An example showing how to apply an existing PLSR model to new data. In this case applying the LMA model from Serbin et al., (2019; DOI - 10.1111/nph.16123) to a dataset collected at CONUS NEON field sites

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Getting Started

Load libraries

```
list.of.packages <- c("pls","dplyr","reshape2","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
## Warning: package 'dplyr' was built under R version 4.0.5
##
## 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/RtmpaW2R1z"
```

Grab PLSR Coefficients from GitHub

```
git_repo <- "https://raw.githubusercontent.com/serbinsh/SSerbin_etal_2019_NewPhytologist/master/"
print("**** Downloading PLSR coefficients ****")
```

```
## [1] "**** Downloading PLSR coefficients ****"
```

```
githubURL <- paste0(git_repo,"SSerbin_multibiome_lma_plsr_model/sqrt_LMA_gDW_m2_PLSR_Coefficients_10comp
LeafLMA.plsr.coeffs <- spectratrait::source_GitHubData(githubURL)
rm(githubURL)
githubURL <- paste0(git_repo,"SSerbin_multibiome_lma_plsr_model/sqrt_LMA_gDW_m2_Jackkife_PLSR_Coefficien
LeafLMA.plsr.jk.coeffs <- spectratrait::source_GitHubData(githubURL)
rm(githubURL)
```

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"
```

Prepare new data for estimation

```
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))
head(Spectra)[1:6,1:10]
```

```
##      Wave_500 Wave_501 Wave_502 Wave_503 Wave_504 Wave_505 Wave_506 Wave_507
## [1,] 0.044226 0.044605 0.044927 0.045473 0.046241 0.046878 0.047826 0.049090
## [2,] 0.046855 0.047601 0.047944 0.048478 0.049381 0.050235 0.051161 0.052191
## [3,] 0.043758 0.044171 0.044869 0.045465 0.045984 0.046933 0.047993 0.049090
```

```
## [4,] 0.041154 0.041603 0.042088 0.042408 0.042639 0.043260 0.044140 0.045058
## [5,] 0.037296 0.037944 0.038209 0.038677 0.039388 0.039948 0.040630 0.041501
## [6,] 0.043878 0.044257 0.044723 0.045295 0.045949 0.046575 0.047378 0.048357
##      Wave_508 Wave_509
## [1,] 0.050268 0.051525
## [2,] 0.053322 0.054357
## [3,] 0.050168 0.051441
## [4,] 0.045700 0.046476
## [5,] 0.042613 0.043731
## [6,] 0.049392 0.050387
```

```
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)
```

```
#### End user needs to do what's appropriate for their data.  This may be an iterative process.
# Keep only complete rows of inVar and spec data before fitting
plsr_data <- plsr_data[complete.cases(plsr_data[,names(plsr_data) %in%
                                                  c(inVar,paste0("Wave_",wv))]),]
```

Example data cleaning.

```
print("**** Applying PLSR model to estimate LMA from spectral observations ****")
```

Prepare PLSR model

```
## [1] "**** Applying PLSR model to estimate LMA from spectral observations ****"
```

```
# setup model
dims <- dim(LeafLMA.plsr.coeffs)
LeafLMA.plsr.intercept <- LeafLMA.plsr.coeffs[1,]
LeafLMA.plsr.coeffs <- data.frame(LeafLMA.plsr.coeffs[2:dims[1],])
names(LeafLMA.plsr.coeffs) <- c("wavelength","coefs")
LeafLMA.plsr.coeffs.vec <- as.vector(LeafLMA.plsr.coeffs[,2])
sub_spec <- droplevels(plsr_data[,which(names(plsr_data) %in%
                                          paste0("Wave_",seq(Start.wave,End.wave,1)))])
```

```
plsr_pred <- as.matrix(sub_spec) %*% LeafLMA.plsr.coeffs.vec + LeafLMA.plsr.intercept[,2]
leafLMA <- plsr_pred[,1]^2  # convert to standard LMA units from sqrt(LMA)
names(leafLMA) <- "PLSR_LMA_gDW_m2"

# organize output
LeafLMA.PLSR.dataset <- data.frame(plsr_data[,which(names(plsr_data) %notin%
                                                      paste0("Wave_",seq(Start.wave,End.wave,1)))],
                                   PLSR_LMA_gDW_m2=leafLMA, PLSR_Residuals=leafLMA-plsr_data[,inVar])
head(LeafLMA.PLSR.dataset)
```

Apply PLSR model

```
##   Domain Functional_type Sample_ID USDA_Species_Code LMA_gDW_m2 PLSR_LMA_gDW_m2
## 1    D02       broadleaf     P0001              JUNI      72.87        96.26243
## 2    D02       broadleaf     L0001              JUNI      72.87        90.09453
## 3    D02       broadleaf     P0002              JUNI      60.77        77.16475
## 4    D02       broadleaf     L0002              JUNI      60.77        60.99039
## 5    D02       broadleaf     P0003              JUNI      85.92       101.22709
## 6    D02       broadleaf     L0003              JUNI      85.92        97.13018
##   PLSR_Residuals
## 1     23.3924343
## 2     17.2245326
## 3     16.3947533
## 4      0.2203913
## 5     15.3070857
## 6     11.2101840
```

```
print("**** Generate PLSR uncertainty estimates ****")
```

Generate PLSR uncertainty estimates

```
## [1] "**** Generate PLSR uncertainty estimates ****"
```

```
jk_coef <- data.frame(LeafLMA.plsr.jk.coeffs[,3:dim(LeafLMA.plsr.jk.coeffs)[2]])
jk_coef <- t(jk_coef)
head(jk_coef)[,1:6]
```

```
##               [,1]      [,2]      [,3]      [,4]      [,5]      [,6]
## Wave_500 1.0005875 0.9952840 0.5652908 0.9793160 1.1052207 0.9370473
## Wave_501 0.9584235 0.9631434 0.5230544 0.9330803 1.0477469 0.9042780
## Wave_502 0.8960202 0.9065954 0.4597413 0.8710298 0.9658130 0.8628370
## Wave_503 0.8722135 0.8936197 0.4420696 0.8456098 0.9272967 0.8513741
```

```
## Wave_504 0.8452831 0.8644923 0.4159567 0.8110004 0.8903192 0.8320347
## Wave_505 0.8240743 0.8378399 0.3902871 0.7829891 0.8570048 0.8150339
```

```
jk_int <- t(LeafLMA.plsr.jk.coeffs[,2])
head(jk_int)[,1:6]
```

```
## [1] 7.787098 7.959443 8.015161 8.018586 7.658080 7.998432
```

```
jk_pred <- as.matrix(sub_spec) %*% jk_coef + matrix(rep(jk_int, length(plsr_data[,inVar])),
                                                    byrow=TRUE, ncol=length(jk_int))
jk_pred <- jk_pred^2
head(jk_pred)[,1:6]
```

```
##       [,1]      [,2]      [,3]     [,4]      [,5]      [,6]
## 1 94.28721  96.77712  96.44452 95.11992  96.72830  95.33877
## 2 90.36051  90.57120  90.77562 89.77821  90.24826  89.61806
## 3 75.71088  77.91861  76.42730 76.11473  77.67179  76.68756
## 4 61.37001  61.30963  60.56606 60.72330  61.63712  60.69649
## 5 99.24456 101.75948 101.22916 99.96305 101.70397 100.16758
## 6 97.40414  97.65463  97.52687 97.00817  97.33677  96.08535
```

```
dim(jk_pred)
```

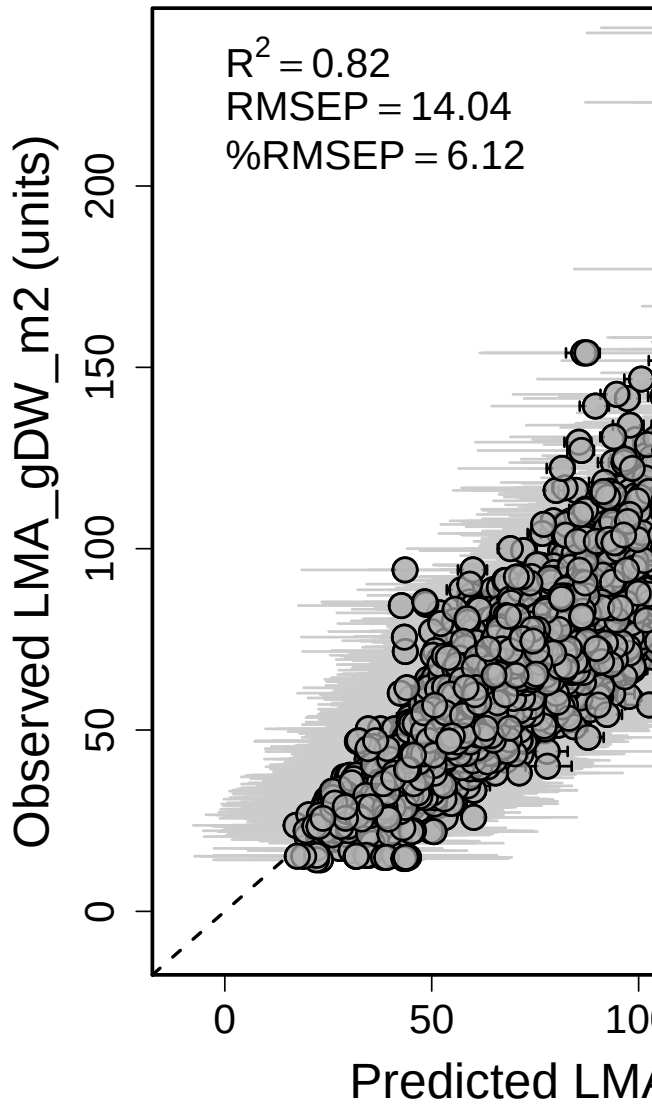
```
## [1] 6312 1000
```

```
interval <- c(0.025,0.975)
Interval_Conf <- apply(X = jk_pred, MARGIN = 1, FUN = quantile,
                       probs=c(interval[1], interval[2]))
sd_mean <- apply(X = jk_pred, MARGIN = 1, FUN =sd)
sd_res <- sd(LeafLMA.PLSR.dataset$PLSR_Residuals)
sd_tot <- sqrt(sd_mean^2+sd_res^2)
LeafLMA.PLSR.dataset$LCI <- Interval_Conf[1,]
LeafLMA.PLSR.dataset$UCI <- Interval_Conf[2,]
LeafLMA.PLSR.dataset$LPI <- LeafLMA.PLSR.dataset$PLSR_LMA_gDW_m2-1.96*sd_tot
LeafLMA.PLSR.dataset$UPI <- LeafLMA.PLSR.dataset$PLSR_LMA_gDW_m2+1.96*sd_tot
head(LeafLMA.PLSR.dataset)
```

```
##   Domain Functional_type Sample_ID USDA_Species_Code LMA_gDW_m2 PLSR_LMA_gDW_m2
## 1    D02       broadleaf     P0001               JUNI      72.87        96.26243
## 2    D02       broadleaf     L0001               JUNI      72.87        90.09453
## 3    D02       broadleaf     P0002               JUNI      60.77        77.16475
## 4    D02       broadleaf     L0002               JUNI      60.77        60.99039
## 5    D02       broadleaf     P0003               JUNI      85.92       101.22709
## 6    D02       broadleaf     L0003               JUNI      85.92        97.13018
##   PLSR_Residuals      LCI       UCI      LPI      UPI
## 1     23.3924343 93.95423  99.03625 71.30476 121.2201
## 2     17.2245326 88.81329  92.00078 65.21071 114.9784
## 3     16.3947533 74.79509  79.85715 52.19722 102.1323
## 4      0.2203913 59.80058  62.29402 36.12678  85.8540
## 5     15.3070857 98.86570 103.97701 76.26586 126.1883
## 6     11.2101840 95.50843  99.66865 72.20971 122.0507
```

```
rmsep_percrmsep <- spectratrait::percent_rmse(plsr_dataset = LeafLMA.PLSR.dataset,
                                              inVar = inVar,
                                              residuals = LeafLMA.PLSR.dataset$PLSR_Residuals,
```

```
                                                range="full")
RMSEP <- rmsep_percrmsep$rmse
perc_RMSEP <- rmsep_percrmsep$perc_rmse
r2 <- round(summary(lm(LeafLMA.PLSR.dataset$PLSR_LMA_gDW_m2~
                         LeafLMA.PLSR.dataset[,inVar]))$adj.r.squared,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(LeafLMA.PLSR.dataset$LPI), max(LeafLMA.PLSR.dataset$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(LeafLMA.PLSR.dataset$PLSR_LMA_gDW_m2,LeafLMA.PLSR.dataset[,inVar],
                li=LeafLMA.PLSR.dataset$LPI, ui=LeafLMA.PLSR.dataset$UPI, gap=0.009,sfrac=0.000,
                lwd=1.6, xlim=c(rng_vals[1], rng_vals[2]), ylim=c(rng_vals[1], rng_vals[2]),
                err="x", pch=21, col="black", pt.bg=scales::alpha("grey70",0.7), scol="grey80",
                cex=2, xlab=paste0("Predicted ", paste(inVar), " (units)"),
                ylab=paste0("Observed ", paste(inVar), " (units)"),
                cex.axis=1.5,cex.lab=1.8)
abline(0,1,lty=2,lw=2)
plotrix::plotCI(LeafLMA.PLSR.dataset$PLSR_LMA_gDW_m2,LeafLMA.PLSR.dataset[,inVar],
                li=LeafLMA.PLSR.dataset$LCI, ui=LeafLMA.PLSR.dataset$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)
```



Generate PLSR estimated LMA observed vs predicted plot

```
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
```

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

```
## [1] "Output directory:  /var/folders/xp/h3k9vf3n2jx181ts786_yjrn9c2gjq/T//RtmpaW2R1z"
```

```
# Observed versus predicted
write.csv(LeafLMA.PLSR.dataset,file=file.path(outdir,
                                              paste0(inVar,'_PLSR_Estimates.csv')),
          row.names=FALSE)
```

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_PLSR_Estimates.csv"
## [2] "LMA_gDW_m2_PLSR_Validation_Scatterplot.png"
```