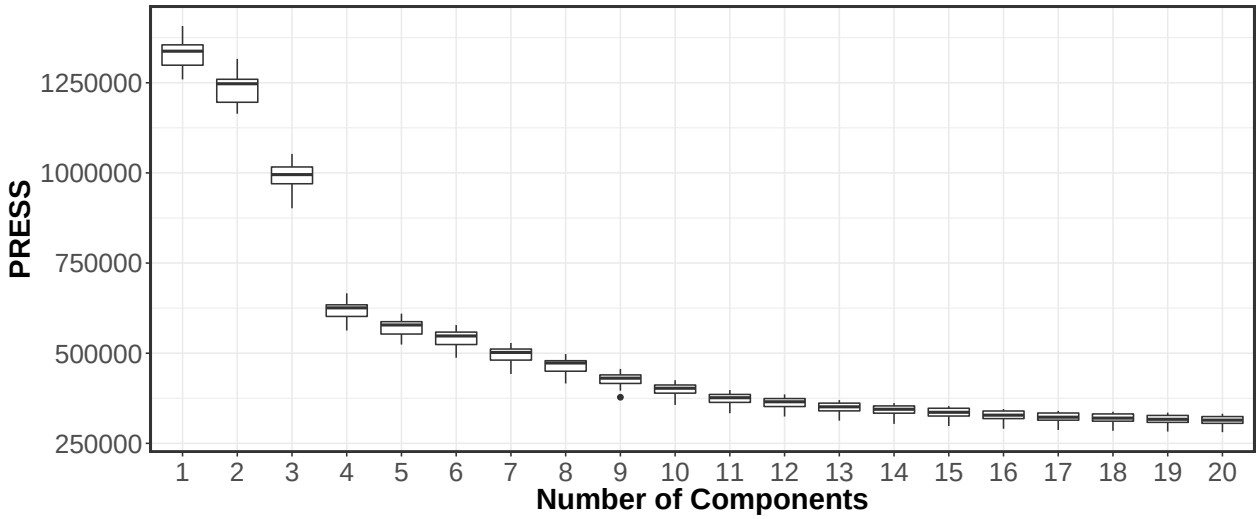

```
par(mfrow=c(1,1))
```

Use Jackknife permutation to determine optimal number of components

```
### Use permutation to determine the optimal number of components
if(grepl("Windows", sessionInfo()$running)){
  pls.options(parallel = NULL)
} else {
  pls.options(parallel = parallel::detectCores()-1)
}

method <- "custom"
random_seed <- 2356812
seg <- 100
maxComps <- 20
iterations <- 20
if (method=="pls") {
  # pls package approach - faster but estimates more components....
  nComps <- find_optimal_components(method=method, maxComps=maxComps, seg=seg,
                                    random_seed=random_seed)
} else {
  # custom method - slow but generally finds the smallest number of components
```

```
  nComps <- find_optimal_components(method=method, maxComps=maxComps, iterations=iterations,
                                    seg=seg, prop=0.70,
                                    random_seed=random_seed)
}
```

```
## [1] "*** Running jacknife permutation test.  Please hang tight, this can take awhile ***"
## Running interation 1
## Running interation 2
## Running interation 3
## Running interation 4
## Running interation 5
## Running interation 6
## Running interation 7
## Running interation 8
## Running interation 9
## Running interation 10
## Running interation 11
## Running interation 12
## Running interation 13
## Running interation 14
## Running interation 15
## Running interation 16
## Running interation 17
## Running interation 18
## Running interation 19
## Running interation 20
## No id variables; using all as measure variables
```




```
## [1] "*** Optimal number of components based on t.test: 14"
```

Fit final model

```
### Fit final model
segs <- 100
plsr.out <- plsr(as.formula(paste(inVar,"~","Spectra")),scale=FALSE,ncomp=nComps,
                 validation="CV",
                 segments=segs, segment.type="interleaved",trace=FALSE,
                 data=cal.plsr.data)
fit <- plsr.out$fitted.values[,1,nComps]
pls.options(parallel = NULL)

# External validation fit stats
par(mfrow=c(1,2)) # B, L, T, R
RMSEP(plsr.out, newdata = val.plsr.data)
```

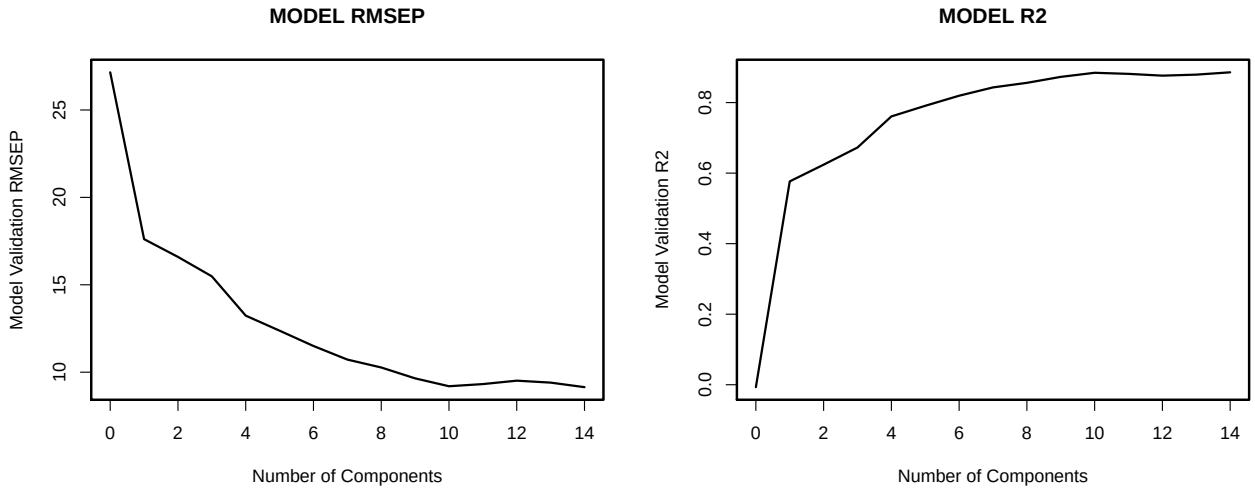
```
## (Intercept)      1 comps      2 comps      3 comps      4 comps      5 comps
##      27.155       17.610       16.595       15.483       13.235       12.374
##     6 comps      7 comps      8 comps      9 comps     10 comps     11 comps
##      11.499       10.722       10.269        9.647        9.197        9.319
##    12 comps     13 comps     14 comps
##       9.515        9.403        9.143
```

```
plot(RMSEP(plsr.out,estimate=c("test"),newdata = val.plsr.data),
     main="MODEL RMSEP",
     xlab="Number of Components",ylab="Model Validation RMSEP",lty=1,col="black",
     cex=1.5,lwd=2)
box(lwd=2.2)

R2(plsr.out, newdata = val.plsr.data)
```

```
## (Intercept)      1 comps      2 comps      3 comps      4 comps      5 comps
##   -0.006901     0.576543     0.623949     0.672643     0.760799     0.790906
##     6 comps      7 comps      8 comps      9 comps     10 comps     11 comps
##    0.819456     0.843031     0.856001     0.872913     0.884511     0.881406
##    12 comps     13 comps     14 comps
```

```
##    0.876368     0.879269     0.885848
```

```
plot(R2(plsr.out,estimate=c("test"),newdata = val.plsr.data), main="MODEL R2",
     xlab="Number of Components",ylab="Model Validation R2",lty=1,col="black",
     cex=1.5,lwd=2)
box(lwd=2.2)
```




```
par(opar)
```

PLSR fit observed vs. predicted plot data

```
#calibration
cal.plsr.output <- data.frame(cal.plsr.data[, which(names(cal.plsr.data) %notin% "Spectra")],
                              PLSR_Predicted=fit,
                              PLSR_CV_Predicted=as.vector(plsr.out$validation$pred[,,nComps]))
cal.plsr.output <- cal.plsr.output %>%
  mutate(PLSR_CV_Residuals = PLSR_CV_Predicted-get(inVar))
head(cal.plsr.output)
```

```
##   Domain Functional_type Sample_ID USDA_Species_Code LMA_gDW_m2 PLSR_Predicted
## 1    D08       broadleaf     L2644              ACBA      44.18       52.25180
## 2    D08       broadleaf     L2646              ACBA      41.71       40.47077
## 3    D08       broadleaf     L2645              ACBA      40.66       44.14454
## 4    D08       broadleaf     P2639              ACBA      44.18       44.96530
## 5    D03       broadleaf     P0614              ACFL      52.91       60.96168
## 6    D03       broadleaf     L0609              ACFL      81.67       91.11058
##   PLSR_CV_Predicted PLSR_CV_Residuals
## 1          52.32370         8.1436968
## 2          40.51303        -1.1969740
## 3          44.34736         3.6873566
## 4          45.12281         0.9428088
## 5          61.15931         8.2493103
## 6          91.19997         9.5299655
```

```
cal.R2 <- round(pls::R2(plsr.out)[[1]][nComps],2)
cal.RMSEP <- round(sqrt(mean(cal.plsr.output$PLSR_CV_Residuals^2)),2)

val.plsr.output <- data.frame(val.plsr.data[, which(names(val.plsr.data) %notin% "Spectra")],
```

```
                              PLSR_Predicted=as.vector(predict(plsr.out,
                                                               newdata = val.plsr.data,
                                                               ncomp=nComps, type="response")[,,1]))
val.plsr.output <- val.plsr.output %>%
  mutate(PLSR_Residuals = PLSR_Predicted-get(inVar))
head(val.plsr.output)
```

```
##   Domain Functional_type Sample_ID USDA_Species_Code LMA_gDW_m2 PLSR_Predicted
## 1    D08       broadleaf     P2462              <NA>      21.10       23.17688
## 2    D08       broadleaf     L2462              SANI     100.72       87.76061
## 3    D08       broadleaf     P2463              <NA>      29.59       30.12776
## 4    D08       broadleaf     L2463              SANI      96.48       89.17843
## 5    D08       broadleaf     P2464              <NA>      31.08       45.66874
## 6    D08       broadleaf     L2464              SANI      61.40       65.10542
##   PLSR_Residuals
## 1      2.0768781
## 2    -12.9593944
## 3      0.5377642
## 4     -7.3015651
## 5     14.5887365
## 6      3.7054219
```

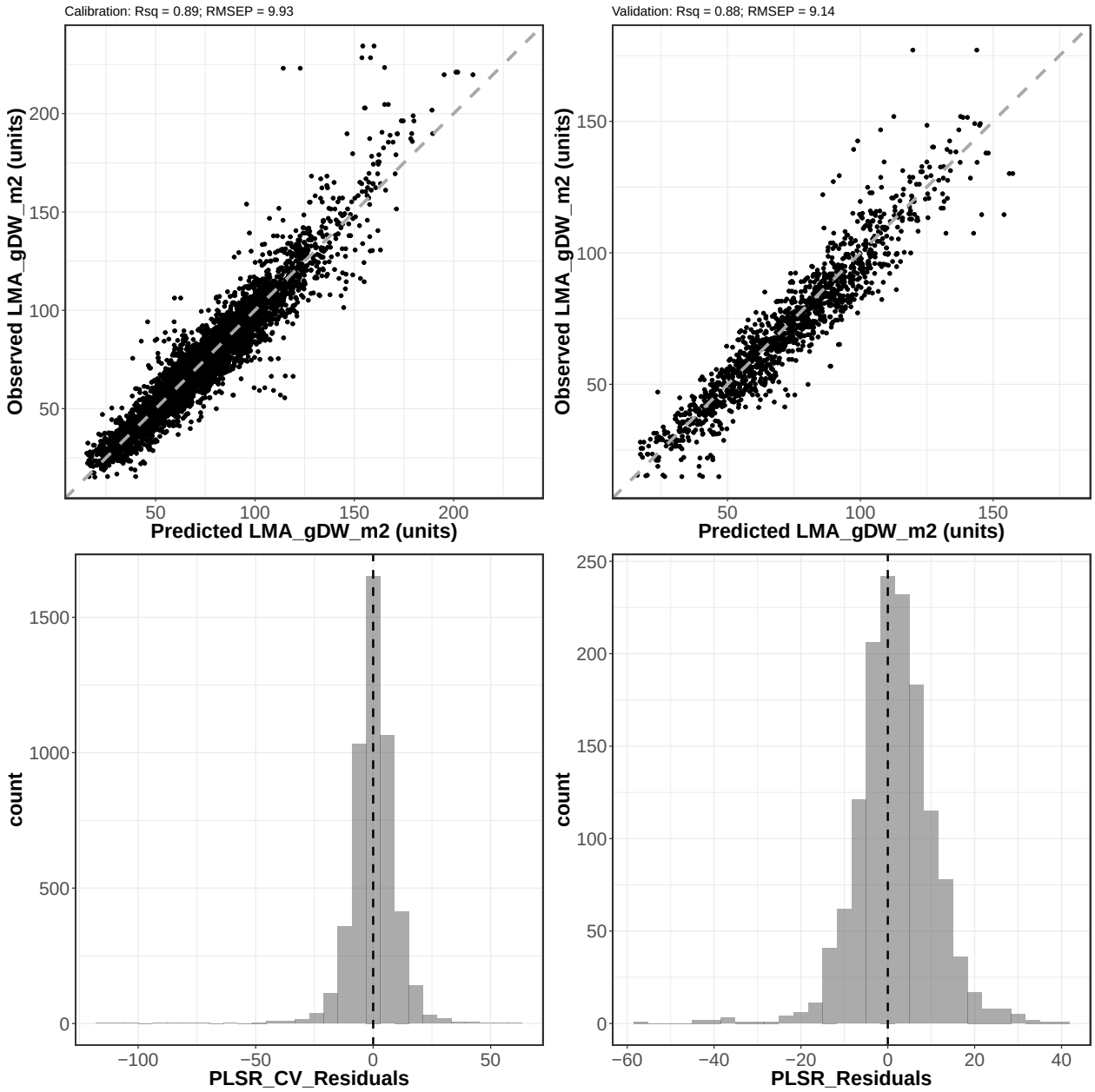
```
val.R2 <- round(pls::R2(plsr.out,newdata=val.plsr.data)[[1]][nComps],2)
val.RMSEP <- round(sqrt(mean(val.plsr.output$PLSR_Residuals^2)),2)

rng_quant <- quantile(cal.plsr.output[,inVar], probs = c(0.001, 0.999))
cal_scatter_plot <- ggplot(cal.plsr.output, aes(x=PLSR_CV_Predicted,
                                                y=get(inVar))) +
  theme_bw() + geom_point() + geom_abline(intercept = 0, slope = 1,
                                          color="dark grey",
                                          linetype="dashed",
                                          size=1.5) +
  xlim(rng_quant[1], rng_quant[2]) +
  ylim(rng_quant[1], rng_quant[2]) +
  labs(x=paste0("Predicted ", paste(inVar), " (units)"),
       y=paste0("Observed ", paste(inVar), " (units)"),
       title=paste0("Calibration: ", paste0("Rsq = ", cal.R2), "; ",
                    paste0("RMSEP = ",
                           cal.RMSEP))) +
  theme(axis.text=element_text(size=18), legend.position="none",
        axis.title=element_text(size=20, face="bold"),
        axis.text.x = element_text(angle = 0,vjust = 0.5),
        panel.border = element_rect(linetype = "solid",
                                    fill = NA, size=1.5))

cal_resid_histogram <- ggplot(cal.plsr.output,
                              aes(x=PLSR_CV_Residuals)) +
  geom_histogram(alpha=.5, position="identity") +
  geom_vline(xintercept = 0, color="black",
             linetype="dashed", size=1) + theme_bw() +
  theme(axis.text=element_text(size=18), legend.position="none",
        axis.title=element_text(size=20, face="bold"),
        axis.text.x = element_text(angle = 0,vjust = 0.5),
        panel.border = element_rect(linetype = "solid",
```

```
                                    fill = NA, size=1.5))

rng_quant <- quantile(val.plsr.output[,inVar],
                      probs = c(0.001, 0.999))
val_scatter_plot <- ggplot(val.plsr.output,
                           aes(x=PLSR_Predicted, y=get(inVar))) +
  theme_bw() + geom_point() +
  geom_abline(intercept = 0, slope = 1, color="dark grey",
              linetype="dashed", size=1.5) +
  xlim(rng_quant[1], rng_quant[2]) +
  ylim(rng_quant[1], rng_quant[2]) +
  labs(x=paste0("Predicted ", paste(inVar), " (units)"),
       y=paste0("Observed ", paste(inVar), " (units)"),
       title=paste0("Validation: ", paste0("Rsq = ", val.R2), "; ",
                    paste0("RMSEP = ",
                           val.RMSEP))) +
  theme(axis.text=element_text(size=18), legend.position="none",
        axis.title=element_text(size=20, face="bold"),
        axis.text.x = element_text(angle = 0,vjust = 0.5),
        panel.border = element_rect(linetype = "solid", fill = NA,
                                    size=1.5))

val_resid_histogram <- ggplot(val.plsr.output, aes(x=PLSR_Residuals)) +
  geom_histogram(alpha=.5, position="identity") +
  geom_vline(xintercept = 0, color="black",
             linetype="dashed", size=1) + theme_bw() +
  theme(axis.text=element_text(size=18), legend.position="none",
        axis.title=element_text(size=20, face="bold"),
        axis.text.x = element_text(angle = 0,vjust = 0.5),
        panel.border = element_rect(linetype = "solid", fill = NA,
                                    size=1.5))

# plot cal/val side-by-side
grid.arrange(cal_scatter_plot, val_scatter_plot, cal_resid_histogram,
             val_resid_histogram,
             nrow=2,ncol=2)
```

```
## Warning: Removed 16 rows containing missing values (geom_point).
```

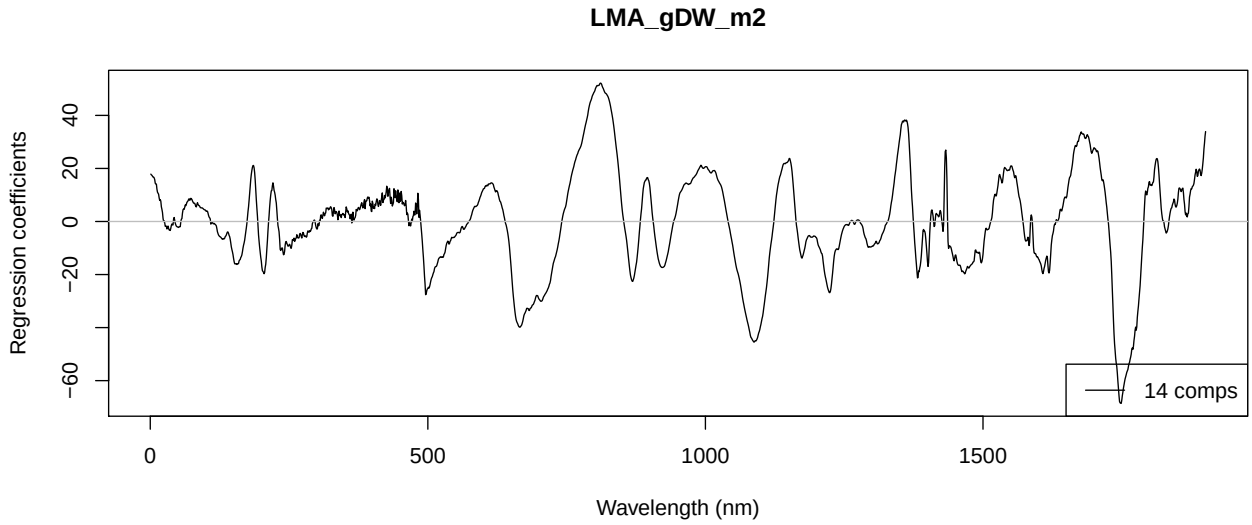
```
## Warning: Removed 7 rows containing missing values (geom_point).
```

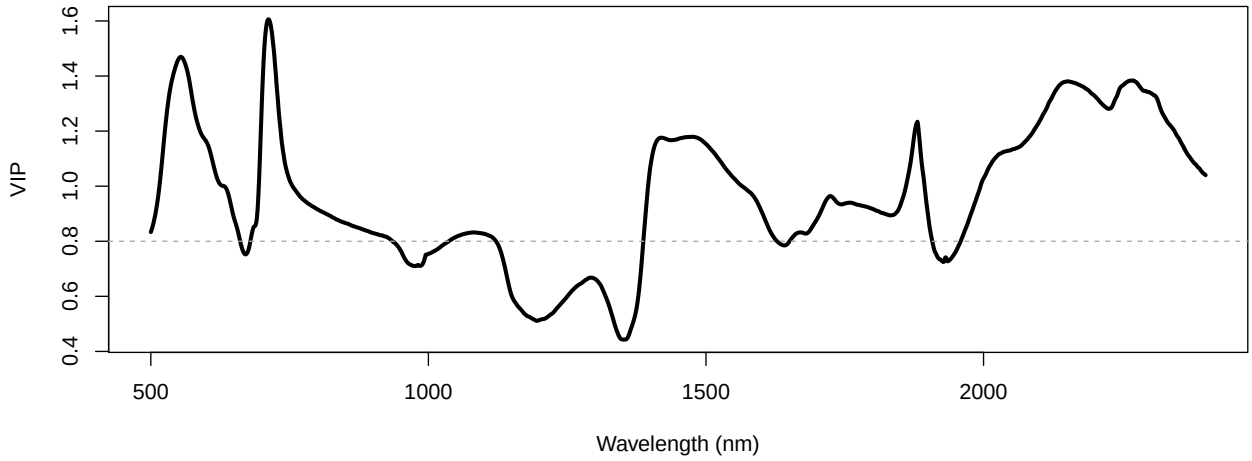
```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



Generate Coefficient and VIP plots

```
vips <- VIP(plsr.out)[nComps,]
par(mfrow=c(2,1))
plot(plsr.out, plottype = "coef",xlab="Wavelength (nm)",
     ylab="Regression coefficients",legendpos = "bottomright",
     ncomp=nComps)

plot(seq(Start.wave,End.wave,1),vips,xlab="Wavelength (nm)",ylab="VIP",
     cex=0.01)
lines(seq(Start.wave,End.wave,1),vips,lwd=3)
abline(h=0.8,lty=2,col="dark grey")
```





Jackknife validation

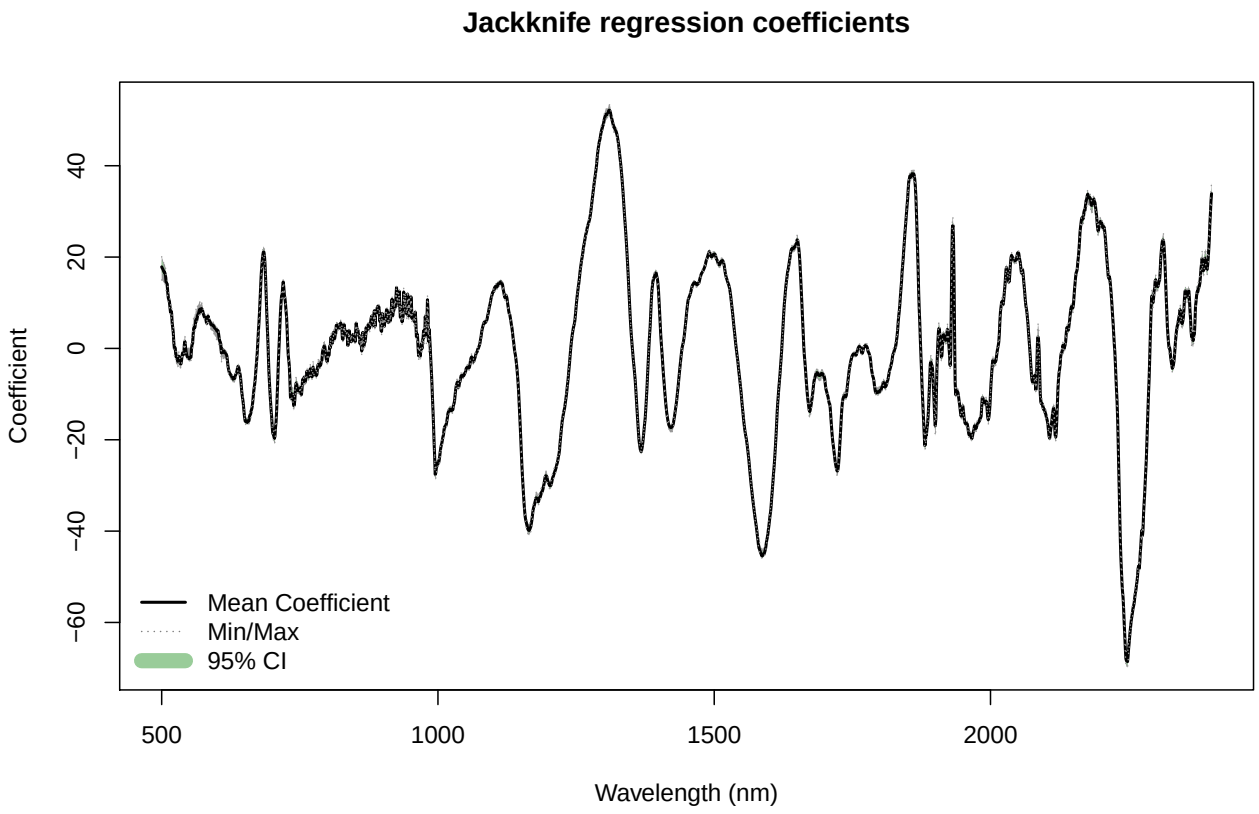
```
if(grepl("Windows", sessionInfo()$running)){
  pls.options(parallel =NULL)
} else {
  pls.options(parallel = parallel::detectCores()-1)
}

seg <- 100
jk.plsr.out <- pls::plsr(as.formula(paste(inVar,"~","Spectra")),
                         scale=FALSE,
                         center=TRUE, ncomp=nComps,
                       validation="CV", segments = seg,
                       segment.type="interleaved",
                       trace=FALSE,
                       jackknife=TRUE, data=cal.plsr.data)
pls.options(parallel = NULL)
```

```
Jackknife_coef <- f.coef.valid(plsr.out = jk.plsr.out,
                               data_plsr = cal.plsr.data,
                               ncomp = nComps)
Jackknife_intercept <- Jackknife_coef[1,,,]
Jackknife_coef <- Jackknife_coef[2:dim(Jackknife_coef)[1],,,]

#interval <- c(0.025,0.975)
interval <- c(0.05,0.95)
Jackknife_Pred <- val.plsr.data$Spectra%*%Jackknife_coef+Jackknife_intercept
Interval_Conf <- apply(X = Jackknife_Pred,MARGIN = 1,
                       FUN = quantile,probs=c(interval[1],interval[2]))
Interval_Pred <- apply(X = Jackknife_Pred,MARGIN = 1,
                       FUN = quantile,probs=c(interval[1],interval[2]))
sd_mean <- apply(X = Jackknife_Pred,MARGIN = 1,FUN =sd)
sd_res <- sd(val.plsr.output$PLSR_Residuals)
sd_tot <- sqrt(sd_mean^2+sd_res^2)
val.plsr.output$LCI <- Interval_Pred[1,]
val.plsr.output$UCI <- Interval_Pred[2,]
val.plsr.output$LPI <- val.plsr.output$PLSR_Predicted+1.96*sd_tot
val.plsr.output$UPI <- val.plsr.output$PLSR_Predicted-1.96*sd_tot
head(val.plsr.output)
```

```
##   Domain Functional_type Sample_ID USDA_Species_Code LMA_gDW_m2 PLSR_Predicted
## 1    D08       broadleaf     P2462              <NA>      21.10       23.17688
## 2    D08       broadleaf     L2462              SANI     100.72       87.76061
## 3    D08       broadleaf     P2463              <NA>      29.59       30.12776
## 4    D08       broadleaf     L2463              SANI      96.48       89.17843
## 5    D08       broadleaf     P2464              <NA>      31.08       45.66874
## 6    D08       broadleaf     L2464              SANI      61.40       65.10542
##   PLSR_Residuals      LCI      UCI       LPI       UPI
## 1      2.0768781 22.71494 23.87684  40.82572  5.528041
## 2    -12.9593944 86.99439 88.32899 105.40986 70.111352
## 3      0.5377642 29.10105 31.53336  47.81203 12.443494
## 4     -7.3015651 88.39579 89.52677 106.82441 71.532455
## 5     14.5887365 45.01835 46.24715  63.31762 28.019855
## 6      3.7054219 64.37264 65.64146  82.75183 47.459017
```

Jackknife coefficient plot

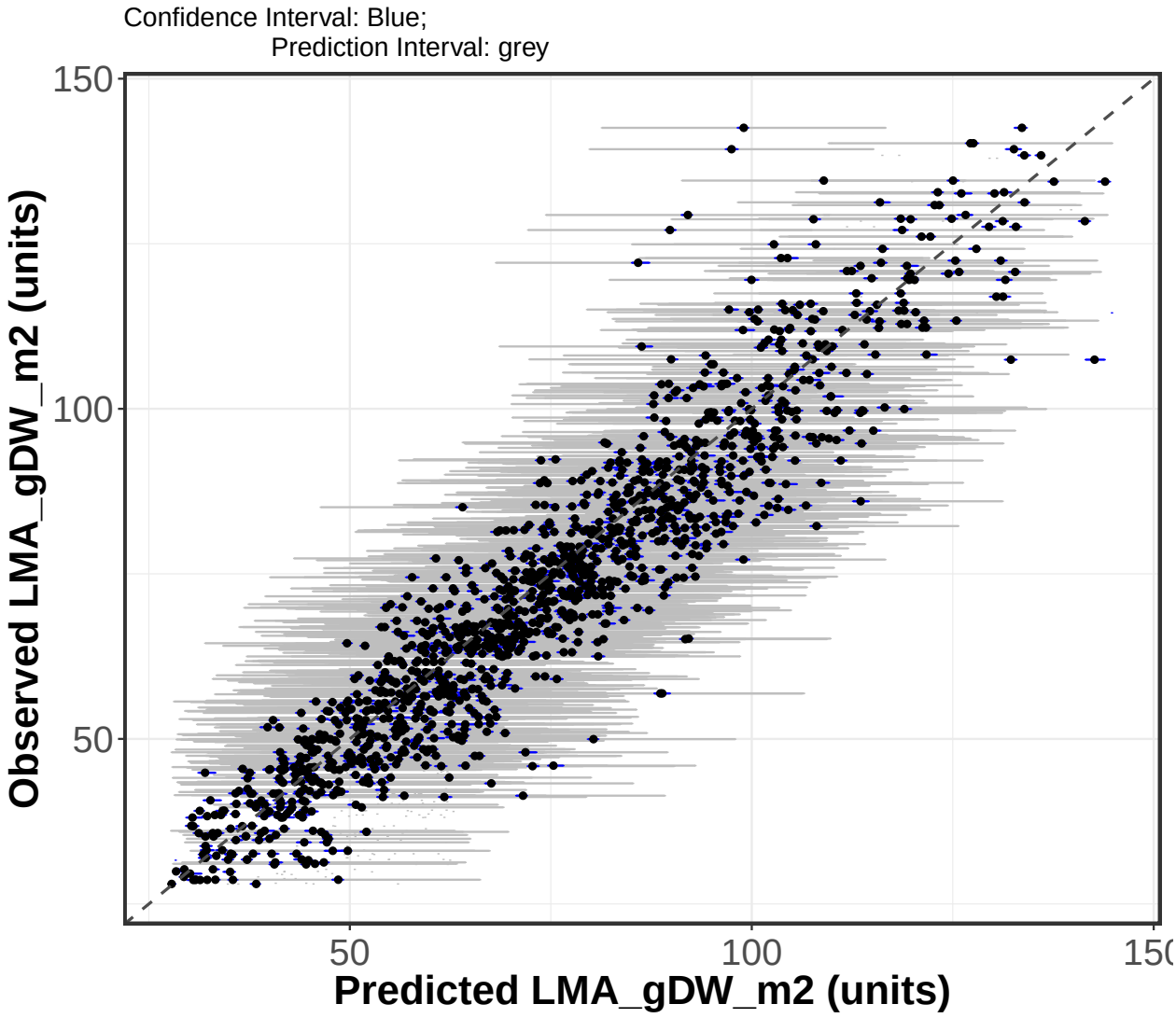
```
f.plot.coef(Z = t(Jackknife_coef), wv = seq(Start.wave,End.wave,1),
            plot_label="Jackknife regression coefficients",
            position = 'bottomleft')
```



Jackknife validation plot

```
#rng_vals <- quantile(val.plsr.output[,inVar], probs = c(0.001, 0.999))
rng_vals <- c(min(val.plsr.output$LPI), max(val.plsr.output$UPI))
jk_val_scatterplot <- ggplot(val.plsr.output, aes(x=PLSR_Predicted,
                                                  y=get(inVar))) +
  theme_bw()+ geom_errorbar(aes(xmin = LPI,xmax = UPI),color='grey',
                            width=0.2) +
  geom_errorbar(aes(xmin = LCI,xmax = UCI),color='blue',width=0.2) +
  geom_point(size=1.3)  +
  geom_abline(intercept = 0, slope = 1, color="grey30",
              linetype="dashed", size=0.7) +
  xlim(rng_vals[1], rng_vals[2]) +
  ylim(rng_vals[1], rng_vals[2]) +
  labs(x=paste0("Predicted ", paste(inVar), " (units)"),
       y=paste0("Observed ", paste(inVar), " (units)"),
       title=paste0("Confidence Interval: Blue;
                    Prediction Interval: grey")) +
  theme(axis.text=element_text(size=18),
        legend.position = 'right',
        axis.title=element_text(size=20, face="bold"),
        axis.text.x = element_text(angle = 0,vjust = 0.5),
        panel.border = element_rect(linetype = "solid",
                                    fill = NA, size=1.5))
jk_val_scatterplot
```

```
## Warning: Removed 84 rows containing missing values (geom_point).
```



Output jackknife results

```
out.jk.coefs <- data.frame(Iteration=seq(1,seg,1),
                           Intercept=Jackknife_intercept,
                           t(Jackknife_coef))
head(out.jk.coefs)[1:6]
```

```
##       Iteration Intercept Wave_500 Wave_501 Wave_502 Wave_503
## Seg 1         1  63.74332 18.24687 17.95401 17.77171 17.38132
## Seg 2         2  63.73713 18.85761 18.62012 18.39545 18.02299
## Seg 3         3  62.92261 19.42642 19.12960 18.88917 18.38110
## Seg 4         4  63.38407 18.33061 17.97824 17.88824 17.56360
## Seg 5         5  63.44702 17.60085 17.39623 17.12976 16.75319
## Seg 6         6  62.81849 17.70992 17.51663 17.39929 16.95014
```

```
write.csv(out.jk.coefs,file=file.path(outdir,
                                      paste0(inVar,
                                             '_Jackkife_PLSR_Coefficients.csv')),
```

```
          row.names=FALSE)
```

Create core PLSR outputs

```
print(paste("Output directory: ", getwd()))
```

```
## [1] "Output directory:  /Users/sserbin/Data/GitHub/PLSR_for_plant_trait_prediction/vignettes"
```

```
# Observed versus predicted
write.csv(cal.plsr.output,file=file.path(outdir,
                                         paste0(inVar,'_Observed_PLSR_CV_Pred_',
                                                nComps,'comp.csv')),
          row.names=FALSE)

# Validation data
write.csv(val.plsr.output,file=file.path(outdir,
                                         paste0(inVar,'_Validation_PLSR_Pred_',
                                                nComps,'comp.csv')),
          row.names=FALSE)

# Model coefficients
coefs <- coef(plsr.out,ncomp=nComps,intercept=TRUE)
write.csv(coefs,file=file.path(outdir,
                               paste0(inVar,'_PLSR_Coefficients_',
                                      nComps,'comp.csv')),
          row.names=TRUE)

# PLSR VIP
write.csv(vips,file=file.path(outdir,
                              paste0(inVar,'_PLSR_VIPs_',
                                     nComps,'comp.csv')))
```

Confirm files were written to temp space

```
print("**** PLSR output files: ")
```

```
## [1] "**** PLSR output files: "
```

```
list.files(outdir)[grep(pattern = inVar, list.files(outdir))]
```

```
## [1] "LMA_gDW_m2_Jackkife_PLSR_Coefficients.csv"
## [2] "LMA_gDW_m2_Observed_PLSR_CV_Pred_14comp.csv"
## [3] "LMA_gDW_m2_PLSR_Coefficients_14comp.csv"
## [4] "LMA_gDW_m2_PLSR_VIPs_14comp.csv"
## [5] "LMA_gDW_m2_Validation_PLSR_Pred_14comp.csv"
```