Spectra-trait PLSR example using leaf-level spectra and leaf nitrogen content (Narea, g/m2) data from eight different crop species growing in a glasshouse at Brookhaven National Laboratory

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Overview

This is an R Markdown Notebook to illustrate how to load an internal dataset ("ely_plsr_data"), choose the "optimal" number of plsr components, and fit a plsr model for leaf nitrogen content (Narea, g/m2)

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
```

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

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

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

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

Load internal Ely et al 2019 dataset

```r
data("ely_plsr_data")
head(ely_plsr_data)[,1:8]
```

```
##   Species_Code      Common_Name C_N_mass   C_g_m2 H20_g_m2 LMA_g_m2   N_g_m2
## 1        HEAN3 common sunflower     7.58 15.61210   167.63    36.40 2.103694
## 2        HEAN3 common sunflower     8.33 14.73724   164.68    34.65 1.231713
## 3        HEAN3 common sunflower     7.70 15.02495   156.95    35.08 1.764752
## 4        CUSA4  garden cucumber     7.40 11.14835   111.52    26.23 1.287963
## 5        CUSA4  garden cucumber     7.47 11.60735   123.58    26.71 1.411361
## 6        CUSA4  garden cucumber     7.43  8.06035   114.36    18.40 1.117704
##   Wave_500
## 1 4.782000
## 2 4.341714
## 3 4.502857
## 4 3.333429
## 5 3.313571
## 6 3.272286
```

```r
# What is the target variable?
inVar <- "N_g_m2"
```

Set working directory (scratch space)

```
## [1] "/private/var/folders/tq/tydmhlwn1bdf_0pmpcq70r2c0000gn/T/RtmpXnZG1h"
```

Full PLSR dataset

```r
Start.wave <- 500
End.wave <- 2400
wv <- seq(Start.wave,End.wave,1)
plsr_data <- ely_plsr_data
head(plsr_data)[,1:6]
```

```
##   Species_Code      Common_Name C_N_mass   C_g_m2 H20_g_m2 LMA_g_m2
## 1        HEAN3 common sunflower     7.58 15.61210   167.63    36.40
## 2        HEAN3 common sunflower     8.33 14.73724   164.68    34.65
## 3        HEAN3 common sunflower     7.70 15.02495   156.95    35.08
```

```
## 4        CUSA4  garden cucumber     7.40 11.14835   111.52    26.23
## 5        CUSA4  garden cucumber     7.47 11.60735   123.58    26.71
## 6        CUSA4  garden cucumber     7.43  8.06035   114.36    18.40
```

Create cal/val datasets

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

method <- "base" #base/dplyr
# base R - a bit slow
# dplyr - much faster
split_data <- spectratrait::create_data_split(dataset=plsr_data, approach=method,
                                             split_seed=23452135, prop=0.7,
                                             group_variables="Species_Code")
```

```
## HEAN3   Cal: 70%

## CUSA4   Cal: 68.182%

## CUPE   Cal: 70.588%

## SOLYL   Cal: 70%

## OCBA   Cal: 68.421%

## POPUL   Cal: 71.429%

## GLMA4   Cal: 70.588%

## PHVU   Cal: 66.667%
```

```r
names(split_data)
```

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

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

```
##    Species_Code      Common_Name C_N_mass   C_g_m2 H20_g_m2 LMA_g_m2   N_g_m2
## 1         HEAN3 common sunflower     7.58 15.61210   167.63    36.40 2.103694
## 2         HEAN3 common sunflower     8.33 14.73724   164.68    34.65 1.231713
## 4         CUSA4  garden cucumber     7.40 11.14835   111.52    26.23 1.287963
## 6         CUSA4  garden cucumber     7.43  8.06035   114.36    18.40 1.117704
## 7          CUPE    field pumpkin     7.20 11.43007   128.42    25.83 1.215333
## 10        SOLYL    garden tomato     7.89 11.61918   142.23    27.40 1.304110
##    Wave_500
## 1  4.782000
## 2  4.341714
## 4  3.333429
## 6  3.272286
## 7  2.943143
## 10 4.145714
```

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

```
##    Species_Code      Common_Name C_N_mass    C_g_m2 H20_g_m2 LMA_g_m2    N_g_m2
## 3         HEAN3 common sunflower     7.70 15.024947   156.95    35.08 1.7647515
## 5         CUSA4  garden cucumber     7.47 11.607347   123.58    26.71 1.4113615
```

```
## 8          CUPE    field pumpkin     7.67 12.466238    124.67     29.22 1.1468413
## 9          CUPE    field pumpkin     7.64 17.100448    142.85     43.39 1.1390174
## 13        SOLYL    garden tomato     7.73  7.938866    129.95     17.96 0.9483533
## 15         OCBA      sweet basil     8.13 16.975969    173.30     38.65 1.1246459
##    Wave_500
## 3  4.502857
## 5  3.313571
## 8  2.868000
## 9  3.338286
## 13 3.960286
## 15 3.744000
```

```r
rm(split_data)

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

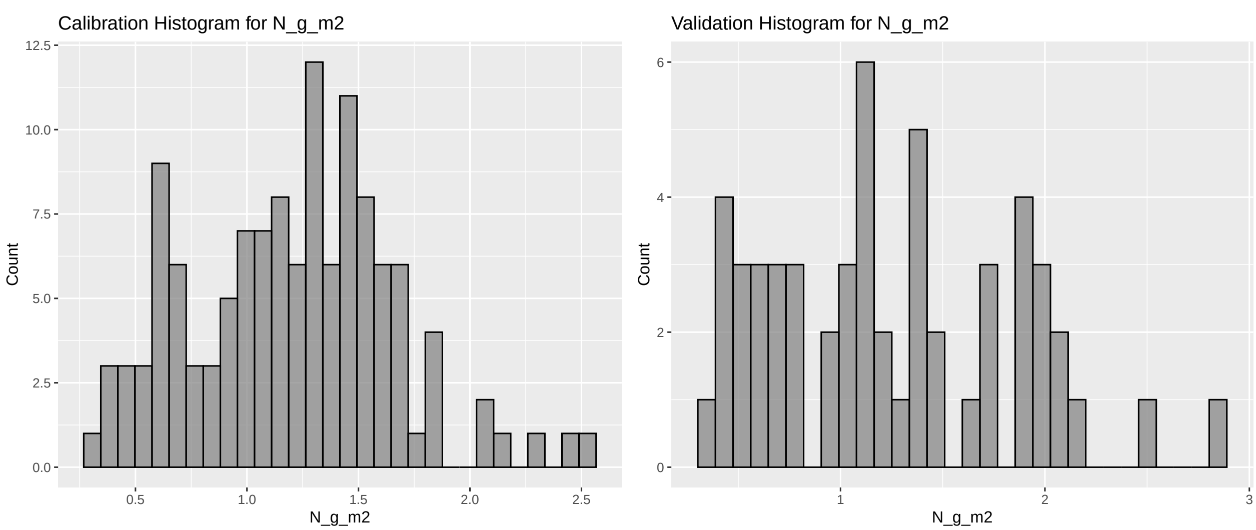
```
## [1] "Cal observations: 124"
```

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

```
## [1] "Val observations: 54"
```

```r
cal_hist_plot <- ggplot(data = cal.plsr.data,
                        aes(x = cal.plsr.data[,paste0(inVar)])) +
  geom_histogram(fill=I("grey50"),col=I("black"),alpha=I(.7)) +
  labs(title=paste0("Calibration Histogram for ",inVar), x = paste0(inVar),
       y = "Count")
val_hist_plot <- ggplot(data = val.plsr.data,
                        aes(x = val.plsr.data[,paste0(inVar)])) +
  geom_histogram(fill=I("grey50"),col=I("black"),alpha=I(.7)) +
  labs(title=paste0("Validation Histogram for ",inVar), x = paste0(inVar),
       y = "Count")
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`.
```



```r
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

```r
### 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]
```

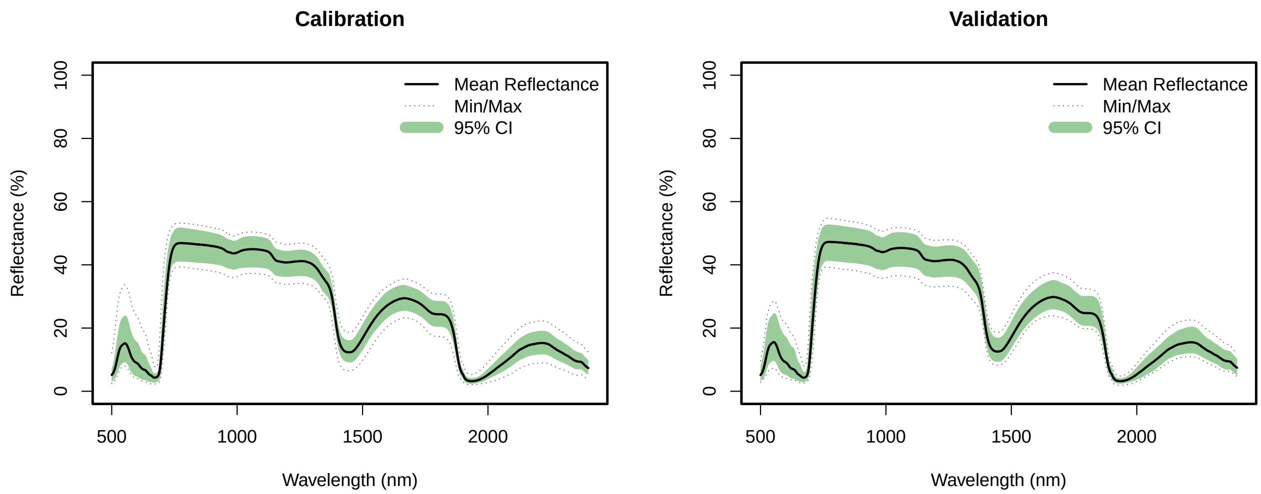
```
##    Species_Code      Common_Name C_N_mass    C_g_m2 H20_g_m2
## 1         HEAN3 common sunflower     7.58 15.61210   167.63
## 2         HEAN3 common sunflower     8.33 14.73724   164.68
## 4         CUSA4  garden cucumber     7.40 11.14835   111.52
## 6         CUSA4  garden cucumber     7.43  8.06035   114.36
## 7          CUPE    field pumpkin     7.20 11.43007   128.42
## 10        SOLYL    garden tomato     7.89 11.61918   142.23
```

```r
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]
```

```
##    Species_Code      Common_Name C_N_mass     C_g_m2 H20_g_m2
## 3         HEAN3 common sunflower     7.70 15.024947   156.95
## 5         CUSA4  garden cucumber     7.47 11.607347   123.58
## 8          CUPE    field pumpkin     7.67 12.466238   124.67
## 9          CUPE    field pumpkin     7.64 17.100448   142.85
## 13        SOLYL    garden tomato     7.73  7.938866   129.95
## 15         OCBA      sweet basil     8.13 16.975969   173.30
```

plot cal and val spectra

```r
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")
```




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

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

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

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

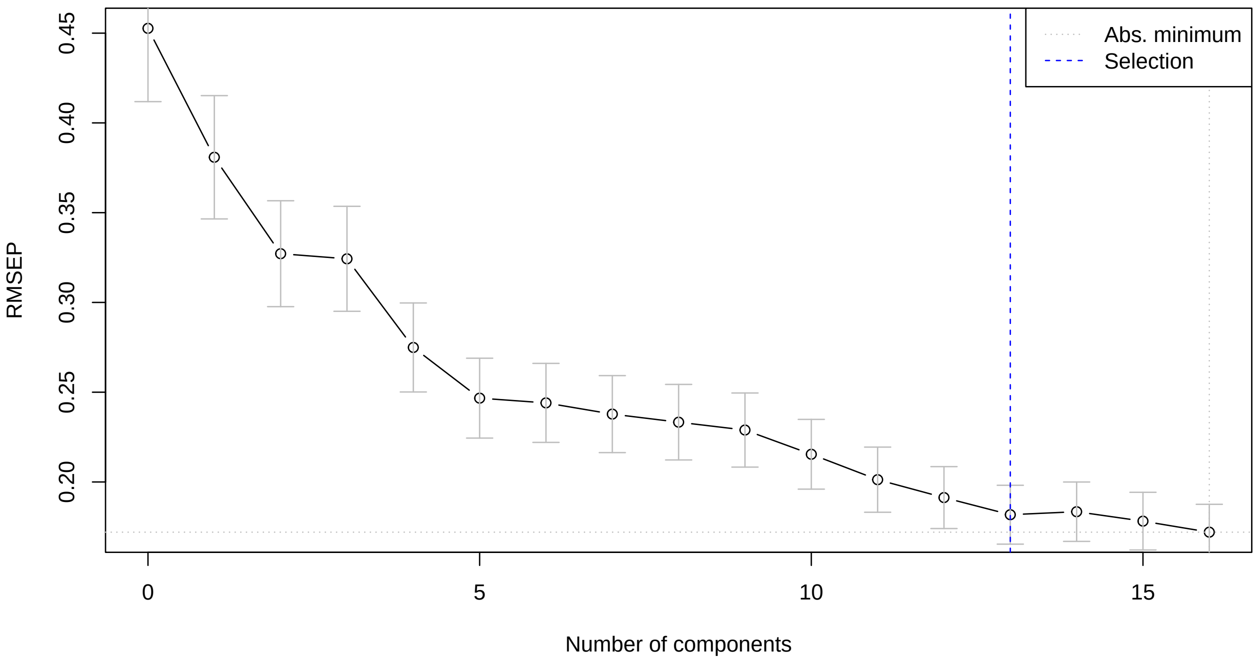
```r
par(mfrow=c(1,1))
```

Use permutation to determine optimal number of components

```r
### 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 <- "pls" #pls, firstPlateau, firstMin
random_seed <- 1245565
seg <- 50
maxComps <- 16
iterations <- 80
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 PLS permutation test ***"
```




```
## [1] "*** Optimal number of components: 13"
```

```
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

```
plsr.out <- plsr(as.formula(paste(inVar,"~","Spectra")),scale=FALSE,ncomp=nComps,validation="LOO",
                  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)
```

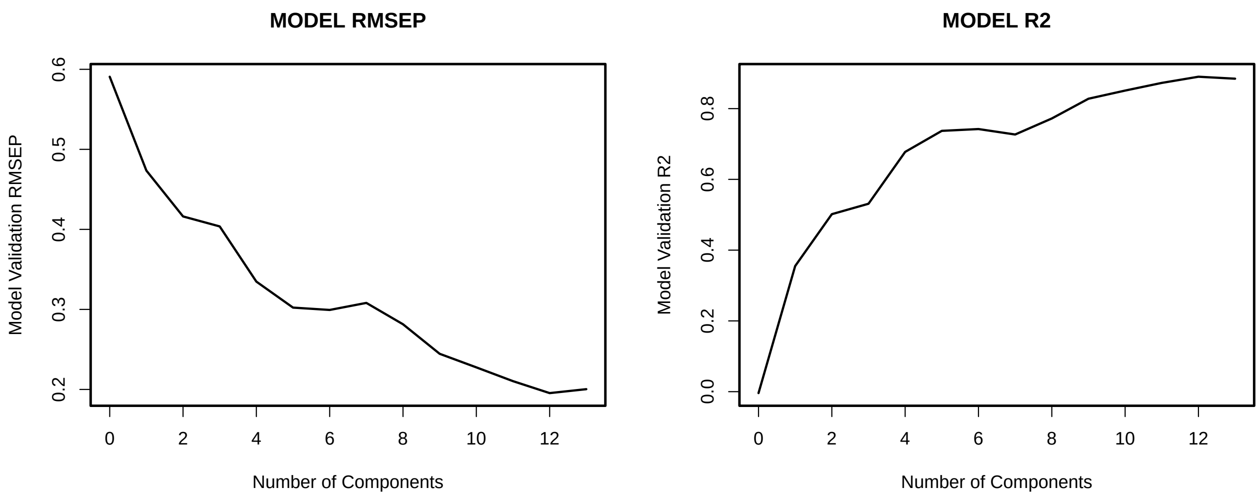
```
## (Intercept)      1 comps      2 comps      3 comps      4 comps      5 comps
##      0.5908       0.4735       0.4162       0.4037       0.3347       0.3023
##     6 comps      7 comps      8 comps      9 comps     10 comps     11 comps
##      0.2993       0.3081       0.2814       0.2445       0.2276       0.2104
##    12 comps     13 comps
```

```
##      0.1954       0.2003
```

```r
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
##   -0.004079     0.355010     0.501632     0.531088     0.677620     0.737143
##     6 comps      7 comps      8 comps      9 comps     10 comps     11 comps
##    0.742224     0.726835     0.772115     0.827942     0.850962     0.872685
##    12 comps     13 comps
##    0.890124     0.884529
```

```r
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)
```




```r
dev.copy(png,file.path(outdir,paste0(paste0(inVar,"_Validation_RMSEP_R2_by_Component.png"))),
         height=2800, width=4800,  res=340)
```

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

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

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

```r
par(opar)
```

PLSR fit observed vs. predicted plot data

```r
#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)
```

```
##    Species_Code      Common_Name C_N_mass   C_g_m2 H20_g_m2 LMA_g_m2   N_g_m2
## 1         HEAN3 common sunflower     7.58 15.61210   167.63    36.40 2.103694
## 2         HEAN3 common sunflower     8.33 14.73724   164.68    34.65 1.231713
## 4         CUSA4  garden cucumber     7.40 11.14835   111.52    26.23 1.287963
## 6         CUSA4  garden cucumber     7.43  8.06035   114.36    18.40 1.117704
## 7          CUPE    field pumpkin     7.20 11.43007   128.42    25.83 1.215333
## 10        SOLYL    garden tomato     7.89 11.61918   142.23    27.40 1.304110
##    PLSR_Predicted PLSR_CV_Predicted PLSR_CV_Residuals
## 1        1.820666          1.702501       -0.40119317
## 2        1.609632          1.711772        0.48005882
## 4        1.364985          1.275526       -0.01243687
## 6        1.126062          1.060119       -0.05758587
## 7        1.227538          1.226708        0.01137583
## 10       1.358638          1.365181        0.06107105
```

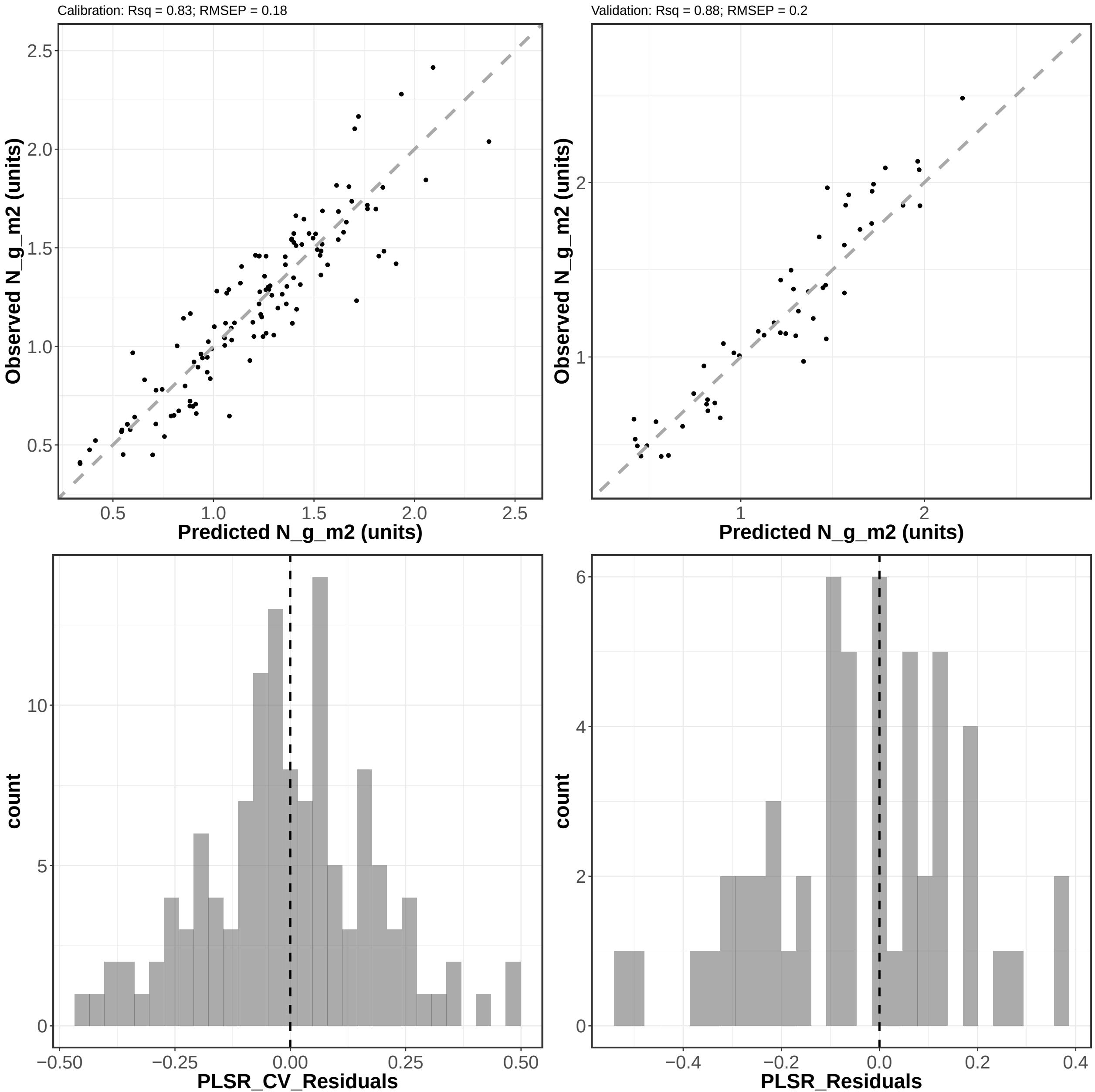
```
cal.R2 <- round(pls::R2(plsr.out,intercept=F)[[1]][nComps],2)
cal.RMSEP <- round(sqrt(mean(cal.plsr.output$PLSR_CV_Residuals^2)),2)

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)
```

```
##    Species_Code      Common_Name C_N_mass    C_g_m2 H20_g_m2 LMA_g_m2    N_g_m2
## 3         HEAN3 common sunflower     7.70 15.024947   156.95    35.08 1.7647515
## 5         CUSA4  garden cucumber     7.47 11.607347   123.58    26.71 1.4113615
## 8          CUPE    field pumpkin     7.67 12.466238   124.67    29.22 1.1468413
## 9          CUPE    field pumpkin     7.64 17.100448   142.85    43.39 1.1390174
## 13        SOLYL    garden tomato     7.73  7.938866   129.95    17.96 0.9483533
## 15         OCBA      sweet basil     8.13 16.975969   173.30    38.65 1.1246459
##    PLSR_Predicted PLSR_Residuals
## 3       1.7125176   -0.052233917
## 5       1.4618447    0.050483171
## 8       1.0951891   -0.051652168
## 9       1.2152379    0.076220509
## 13      0.7992342   -0.149119020
## 15      1.1267054    0.002059572
```

```
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", linewidth=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",
```

```r
        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, linewidth=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", linewidth=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, linewidth=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", linewidth=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, linewidth=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", linewidth=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, linewidth=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 3 rows containing missing values or values outside the scale range
## (`geom_point()`).
## Removed 3 rows containing missing values or values outside the scale range
## (`geom_point()`).

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

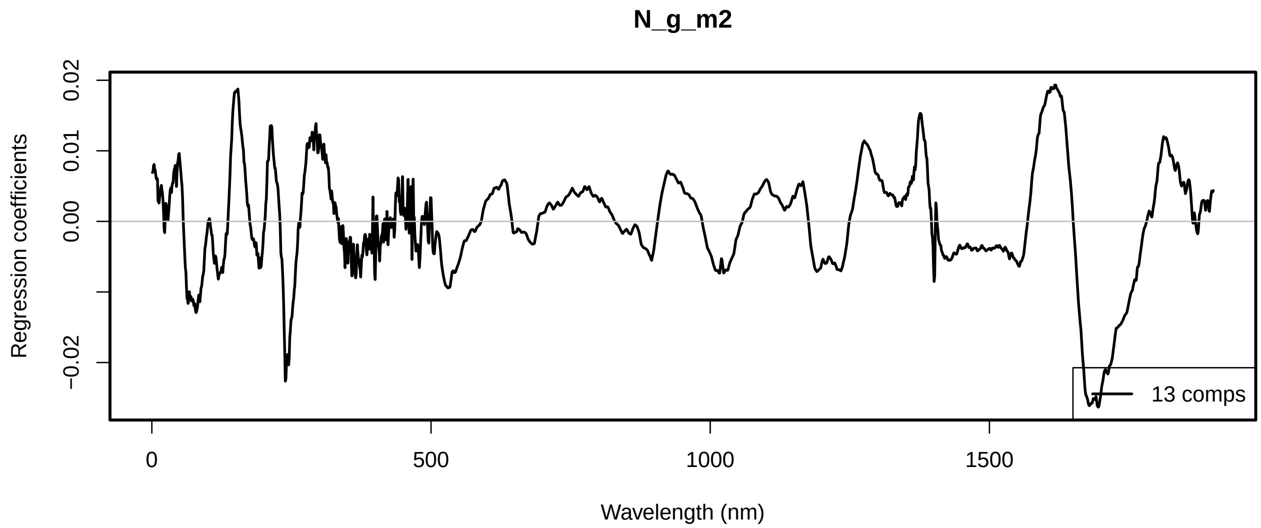


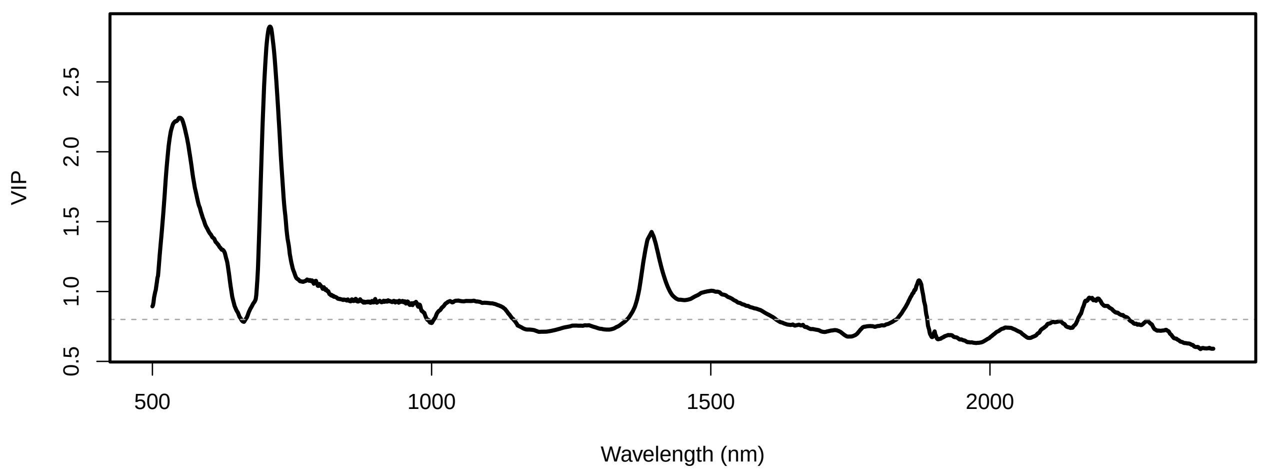

```r
ggsave(filename = file.path(outdir,paste0(inVar,"_Cal_Val_Scatterplots.png")),
       plot = scatterplots, device="png",
       width = 32,
       height = 30, units = "cm",
       dpi = 300)
```

Generate Coefficient and VIP plots

```r
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)
```

```r
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)
```






```r
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
```

Bootstrap validation

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

### PLSR bootstrap permutation uncertainty analysis
iterations <- 500    # how many permutation iterations to run
prop <- 0.70          # fraction of training data to keep for each iteration
plsr_permutation <- spectratrait::pls_permutation(dataset=cal.plsr.data, targetVariable=inVar,
                                                  maxComps=nComps,
                                                  iterations=iterations, prop=prop,
                                                  verbose = FALSE)
```

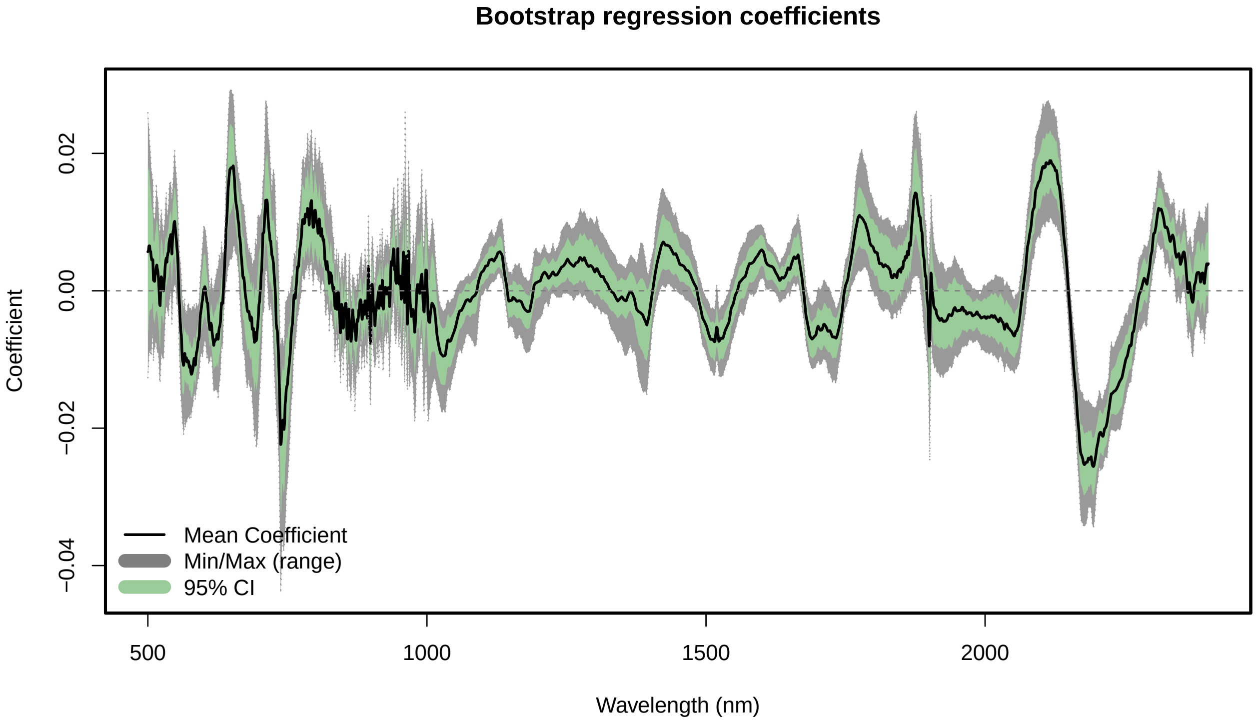
```
## [1] "*** Running permutation test.  Please hang tight, this can take awhile ***"
## [1] "Options:"
## [1] "Max Components: 13 Iterations: 500 Data Proportion (percent): 70"
## [1] "*** Providing PRESS and coefficient array output ***"
```

```r
bootstrap_intercept <- plsr_permutation$coef_array[1,,nComps]
bootstrap_coef <- plsr_permutation$coef_array[2:length(plsr_permutation$coef_array[,1,nComps]),
                                              ,nComps]
rm(plsr_permutation)

# apply coefficients to left-out validation data
interval <- c(0.025,0.975)
Bootstrap_Pred <- val.plsr.data$Spectra %*% bootstrap_coef +
  matrix(rep(bootstrap_intercept, length(val.plsr.data[,inVar])), byrow=TRUE,
         ncol=length(bootstrap_intercept))
Interval_Conf <- apply(X = Bootstrap_Pred, MARGIN = 1, FUN = quantile,
                       probs=c(interval[1], interval[2]))
sd_mean <- apply(X = Bootstrap_Pred, MARGIN = 1, FUN = sd)
sd_res <- sd(val.plsr.output$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)
```

```
##    Species_Code      Common_Name C_N_mass    C_g_m2 H20_g_m2 LMA_g_m2    N_g_m2
## 3         HEAN3 common sunflower     7.70 15.024947   156.95    35.08 1.7647515
## 5         CUSA4  garden cucumber     7.47 11.607347   123.58    26.71 1.4113615
## 8          CUPE    field pumpkin     7.67 12.466238   124.67    29.22 1.1468413
## 9          CUPE    field pumpkin     7.64 17.100448   142.85    43.39 1.1390174
## 13        SOLYL    garden tomato     7.73  7.938866   129.95    17.96 0.9483533
## 15         OCBA      sweet basil     8.13 16.975969   173.30    38.65 1.1246459
##    PLSR_Predicted PLSR_Residuals       LCI       UCI       LPI      UPI
## 3       1.7125176   -0.052233917 1.5070086 1.8760564 1.2810247 2.144011
## 5       1.4618447    0.050483171 1.2909822 1.5475356 1.0541359 1.869553
## 8       1.0951891   -0.051652168 0.9595488 1.2335912 0.6846083 1.505770
## 9       1.2152379    0.076220509 1.0746965 1.3367675 0.8068229 1.623653
## 13      0.7992342   -0.149119020 0.6820207 0.9451323 0.3899050 1.208563
## 15      1.1267054    0.002059572 1.0316572 1.2737521 0.7209233 1.532488
```

Jackknife coefficient plot

```r
# Bootstrap regression coefficient plot
spectratrait::f.plot.coef(Z = t(bootstrap_coef), wv = wv,
            plot_label="Bootstrap regression coefficients",position = 'bottomleft')
abline(h=0,lty=2,col="grey50")
box(lwd=2.2)
```




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

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

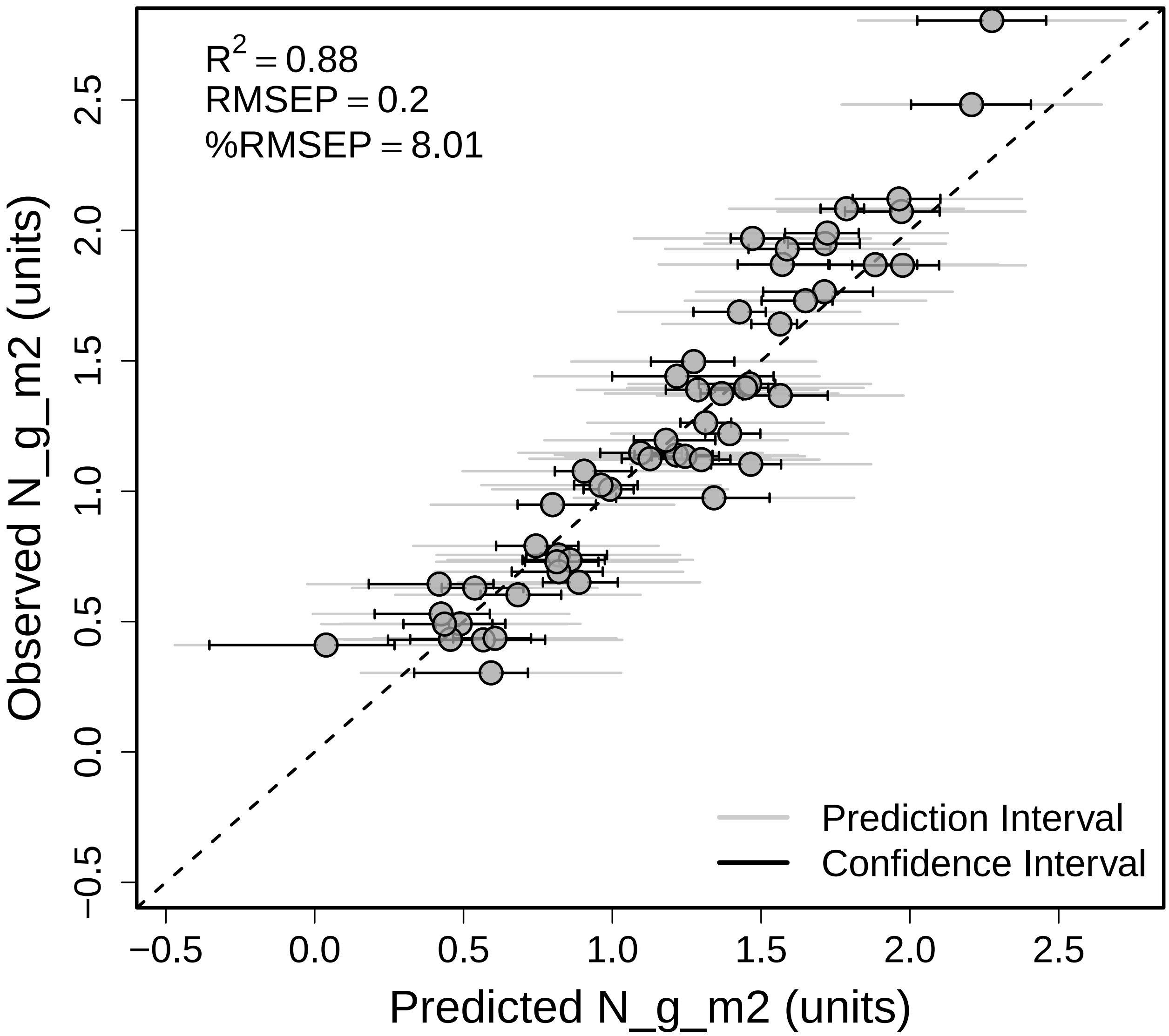
```r
dev.off();
```

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

Bootstrap validation plot

```r
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)))
```

```r
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$UPI, gap=0.009,sfrac=0.000,
       lwd=1.6, xlim=c(rng_vals[1], rng_vals[2]), ylim=c(rng_vals[1], rng_vals[2]),
       err="x", pch=21, col="black", pt.bg=scales::alpha("grey70",0.7), scol="grey80",
       cex=2, xlab=paste0("Predicted ", paste(inVar), " (units)"),
       ylab=paste0("Observed ", paste(inVar), " (units)"),
       cex.axis=1.5,cex.lab=1.8)
abline(0,1,lty=2,lw=2)
plotrix::plotCI(val.plsr.output$PLSR_Predicted,val.plsr.output[,inVar],
       li=val.plsr.output$LCI, ui=val.plsr.output$UCI, 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="black",
       cex=2, xlab=paste0("Predicted ", paste(inVar), " (units)"),
       ylab=paste0("Observed ", paste(inVar), " (units)"),
       cex.axis=1.5,cex.lab=1.8, add=T)
legend("topleft", legend=expr, bty="n", cex=1.5)
legend("bottomright", legend=c("Prediction Interval","Confidence Interval"),
       lty=c(1,1), col = c("grey80","black"), lwd=3, bty="n", cex=1.5)
box(lwd=2.2)
```




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

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

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

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

Output bootstrap results

```r
# Bootstrap Coefficients
out.jk.coefs <- data.frame(Iteration=seq(1,length(bootstrap_intercept),1),
                           Intercept=bootstrap_intercept,t(bootstrap_coef))
names(out.jk.coefs) <- c("Iteration","Intercept",paste0("Wave_",wv))
head(out.jk.coefs)[1:6]
```

```
##    Iteration  Intercept      Wave_500      Wave_501      Wave_502      Wave_503
```

```
## 1         1 -0.6617899 -0.0067918917 -0.006451152 -0.005571355 -0.004909648
## 2         2 -0.4636504 -0.0040384348 -0.001804902  0.001375426  0.002477500
## 3         3 -0.8146267  0.0031055624  0.003529288  0.005078394  0.005883173
## 4         4  0.7030872  0.0003883207  0.002887701  0.003961071  0.003223096
## 5         5  0.4765138  0.0045652557  0.005822813  0.005979498  0.004861387
## 6         6  0.4146289  0.0085296345  0.009692141  0.010451131  0.009300204
```

```r
write.csv(out.jk.coefs,file=file.path(outdir,paste0(inVar,
                                                    '_Bootstrap_PLSR_Coefficients.csv')),
          row.names=FALSE)
```

Create core PLSR outputs

```r
print(paste("Output directory: ", outdir))
```

```
## [1] "Output directory:  /var/folders/tq/tydmhlwn1bdf_0pmpcq70r2c0000gn/T//RtmpXnZG1h"
```

```r
# 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

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

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

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

```
##  [1] "N_g_m2_Bootstrap_PLSR_Coefficients.csv"
##  [2] "N_g_m2_Bootstrap_Regression_Coefficients.png"
##  [3] "N_g_m2_Cal_PLSR_Dataset.csv"
##  [4] "N_g_m2_Cal_Val_Histograms.png"
##  [5] "N_g_m2_Cal_Val_Scatterplots.png"
##  [6] "N_g_m2_Cal_Val_Spectra.png"
```

```
##  [7] "N_g_m2_Coefficient_VIP_plot.png"
##  [8] "N_g_m2_Observed_PLSR_CV_Pred_13comp.csv"
##  [9] "N_g_m2_PLSR_Coefficients_13comp.csv"
## [10] "N_g_m2_PLSR_Component_Selection.png"
## [11] "N_g_m2_PLSR_Validation_Scatterplot.png"
## [12] "N_g_m2_PLSR_VIPs_13comp.csv"
## [13] "N_g_m2_Val_PLSR_Dataset.csv"
## [14] "N_g_m2_Validation_PLSR_Pred_13comp.csv"
## [15] "N_g_m2_Validation_RMSEP_R2_by_Component.png"
```