

# 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 pls components, and fit a pls model for leaf-mass area (LMA)

## Getting Started

### Installation

```
## Loading required package: usethis
##
## Attaching package: 'remotes'
## The following objects are masked from 'package:devtools':
##
##   dev_package_deps, install_bioc, install_bitbucket, install_cran,
##   install_deps, install_dev, install_git, install_github,
##   install_gitlab, install_local, install_svn, install_url,
##   install_version, update_packages
## The following object is masked from 'package:usethis':
##
##   git_credentials
##
## 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 <- TRUE
if (source_from_gh) {
  # Source helper functions from GitHub
  print("*** GitHub hash of functions.R file:")
  devtools::source_url("https://raw.githubusercontent.com/TESTgroup-BNL/PLSR_for_plant_trait_prediction")
} else {
  functions <- file.path(github_dir, "functions.R")
  source(functions)
}

## [1] "*** GitHub hash of functions.R file:"
## SHA-1 hash of file is 8c6b457e931a5879e8c975f4d6529f61b52c4453

# 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"

# Specify output directory, output_dir
# Options:
# tempdir - use a OS-specified temporary directory
# user defined PATH - e.g. "~/scratch/PLSR"
output_dir <- "tempdir"
```

## Set working directory (scratch space)

```
## [1] "/private/var/folders/xp/h3k9vf3n2jx181ts786_yjrn9c2gjq/T/RtmpdcpZRq"
```

## 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...
```

```
##
```

```
## -- 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()
```

```
## )
```

```
## i Use `spec()` for the 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 pls dataset

```
### Create pls 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"
```

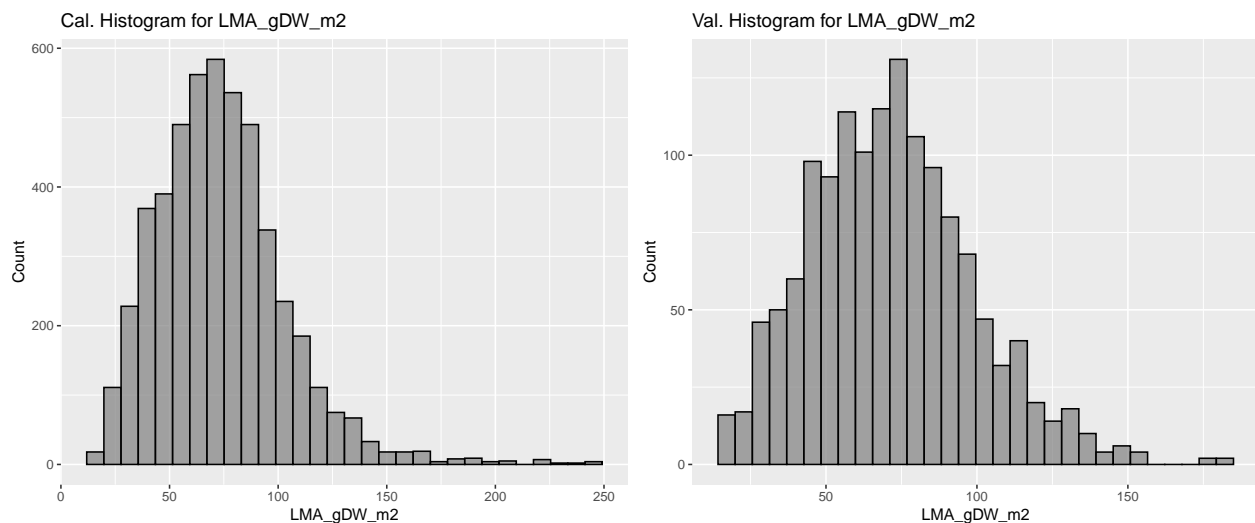
```
print(paste("Val observations: ",dim(val.plsr.data)[1],sep=""))
```

```
## [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))
histograms <- 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`.
```



```
ggsave(filename = file.path(outdir,paste0(inVar,"_Cal_Val_Histograms.png")),
  plot = histograms, device="png", width = 30, height = 12, units = "cm",
  dpi = 300)
# output cal/val data
write.csv(cal.plsr.data,file=file.path(outdir,paste0(inVar,'_Cal_PLSR_Dataset.csv')),
  row.names=FALSE)
write.csv(val.plsr.data,file=file.path(outdir,paste0(inVar,'_Val_PLSR_Dataset.csv')),
  row.names=FALSE)
```

## 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]

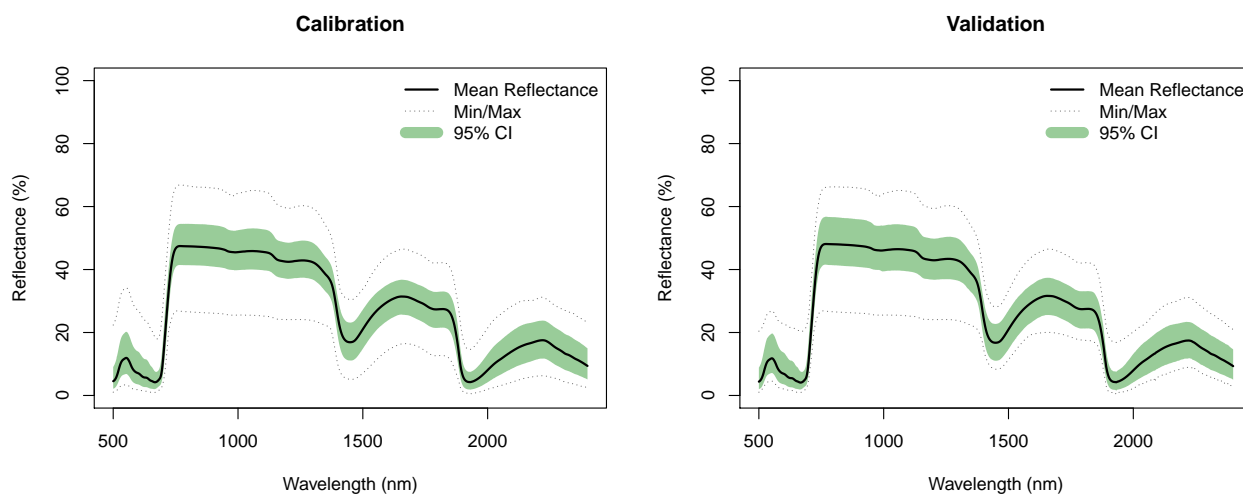
##   Domain Functional_type Sample_ID USDA_Species_Code LMA_gDW_m2
## 1   D08      broadleaf    L2644                ACBA      44.18
## 2   D08      broadleaf    L2646                ACBA      41.71
## 3   D08      broadleaf    L2645                ACBA      40.66
## 4   D08      broadleaf    P2639                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")
```



```
dev.copy(png,file.path(outdir,paste0(inVar,'_Cal_Val_Spectra.png')),
         height=2500,width=4900, res=340)
```

```
## quartz_off_screen
##          3
```

```
dev.off();
```

```
## pdf
##    2
```

```
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 <- "firstPlateau" #pls, firstPlateau, firstMin
random_seed <- 2356812
seg <- 250
maxComps <- 20
iterations <- 40
prop <- 0.70
if (method=="pls") {
  nComps <- find_optimal_components(dataset=cal.plsr.data, method=method, maxComps=maxComps,
                                   seg=seg, random_seed=random_seed)
  print(paste0("*** Optimal number of components: ", nComps))
} else {
  nComps <- find_optimal_components(dataset=cal.plsr.data, method=method, maxComps=maxComps,
                                   iterations=iterations, seg=seg, prop=prop,
                                   random_seed=random_seed)
}
```

```
## [1] "*** Running permutation test. Please hang tight, this can take awhile ***"
```

```
## [1] "Options: 20 40 250 0.7"
```

```
## Running iteration 1
```

```
## Running iteration 2
```

```
## Running iteration 3
```

```
## Running iteration 4
```

```
## Running iteration 5
```

```
## Running iteration 6
```

```
## Running iteration 7
```

```
## Running iteration 8
```

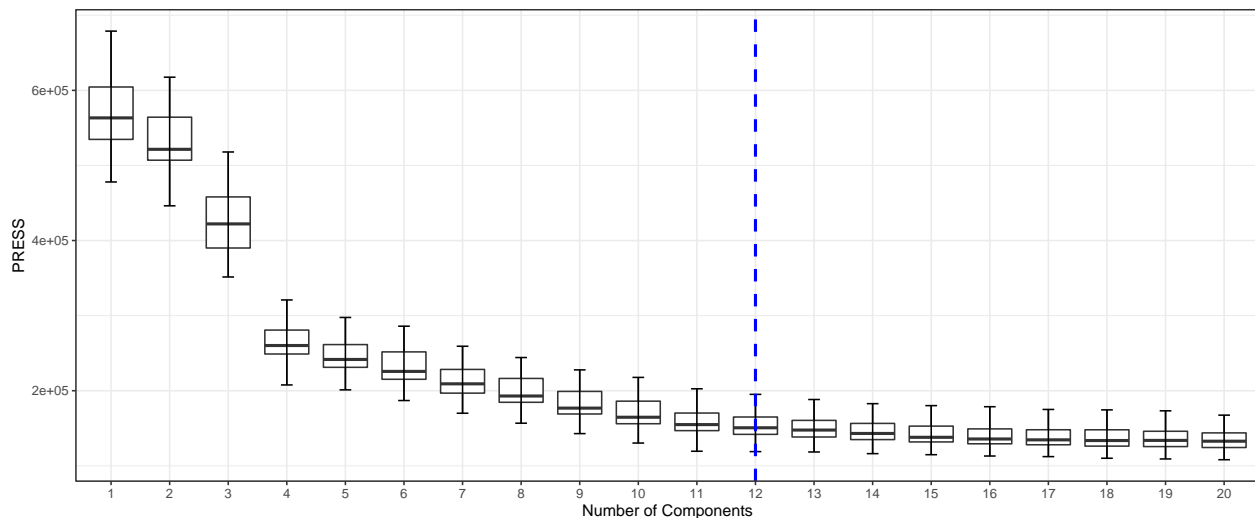
```
## Running iteration 9
```

```
## Running iteration 10
```

```
## Running iteration 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
## Running interation 21
## Running interation 22
## Running interation 23
## Running interation 24
## Running interation 25
## Running interation 26
## Running interation 27
## Running interation 28
## Running interation 29
## Running interation 30
## Running interation 31
## Running interation 32
## Running interation 33
## Running interation 34
## Running interation 35
## Running interation 36
## Running interation 37
## Running interation 38
## Running interation 39
## Running interation 40
## No id variables; using all as measure variables
## [1] "*** Optimal number of components based on t.test: 12"
```



```
dev.copy(png,file.path(outdir,paste0(paste0(inVar,"_PLSR_Component_Selection.png"))),
         height=2800, width=3400, res=340)
```

```
## quartz_off_screen
##                               3
```

```
dev.off();
```

```
## pdf
##    2
```

## 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)
```

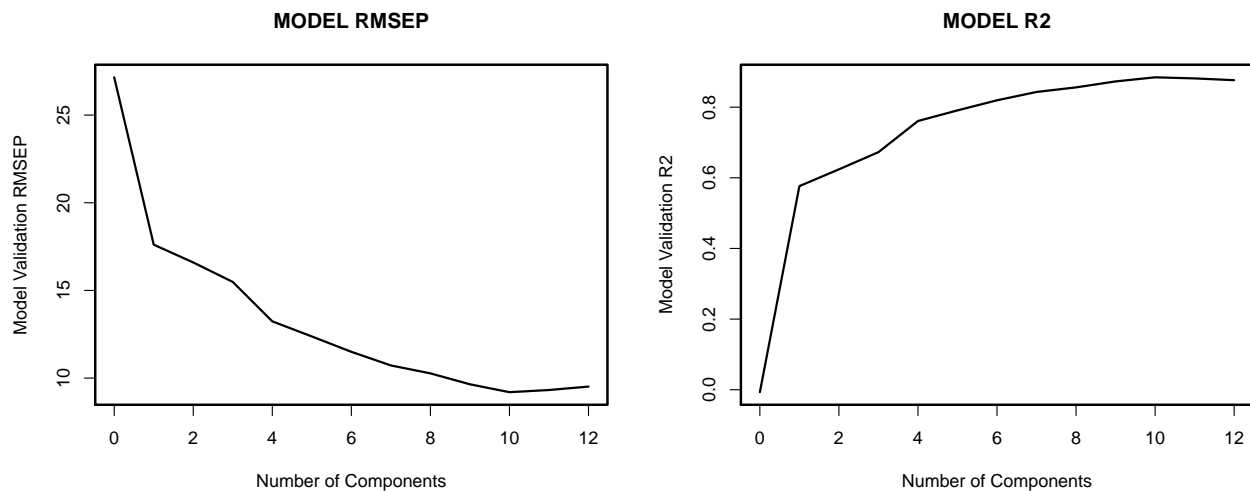
```
## (Intercept)      1 comps      2 comps      3 comps      4 comps      5 comps
##      27.155      17.610      16.595      15.483      13.235      12.374
##      6 comps      7 comps      8 comps      9 comps     10 comps     11 comps
##      11.499      10.722      10.269      9.647       9.197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

```
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
##    0.876368
```

```
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      53.00773
## 2   D08      broadleaf    L2646             ACBA      41.71      44.02712
## 3   D08      broadleaf    L2645             ACBA      40.66      46.76972
## 4   D08      broadleaf    P2639             ACBA      44.18      49.62804
## 5   D03      broadleaf    P0614             ACFL      52.91      64.78900
## 6   D03      broadleaf    L0609             ACFL      81.67      96.85291
##   PLSR_CV_Predicted PLSR_CV_Residuals
## 1          53.03952           8.859523
## 2          44.03282           2.322823
## 3          46.90528           6.245280
```

```
## 4          49.80084          5.620843
## 5          64.98964          12.079641
## 6          96.86039          15.190390

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      21.14155
## 2   D08      broadleaf   L2462          SANI      100.72      89.65467
## 3   D08      broadleaf   P2463          <NA>      29.59      27.94765
## 4   D08      broadleaf   L2463          SANI      96.48      92.46121
## 5   D08      broadleaf   P2464          <NA>      31.08      40.73367
## 6   D08      broadleaf   L2464          SANI      61.40      65.94687
##   PLSR_Residuals
## 1      0.04155041
## 2     -11.06533484
## 3     -1.64234512
## 4     -4.01879017
## 5      9.65367301
## 6      4.54686556
```

```
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("Rsqr = ", 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))

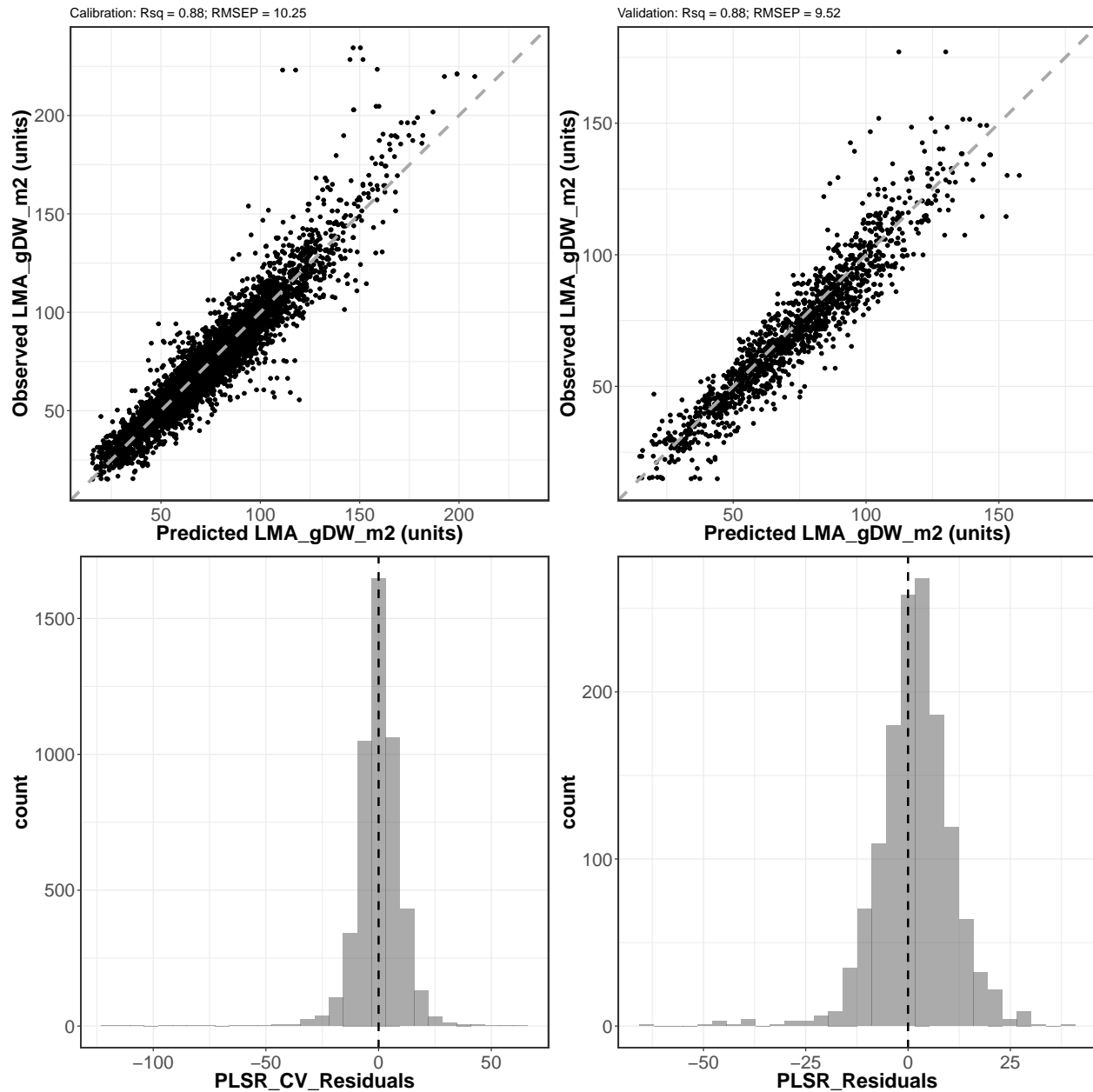
rng_quant <- quantile(val.plsr.output[,inVar],
                     probs = c(0.001, 0.999))
val_scatter_plot <- ggplot(val.plsr.output,
                          aes(x=PLSR_Predicted, y=get(inVar))) +
  theme_bw() + geom_point() +
  geom_abline(intercept = 0, slope = 1, color="dark grey",
             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("Rsqr = ", 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
scatterplots <- grid.arrange(cal_scatter_plot, val_scatter_plot, cal_resid_histogram,
                             val_resid_histogram, nrow=2, ncol=2)

## Warning: Removed 21 rows containing missing values (geom_point).
## Warning: Removed 5 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`.

```



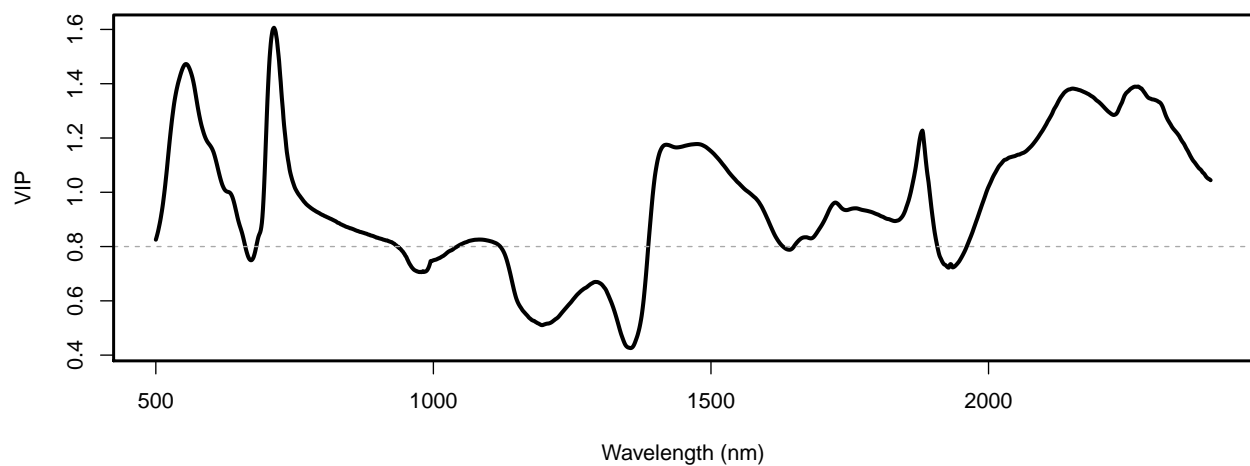
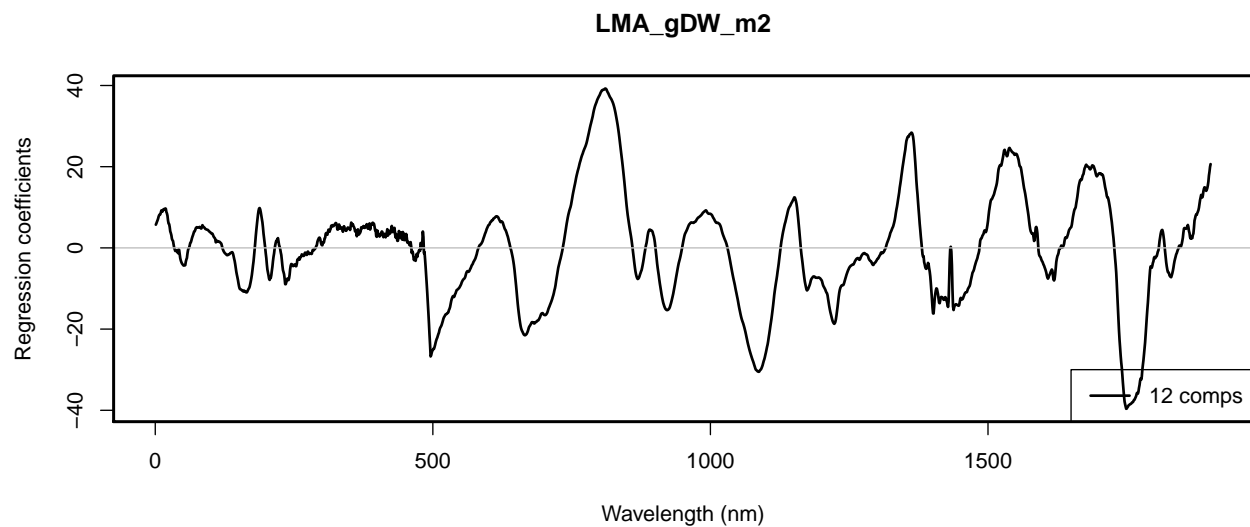
```
ggsave(filename = file.path(outdir, paste0(inVar, "_Cal_Val_scatterplots.png")),
        plot = scatterplots, device = "png", width = 32, height = 30, units = "cm",
        dpi = 300)
```

## 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, lwd=2)
box(lwd=2.2)
```

```
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")
box(lwd=2.2)
```



```
dev.copy(png,file.path(outdir,paste0(inVar,'_Coefficient_VIP_plot.png')),
         height=3100, width=4100, res=340)
```

```
## quartz_off_screen
##           3
```

```
dev.off();
```

```
## pdf
##    2
par(opar)
```

## 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, inVar=inVar)
Jackknife_intercept <- Jackknife_coef[1,,]
Jackknife_coef <- Jackknife_coef[2:dim(Jackknife_coef)[1],,,]

interval <- c(0.025,0.975)
Jackknife_Pred <- val.plsr.data$Spectra %*% Jackknife_coef +
  matrix(rep(Jackknife_intercept, length(val.plsr.data[,inVar])), byrow=TRUE,
          ncol=length(Jackknife_intercept))
Interval_Conf <- apply(X = Jackknife_Pred,MARGIN = 1,
                      FUN = quantile,probs=c(interval[1],interval[2]))
sd_mean <- apply(X = Jackknife_Pred,MARGIN = 1,FUN =sd)
sd_res <- sd(val.plsr.output$PLSR_Residuals)
sd_tot <- sqrt(sd_mean^2+sd_res^2)
val.plsr.output$LCI <- Interval_Conf[1,]
val.plsr.output$UCI <- Interval_Conf[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)

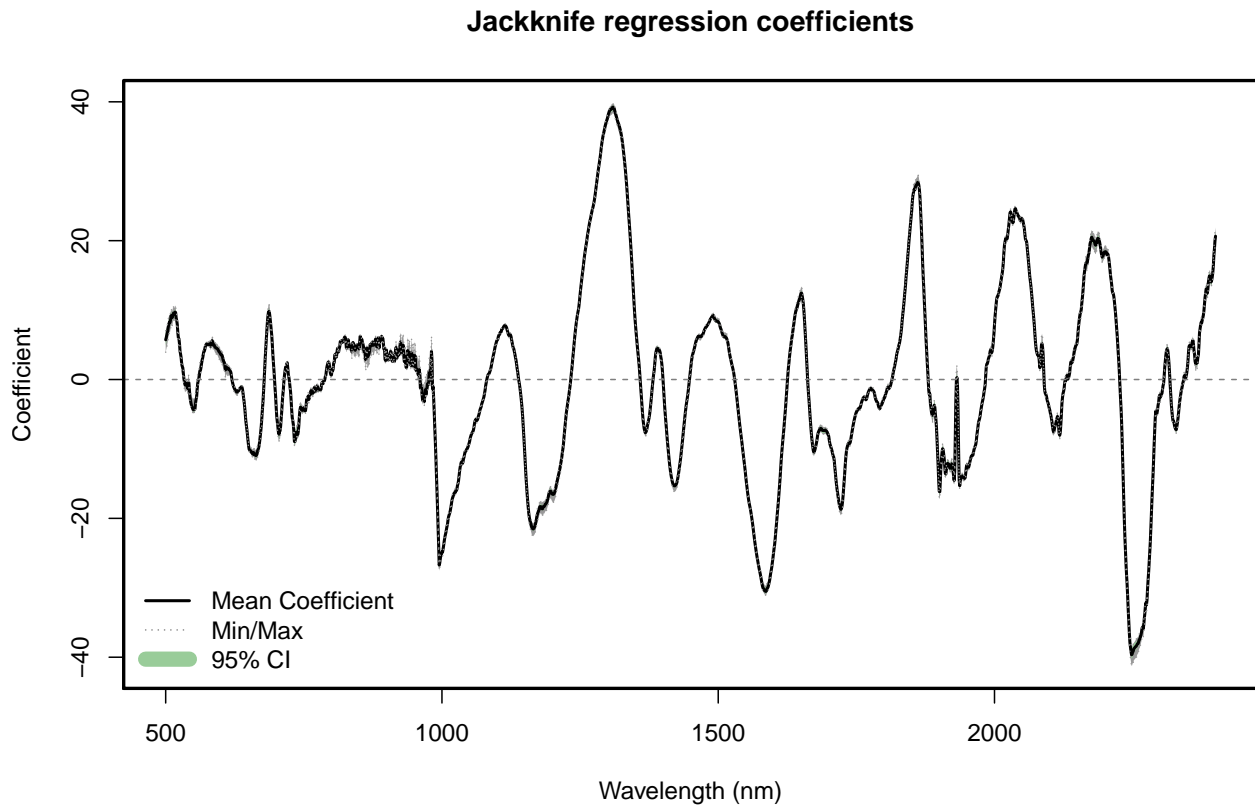
##   Domain Functional_type Sample_ID USDA_Species_Code LMA_gDW_m2 PLSR_Predicted
## 1    D08      broadleaf   P2462                <NA>    21.10      21.14155
## 2    D08      broadleaf   L2462                SANI    100.72     89.65467
## 3    D08      broadleaf   P2463                <NA>    29.59     27.94765
## 4    D08      broadleaf   L2463                SANI    96.48     92.46121
## 5    D08      broadleaf   P2464                <NA>    31.08     40.73367
## 6    D08      broadleaf   L2464                SANI    61.40     65.94687
##   PLSR_Residuals      LCI      UCI      LPI      UPI
## 1    0.04155041 20.94847 21.30604  2.789108 39.49399
## 2   -11.06533484 89.45021 89.97246 71.301221 108.00811
## 3    -1.64234512 27.73172 28.16789  9.594597  46.30071
## 4    -4.01879017 92.26489 92.73225 74.107998 110.81442
## 5     9.65367301 40.50065 40.92588 22.380204  59.08714
## 6     4.54686556 65.77618 66.17712 47.594178  84.29955

```



## Jackknife coefficient plot

```
f.plot.coef(Z = t(Jackknife_coef), wv = seq(Start.wave,End.wave,1),
            plot_label="Jackknife regression coefficients",position = 'bottomleft')
abline(h=0,lty=2,col="grey50")
box(lwd=2.2)
```



```
dev.copy(png,file.path(outdir,paste0(inVar,'_Jackknife_Regression_Coefficients.png')),
         height=2100, width=3800, res=340)
```

```
## quartz_off_screen
##                 3
```

```
dev.off();
```

```
## pdf
##    2
```

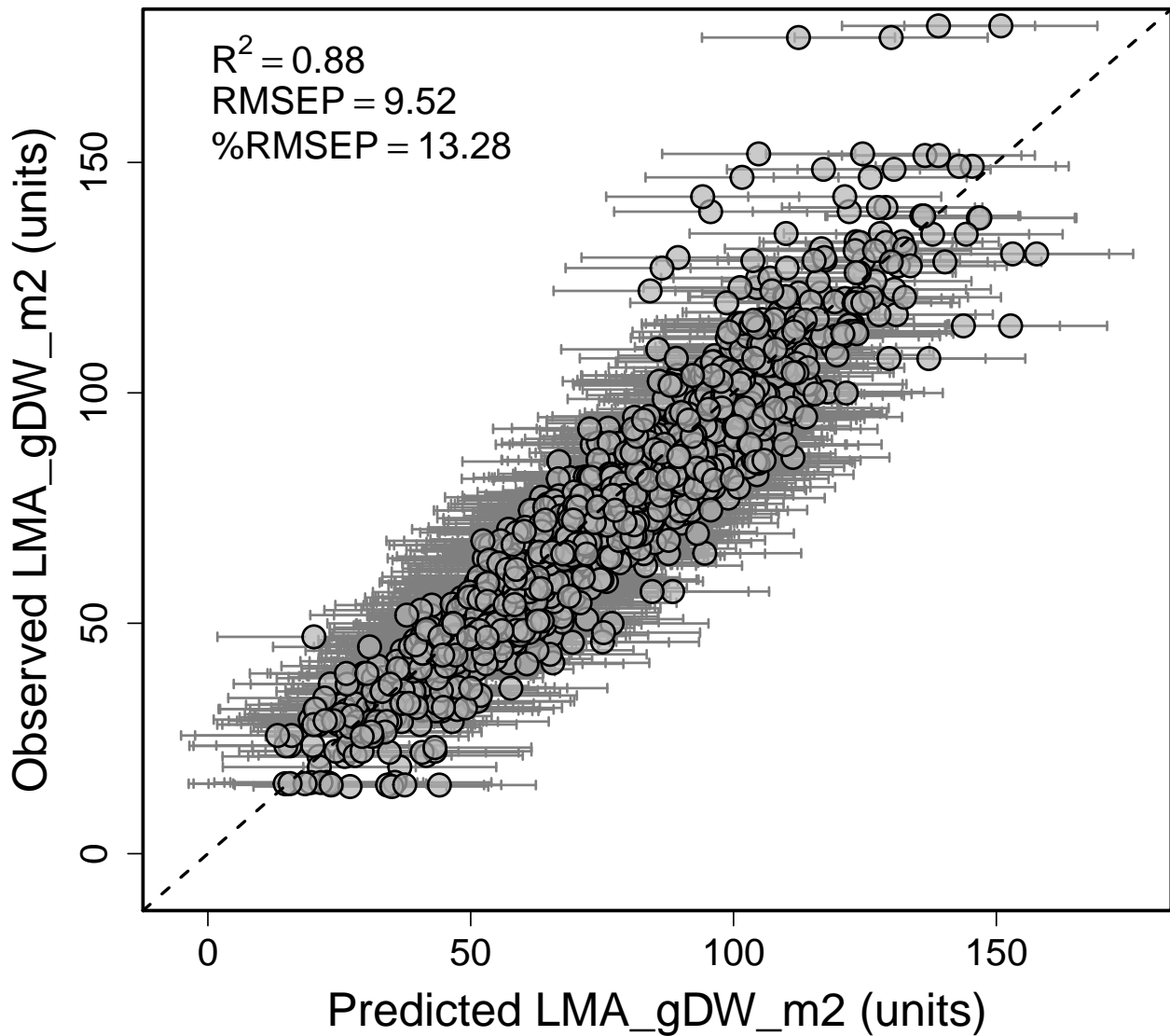
## Jackknife validation plot

```
RMSEP <- sqrt(mean(val.plsr.output$PLSR_Residuals^2))
pecr_RMSEP <- RMSEP/mean(val.plsr.output[,inVar])*100
r2 <- round(pls::R2(plsr.out, newdata = val.plsr.data)$val[nComps+1],2)
expr <- vector("expression", 3)
expr[[1]] <- bquote(R^2==.(r2))
expr[[2]] <- bquote(RMSEP==.(round(RMSEP,2)))
expr[[3]] <- bquote("%RMSEP"==.(round(pecr_RMSEP,2)))
rng_vals <- c(min(val.plsr.output$LPI), max(val.plsr.output$UPI))
```

```

par(mfrow=c(1,1), mar=c(4.2,5.3,1,0.4), oma=c(0, 0.1, 0, 0.2))
plotCI(val.plsr.output$PLSR_Predicted, val.plsr.output[, inVar],
      li=val.plsr.output$LPI, ui=val.plsr.output$UPI, gap=0.009, sfrac=0.004,
      lwd=1.6, xlim=c(rng_vals[1], rng_vals[2]), ylim=c(rng_vals[1], rng_vals[2]),
      err="x", pch=21, col="black", pt.bg=alpha("grey70", 0.7), scol="grey50",
      cex=2, xlab=paste0("Predicted ", paste(inVar, " (units)"),
      ylab=paste0("Observed ", paste(inVar, " (units)"),
      cex.axis=1.5, cex.lab=1.8)
abline(0, 1, lty=2, lw=2)
legend("topleft", legend=expr, bty="n", cex=1.5)
box(lwd=2.2)

```



```

dev.copy(png, file.path(outdir, paste0(inVar, "_PLSR_Validation_Scatterplot.png")),
      height=2800, width=3200, res=340)

```

```

## quartz_off_screen
## 3

```

```
dev.off();
```

```
## pdf  
## 2
```

## 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  69.44171  5.796399  6.112194  6.482897  6.814518  
## Seg 2         2  69.36719  6.316698  6.662910  7.031691  7.382632  
## Seg 3         3  68.73866  6.729135  7.031912  7.372056  7.650510  
## Seg 4         4  69.09350  5.899933  6.199538  6.614751  6.975426  
## Seg 5         5  69.12959  5.355288  5.701339  6.043622  6.383870  
## Seg 6         6  68.67202  5.615024  5.968986  6.358249  6.654510
```

```
write.csv(out.jk.coefs,file=file.path(outdir,  
                                       paste0(inVar,  
                                                '_Jackknife_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_Cal_PLSR_Dataset.csv"  
## [2] "LMA_gDW_m2_Cal_Val_Histograms.png"  
## [3] "LMA_gDW_m2_Cal_Val_scatterplots.png"  
## [4] "LMA_gDW_m2_Cal_Val_Spectra.png"  
## [5] "LMA_gDW_m2_Coefficient_VIP_plot.png"  
## [6] "LMA_gDW_m2_Jackknife_PLSR_Coefficients.csv"  
## [7] "LMA_gDW_m2_Jackknife_Regression_Coefficients.png"  
## [8] "LMA_gDW_m2_Observed_PLSR_CV_Pred_12comp.csv"  
## [9] "LMA_gDW_m2_PLSR_Coefficients_12comp.csv"  
## [10] "LMA_gDW_m2_PLSR_Component_Selection.png"  
## [11] "LMA_gDW_m2_PLSR_Validation_Scatterplot.png"  
## [12] "LMA_gDW_m2_PLSR_VIPs_12comp.csv"  
## [13] "LMA_gDW_m2_Val_PLSR_Dataset.csv"  
## [14] "LMA_gDW_m2_Validation_PLSR_Pred_12comp.csv"
```