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

Shawn P. Serbin, Julien Lamour, & Jeremiah Anderson

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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

Load libraries

```
list.of.packages <- c("pls","dplyr","here","plotrix","ggplot2","gridExtra","spectratrait")
invisible(lapply(list.of.packages, library, character.only = TRUE))
```

```
##
## 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/spectratrait

##
## Attaching package: 'gridExtra'

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

Setup other functions and options

```
### Setup options

# 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/Rtmp8wAkD7"
```

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/spectratrait/vignettes"
```

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

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

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

```
## Rows: 6312 Columns: 2162
## -- Column specification --------------------------------------------------------
## Delimiter: ","
## chr   (10): Affiliation, Common Name, Domain, Functional_type, Latin Genus, ...
## dbl (2152): LMA, 350, 351, 352, 353, 354, 355, 356, 357, 358, 359, 360, 361,...
##
## i Use `spec()` to retrieve the full column specification for this data.
## i Specify the column types or set `show_col_types = FALSE` to quiet this message.
## 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 of Wiscon~ black walnut  D02    broadleaf        72.9 Juglans
## 2 University of Wiscon~ black walnut  D02    broadleaf        72.9 Juglans
## 3 University of Wiscon~ black walnut  D02    broadleaf        60.8 Juglans
## 4 University of Wiscon~ black walnut  D02    broadleaf        60.8 Juglans
## 5 University of Wiscon~ black walnut  D02    broadleaf        85.9 Juglans
## 6 University of Wiscon~ 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>, ...
```

```
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 of Wiscon~ black walnut  D02    broadleaf        72.9 Juglans
## 2 University of Wiscon~ black walnut  D02    broadleaf        72.9 Juglans
## 3 University of Wiscon~ black walnut  D02    broadleaf        60.8 Juglans
## 4 University of Wiscon~ black walnut  D02    broadleaf        60.8 Juglans
## 5 University of Wiscon~ black walnut  D02    broadleaf        85.9 Juglans
## 6 University of Wiscon~ 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 <- spectratrait::create_data_split(dataset=plsr_data,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
## 3     D02       broadleaf     P0002              JUNI      60.77 0.043758
## 12    D02       broadleaf     L0006              JUNI      42.54 0.044338
## 13    D02       broadleaf     P0007              QUVE     106.57 0.015643
## 19    D02       broadleaf     P0010              PRSE      78.82 0.033019
## 21    D02       broadleaf     P0011              PRSE      86.09 0.024819
## 28    D02       broadleaf     L0014              PRSE      67.11 0.040095
##    Wave_501 Wave_502
## 3  0.044171 0.044869
## 12 0.044748 0.045294
## 13 0.015579 0.015431
## 19 0.033102 0.033245
## 21 0.024826 0.025045
## 28 0.040397 0.040864
```

```
rm(split_data)

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

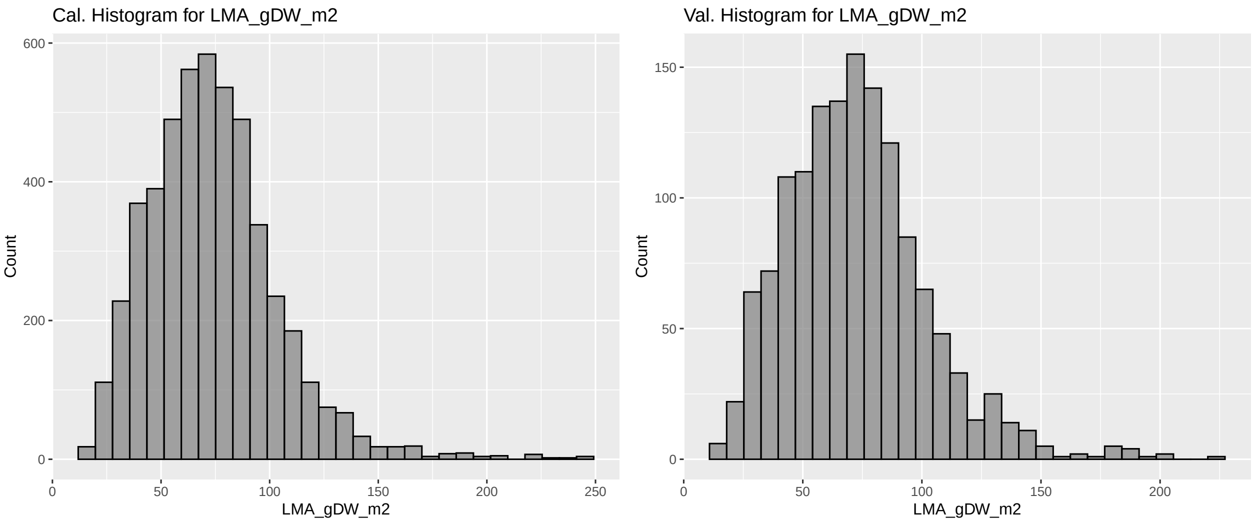
```
## [1] "Cal observations: 4922"
```

```
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]
```

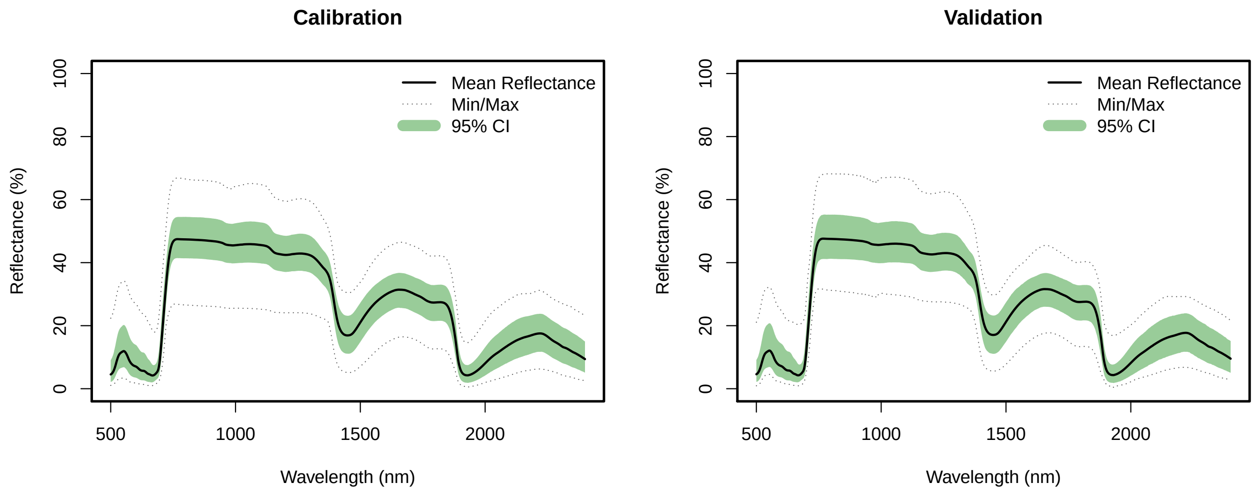
```
##   Domain Functional_type Sample_ID USDA_Species_Code LMA_gDW_m2
## 1    D08       broadleaf     L2644              ACBA      44.18
## 2    D08       broadleaf     L2646              ACBA      41.71
## 3    D08       broadleaf     L2645              ACBA      40.66
## 4    D08       broadleaf     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
## 3     D02       broadleaf     P0002              JUNI      60.77
## 12    D02       broadleaf     L0006              JUNI      42.54
## 13    D02       broadleaf     P0007              QUVE     106.57
## 19    D02       broadleaf     P0010              PRSE      78.82
## 21    D02       broadleaf     P0011              PRSE      86.09
## 28    D02       broadleaf     L0014              PRSE      67.11
```

plot cal and val spectra

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

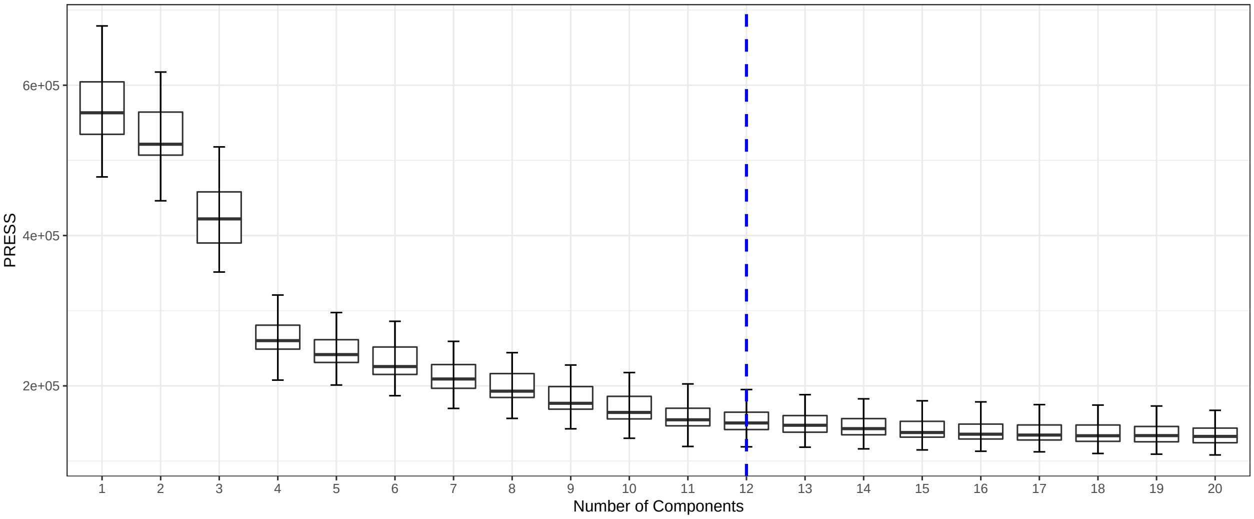
Use Jackknife permutation to determine optimal number of components

```
### 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 <- spectratrait::find_optimal_components(dataset=cal.plsr.data, targetVariable=inVar,
                                                  method=method,
                                                  maxComps=maxComps, seg=seg,
                                                  random_seed=random_seed)
  print(paste0("*** Optimal number of components: ", nComps))
} else {
  nComps <- spectratrait::find_optimal_components(dataset=cal.plsr.data, targetVariable=inVar,
                                                  method=method,
                                                  maxComps=maxComps, iterations=iterations,
                                                  seg=seg, prop=prop,
                                                  random_seed=random_seed)
}
```

```
## [1] "*** Identifying optimal number of PLSR components ***"
## [1] "*** Running permutation test.  Please hang tight, this can take awhile ***"
## [1] "Options:"
## [1] "Max Components: 20 Iterations: 40 Data Proportion (percent): 70"
## [1] "*** Providing PRESS and coefficient array output ***"
```

```
## 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
```

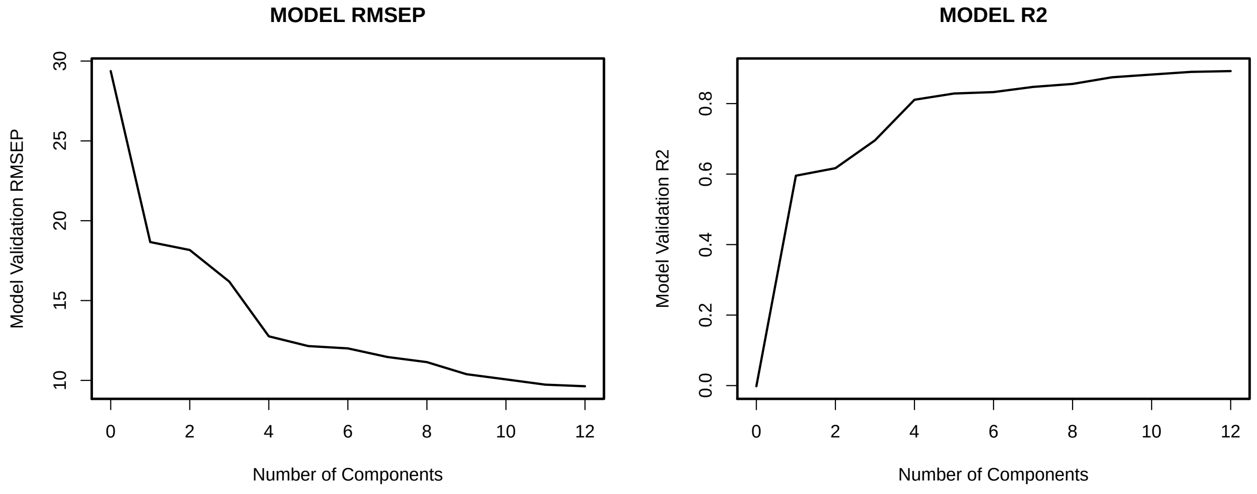
```
par(mfrow=c(1,2)) # B, L, T, R
pls::RMSEP(plsr.out, newdata = val.plsr.data)
```

```
## (Intercept)      1 comps      2 comps      3 comps      4 comps      5 comps
##      29.372       18.664       18.166       16.187       12.760       12.149
##     6 comps      7 comps      8 comps      9 comps     10 comps     11 comps
##      12.004       11.465       11.144       10.389       10.063        9.732
##    12 comps
##       9.633
```

```
plot(pls::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)

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

```
## (Intercept)      1 comps      2 comps      3 comps      4 comps      5 comps
##   -0.001908     0.595475     0.616770     0.695732     0.810908     0.828593
##     6 comps      7 comps      8 comps      9 comps     10 comps     11 comps
##    0.832656     0.847338     0.855775     0.874647     0.882410     0.890000
##    12 comps
##    0.892247
```

```
plot(pls::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
```

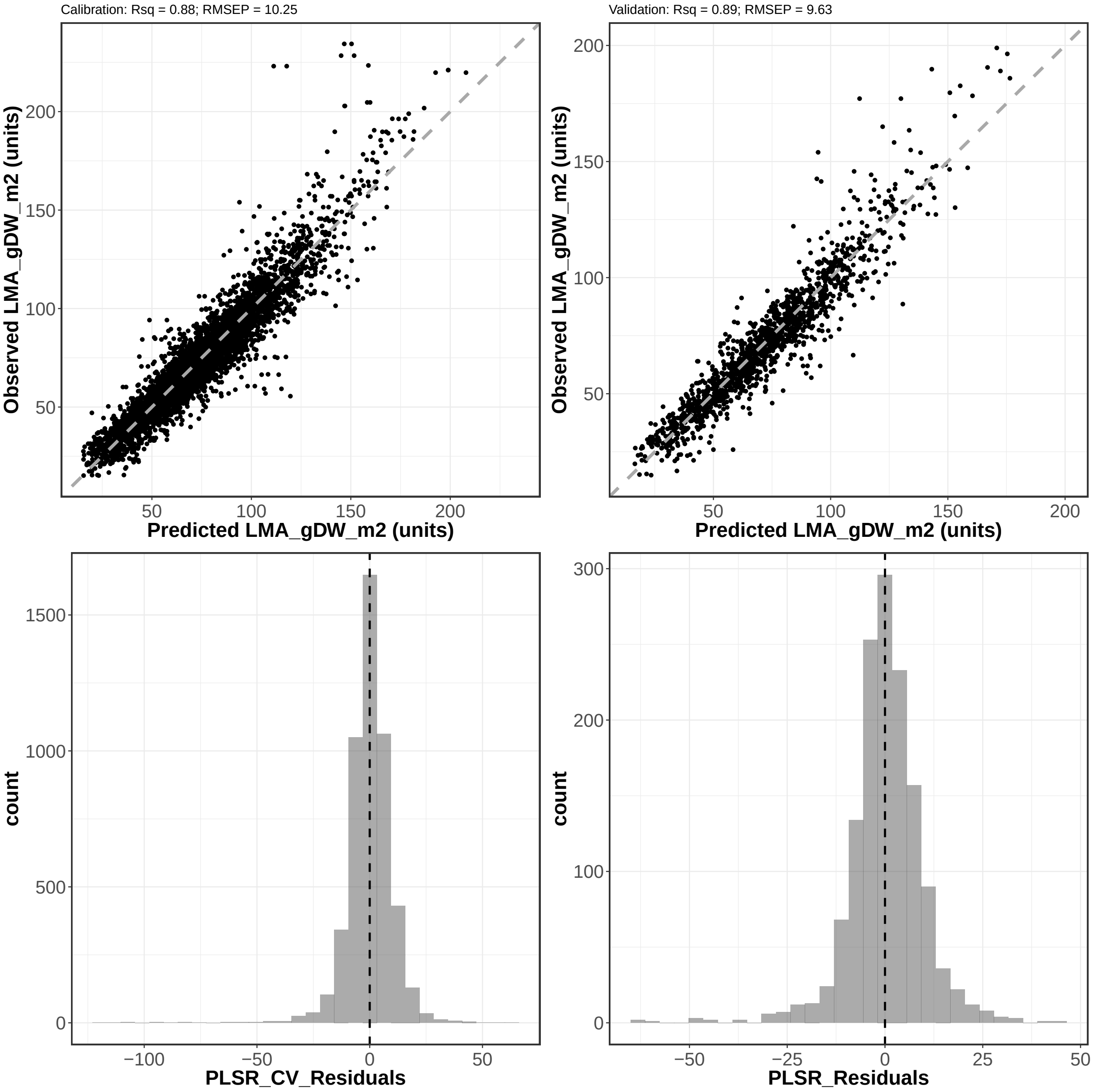
```
cal.R2 <- round(pls::R2(plsr.out,intercept=F)[[1]][nComps],2)
cal.RMSEP <- round(sqrt(mean(cal.plsr.output$PLSR_CV_Residuals^2)),2)

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
## 3     D02       broadleaf     P0002              JUNI      60.77       63.90905
## 12    D02       broadleaf     L0006              JUNI      42.54       41.54133
## 13    D02       broadleaf     P0007              QUVE     106.57       99.99662
## 19    D02       broadleaf     P0010              PRSE      78.82       89.03078
## 21    D02       broadleaf     P0011              PRSE      86.09       85.17273
## 28    D02       broadleaf     L0014              PRSE      67.11       67.95549
##    PLSR_Residuals
## 3       3.1390459
## 12     -0.9986720
## 13     -6.5733831
## 19     10.2107788
## 21     -0.9172668
## 28      0.8454930
```

```
val.R2 <- round(pls::R2(plsr.out,newdata=val.plsr.data,intercept=F)[[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
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 8 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`.
```



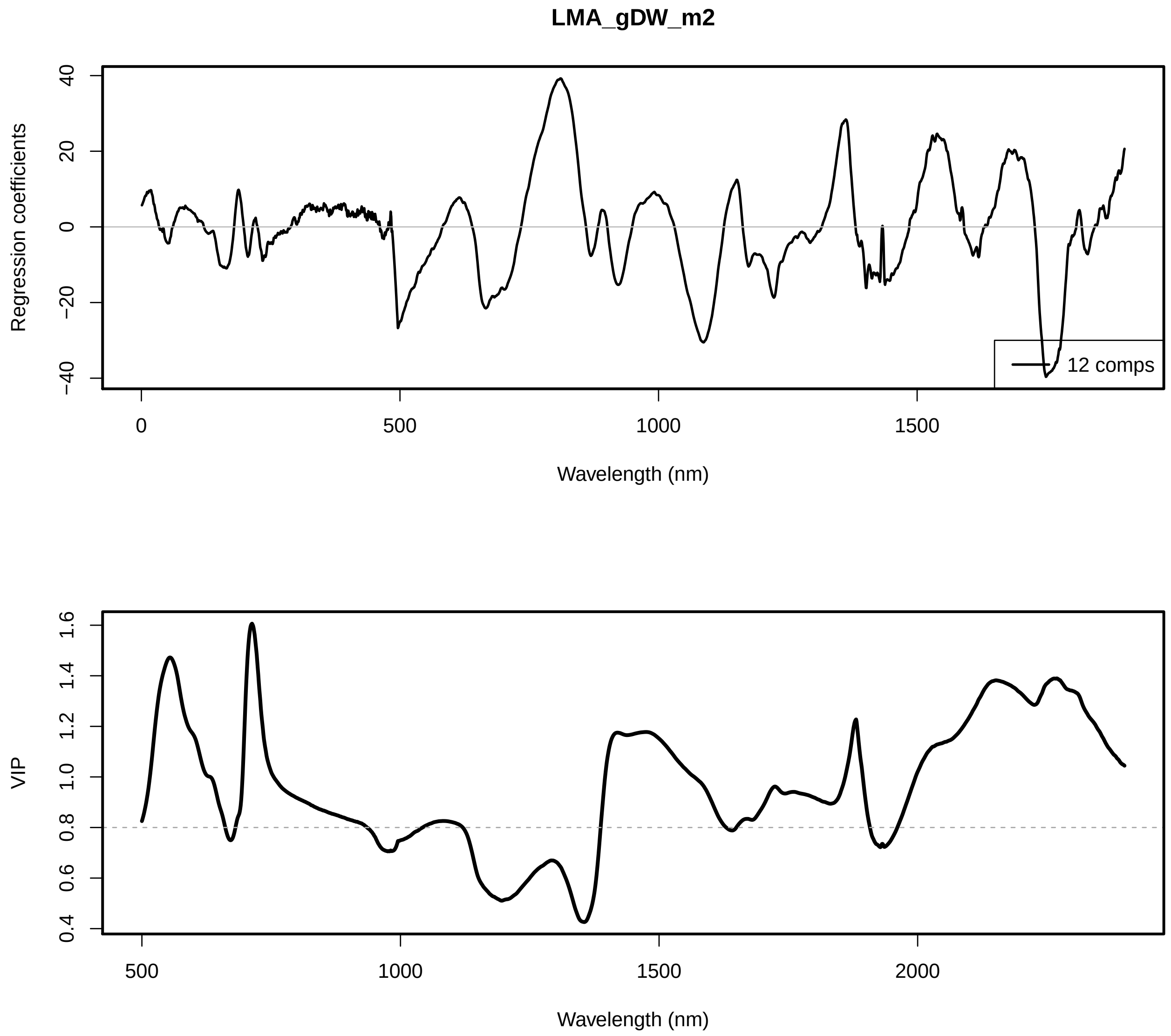
Calibration: Rsq = 0.88; RMSEP = 10.25

Validation: Rsq = 0.89; RMSEP = 9.63

```
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 <- spectratrait::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
```

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

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

```r
par(opar)
```

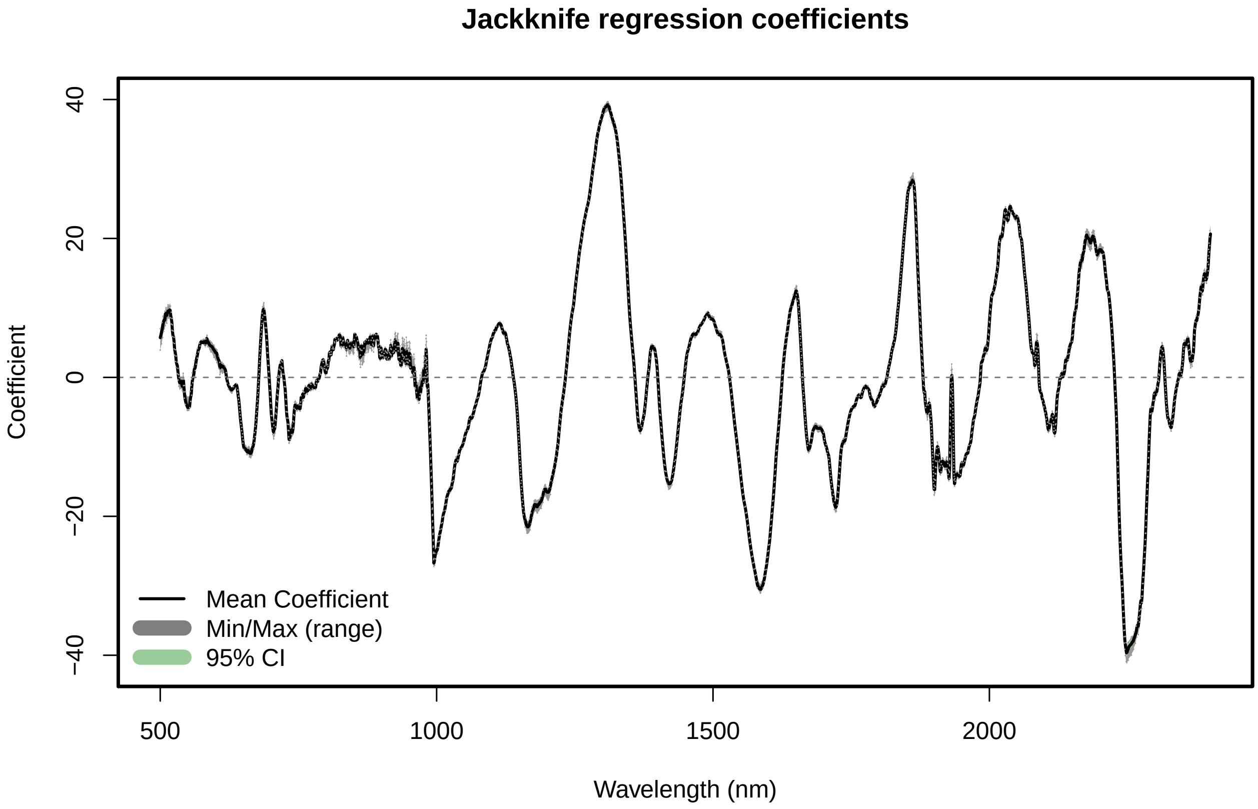
Jackknife validation

```r
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 <- spectratrait::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
## 3     D02       broadleaf     P0002              JUNI      60.77       63.90905
## 12    D02       broadleaf     L0006              JUNI      42.54       41.54133
## 13    D02       broadleaf     P0007              QUVE     106.57       99.99662
## 19    D02       broadleaf     P0010              PRSE      78.82       89.03078
## 21    D02       broadleaf     P0011              PRSE      86.09       85.17273
## 28    D02       broadleaf     L0014              PRSE      67.11       67.95549
##    PLSR_Residuals       LCI       UCI       LPI       UPI
## 3       3.1390459 63.75673  64.12043 45.02836  82.78973
## 12     -0.9986720 41.42248  41.69728 22.66069  60.42196
## 13     -6.5733831 99.88029 100.11962 81.11612 118.87712
## 19     10.2107788 88.83274  89.21623 70.14949 107.91207
## 21     -0.9172668 85.02330  85.32067 66.29194 104.05353
## 28      0.8454930 67.82558  68.15298 49.07457  86.83642
```

Jackknife coefficient plot

```
spectratrait::f.plot.coef(Z = t(Jackknife_coef), wv = wv,
            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)
```

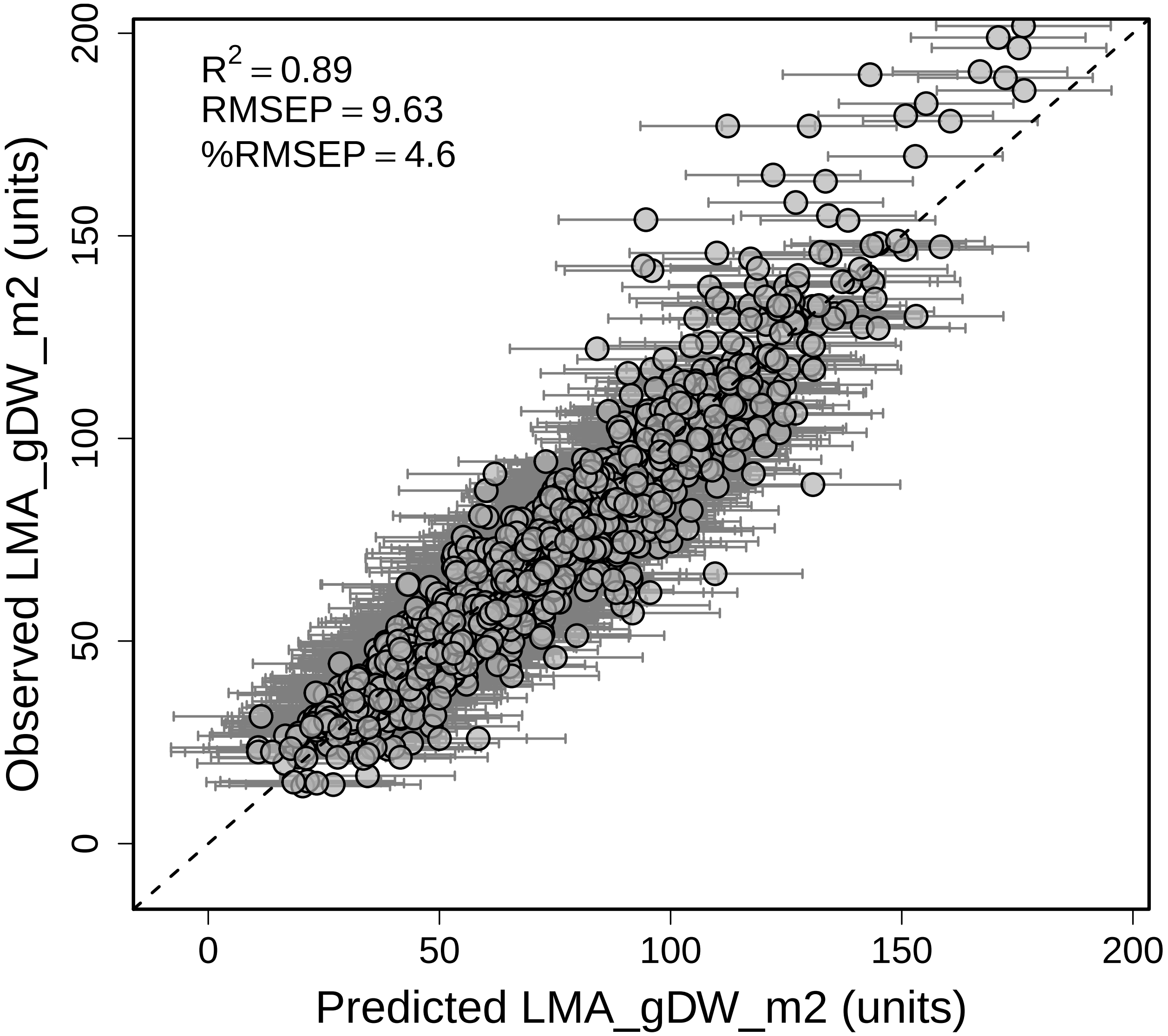
```
## quartz_off_screen
##                 3
```

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

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

Jackknife validation plot

```
rmsep_percrmsep <- spectratrait::percent_rmse(plsr_dataset = val.plsr.output,
                                              inVar = inVar,
                                              residuals = val.plsr.output$PLSR_Residuals,
                                              range="full")
RMSEP <- rmsep_percrmsep$rmse
perc_RMSEP <- rmsep_percrmsep$perc_rmse
r2 <- round(pls::R2(plsr.out, newdata = val.plsr.data, intercept=F)$val[nComps],2)
expr <- vector("expression", 3)
expr[[1]] <- bquote(R^2==.(r2))
expr[[2]] <- bquote(RMSEP==.(round(RMSEP,2)))
expr[[3]] <- bquote("%RMSEP"==.(round(perc_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))
plotrix::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=scales::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,
                                             '_Jackkife_PLSR_Coefficients.csv')),
          row.names=FALSE)
```

Create core PLSR outputs

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

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

```
print(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_Jackkife_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"
```