

Development of an intertidal foraminifera training set for the North Sea and an assessment of its application for Holocene sea-level reconstructions

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The code is run in R 4.4.1

This is the R code to accompany the journal article: “Development of an intertidal foraminifera training set for the North Sea and an assessment of its application for Holocene sea-level reconstructions” by Rush et al. 2021 published in Marine Micropalaeontology. <https://doi.org/10.1016/j.marmicro.2021.102055>

The code, functions and data are provided are available to download on Figshare: https://figshare.com/authors/Graham_Rush/11546401

If you use any of this code please reference the article above and any incorporated packages.

The code is provided as a guide for carrying out an assessment of the most appropriate transfer function and training set to use. In order to assess different regions you will need to run the code multiple times. The core data provided is synthetic data and not intended for further analysis beyond this example.

If you try to run the code on your own data please contact me if you come across any problems.

This is an R Markdown Notebook. When you execute code within the notebook, the results appear beneath the code.

R code

Set up the workspace

Set up the workspace by clearing it and linking to our data files

```
rm(list = ls())  
options(scipen = 6, digits = 4) # I prefer to view outputs in non-scientific notation
```

Set to the directory that you saved the download

```
# wd <- paste("Your working directory")  
# setwd(wd)
```

Load up the packages we will need

```
library(rioja)
library(RColorBrewer)
library(viridis)
library(palaeoSigs)
library(vegan)
library(fpc)
library(cluster)
library(dplyr)
library(plyr)
```

Load up Grahams functions into memory. These have been written by Graham Rush and incorporate functions written in the above packages. Refer to the individual functions for details.

```
setwd(paste(wd, "/functions", sep = ""))
sapply(list.files(pattern = "[.]R$", recursive = TRUE), source) # loads all the functions in the functions folder
setwd(wd)
```

Read in the raw data Note: the core data is not provided as part of this data

```
mod_data <- read.csv("data/northsea_forams.csv", row.names = "ID", check.names = FALSE) # read in the mod data
core_data <- read.csv("data/Ythan-core.csv") # read in the core data
```

Set-up and clean the data. This creates a list with colours and names to help with the plotting and analysis later and to add the cleaned data to

```
training_sets <- list() # create a list to store the sub-regional training sets in

## set up the colours
training_sets$cols$northsea <- viridis(9, alpha = 1) # for viridis colours
training_sets$cols$northsea <- c("#999999", "#F0E442", "#0072B2", "#E69F00", "#009E73", "#56B4E9", "#D56014", "#F08080", "#000000")
training_sets$cols$west <- training_sets$cols$northsea[c(1:3, 7:9)]
training_sets$cols$northwest <- training_sets$cols$northsea[c(1,3,9)]
training_sets$cols$southwest <- training_sets$cols$northsea[c(2,7,8)]
training_sets$cols$east <- training_sets$cols$northsea[c(4:6)]
training_sets$cols$ythan <- training_sets$cols$northsea[c(9)]

## set up the labels
training_sets$names$northsea <- c("Alnmouth", "Brancaster", "Cowpen", "Kjelst", "Rantum", "Sonderho", "Thor", "Ythan")
training_sets$names$west <- training_sets$names$northsea[c(1:3, 7:9)]
training_sets$names$northwest <- training_sets$names$northsea[c(1,3,9)]
training_sets$names$southwest <- training_sets$names$northsea[c(2,7,8)]
training_sets$names$east <- training_sets$names$northsea[c(4:6)]
training_sets$names$ythan <- training_sets$names$northsea[c(9)]
```

Run grahams function in 'clean_regions.R' and 'cleaning.R' to clean the data 'clean_data' and remove samples with counts less than 'min.count' with the option to remove rare taxa (< 5 % in no more than 1 % of the samples)

```
training_sets$data <- clean_regions(n = 50, rare_species = FALSE, save_file = FALSE)
```

To avoid setting up and cleaning the data each time save the data using the below code and read it in and prevent re-running the above chunk use the following code

```
save(training_sets, file="data/training_sets.RData")    # save the data
load("data/training_sets.RData")    # this line can be run to load the saved data
```

Set the workspace for each training set

Set up the data ready to analyse training sets and transfer functions. Set the region 'reg' to the region of choice. You will need to repeat the code from here on for the different regions

```
reg <- "West"      # set this to the region of choice
training.set <- training_sets$data$west    # set this to the region of choice
name <- training_sets$names$west    # set this to the region of choice

colr <- training_sets$cols$northsea
training.set$Site <- as.factor(training.set$Site)
ts.sp <- ncol(training.set)
df <- df.split(training.set, ts.sp)
env$colour <- colr[env$Site]
```

Test whether to add extra components by running a WAPLS transfer function

```
fit.wapls <- WAPLS(spec, env$SWLI)
cv.loo <- crossval(fit.wapls, cv.method = "boot", nboot = 1000)
```

Show the outcome to test whether a significant improvement occurs to justify choosing more than one component. An increase of > 5% should occur with a p value < 0.05

```
rand.t.test(cv.loo)
```

##		RMSE	R2	Avg.Bias	Max.Bias	Skill	delta.RMSE	p
##	Comp01	18.72	0.6329	-0.03947	62.83	63.29	-38.573	0.001
##	Comp02	17.73	0.6853	0.19955	62.34	68.41	-5.245	0.009
##	Comp03	17.37	0.7306	0.35585	53.69	72.88	-2.064	0.020
##	Comp04	17.82	0.7372	0.47816	48.31	73.41	2.595	0.358
##	Comp05	19.02	0.7344	0.86683	43.76	72.67	6.753	0.774

Adjust the number of desired components and create a label for later

```
wapls.mod <- 2    # adjust this to fit the best choice of components
main1 = paste("WAPLS Component", wapls.mod, " ")
```

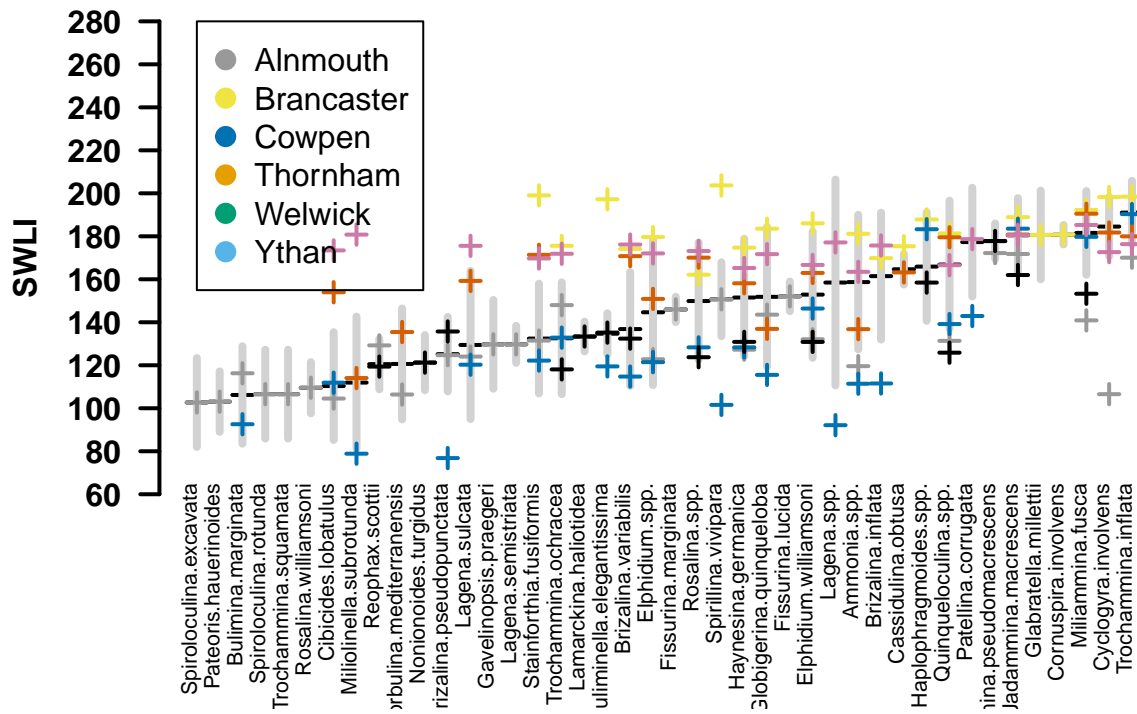
Analysis of training set

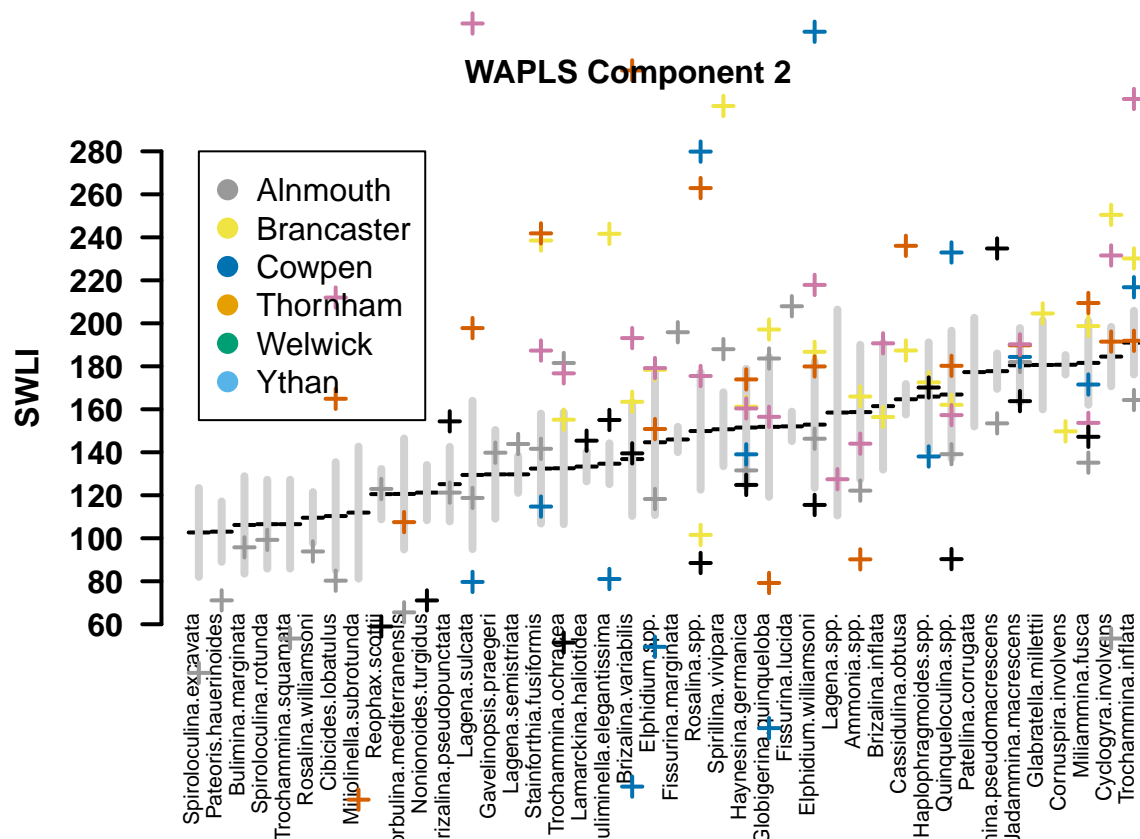
Plot species optimas

Use graham's functions in plot_optimas to plot the species tolerances

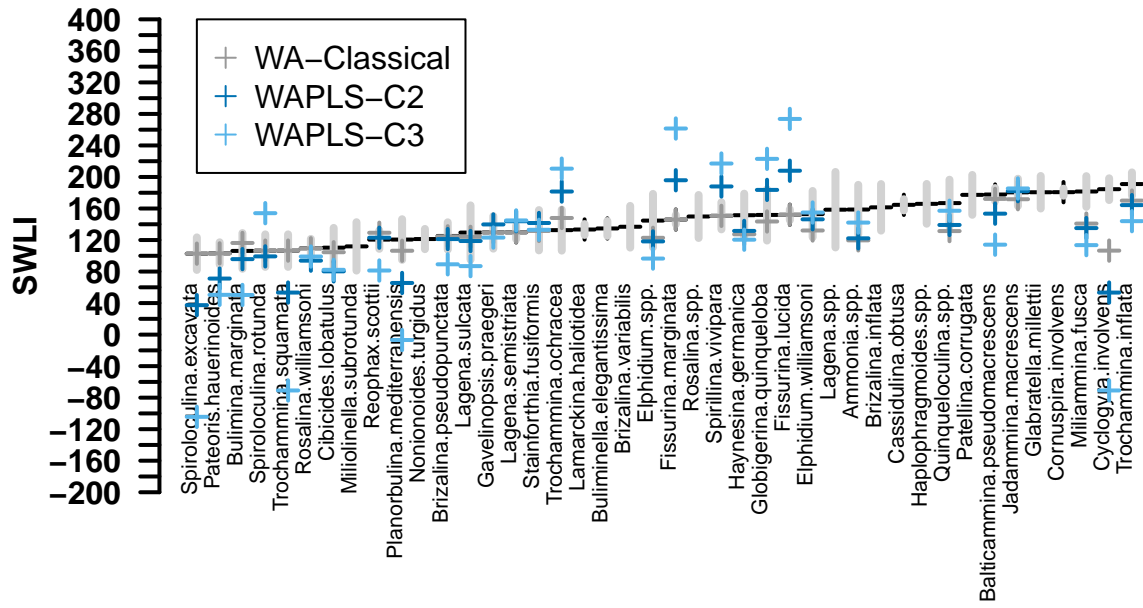
```
plot_species_tolerances(model = 2, y_0 = 60, y_1 = 280, x_1 = ncol(spec), wa = TRUE, wapls = TRUE, comp
```

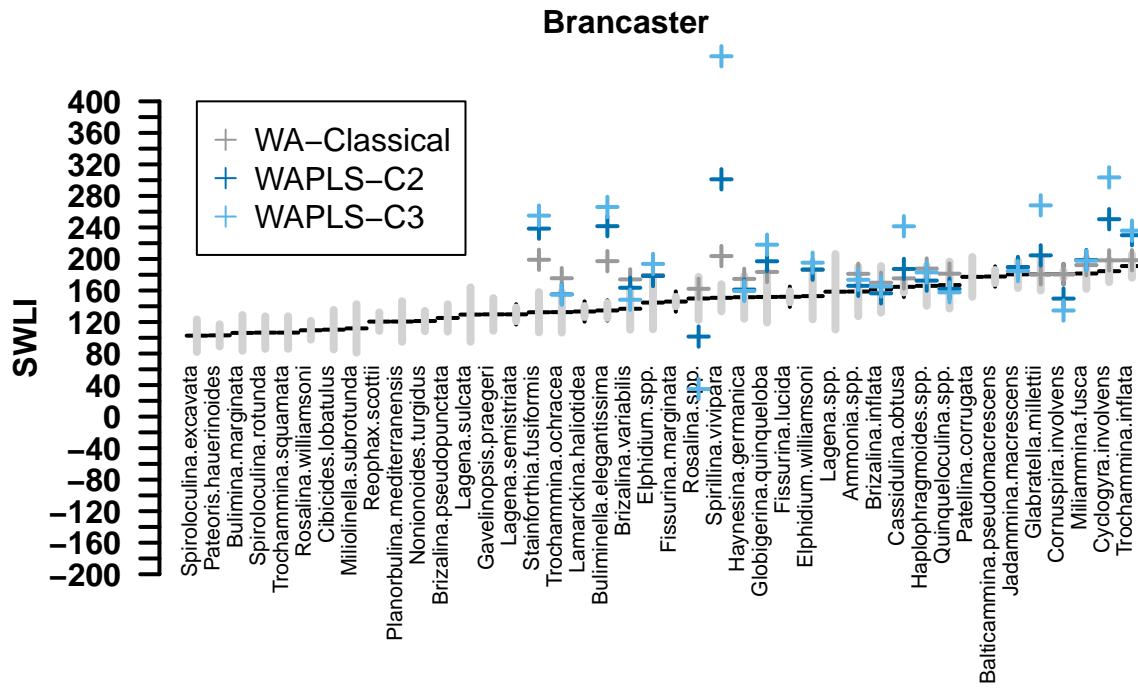
WA Classical

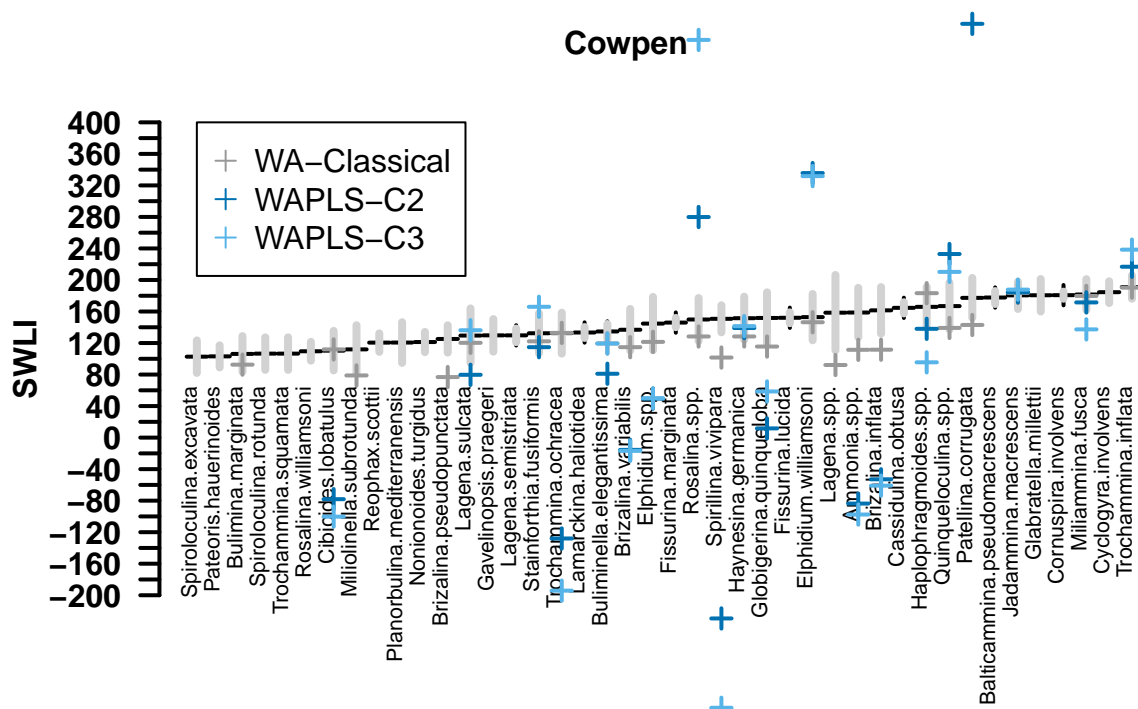


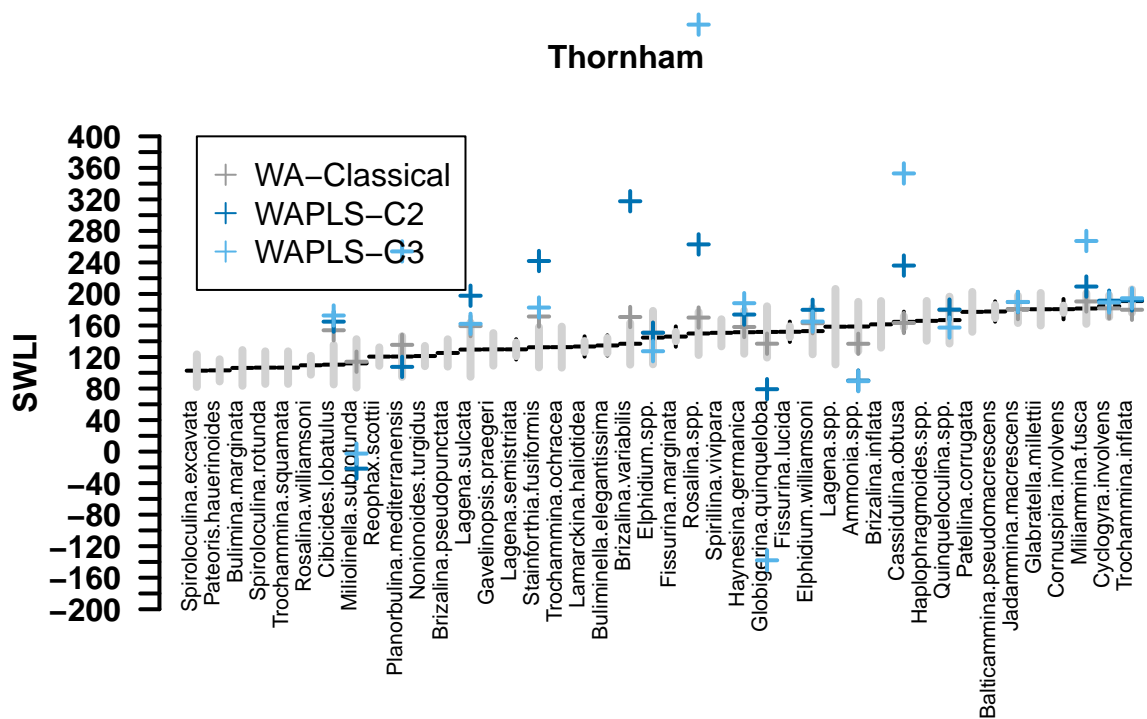


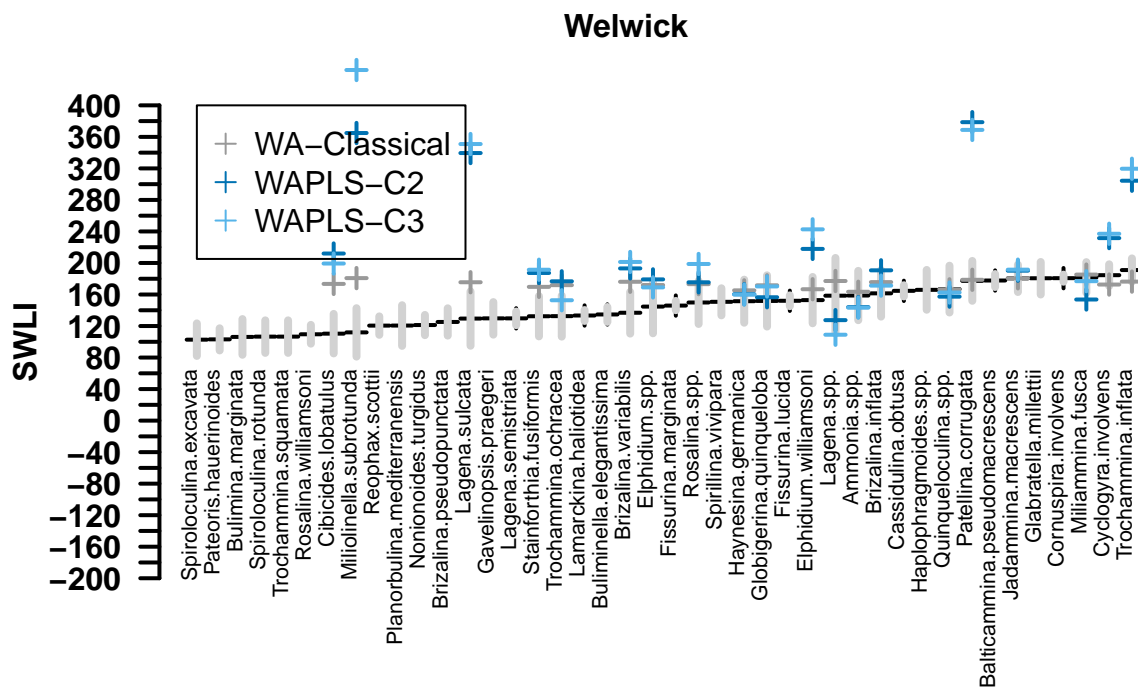
Alnmouth



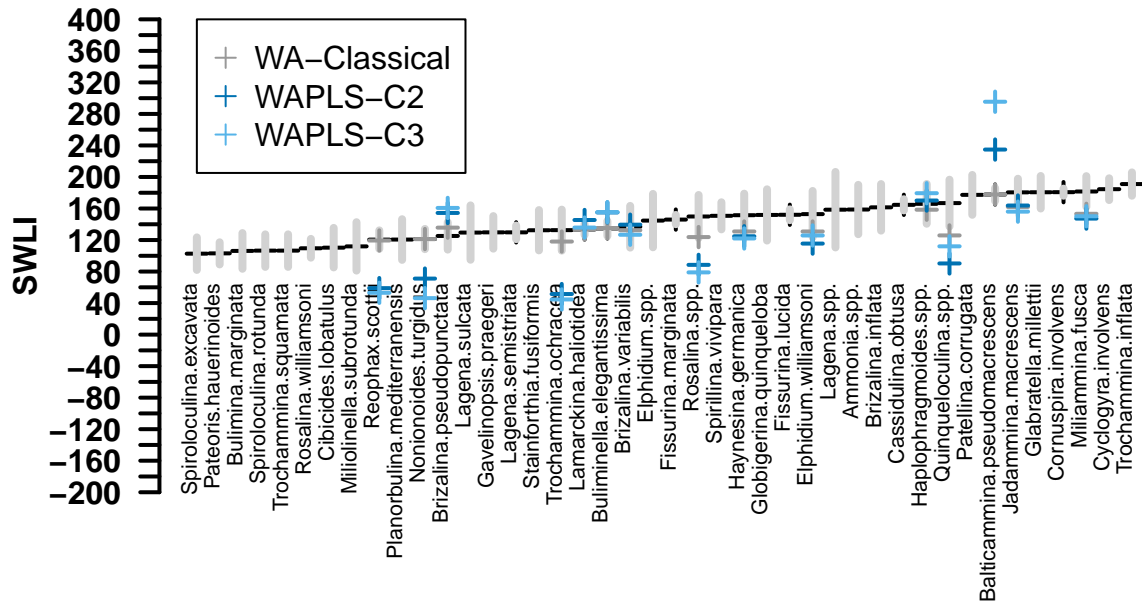








Ythan



Cluster Analysis

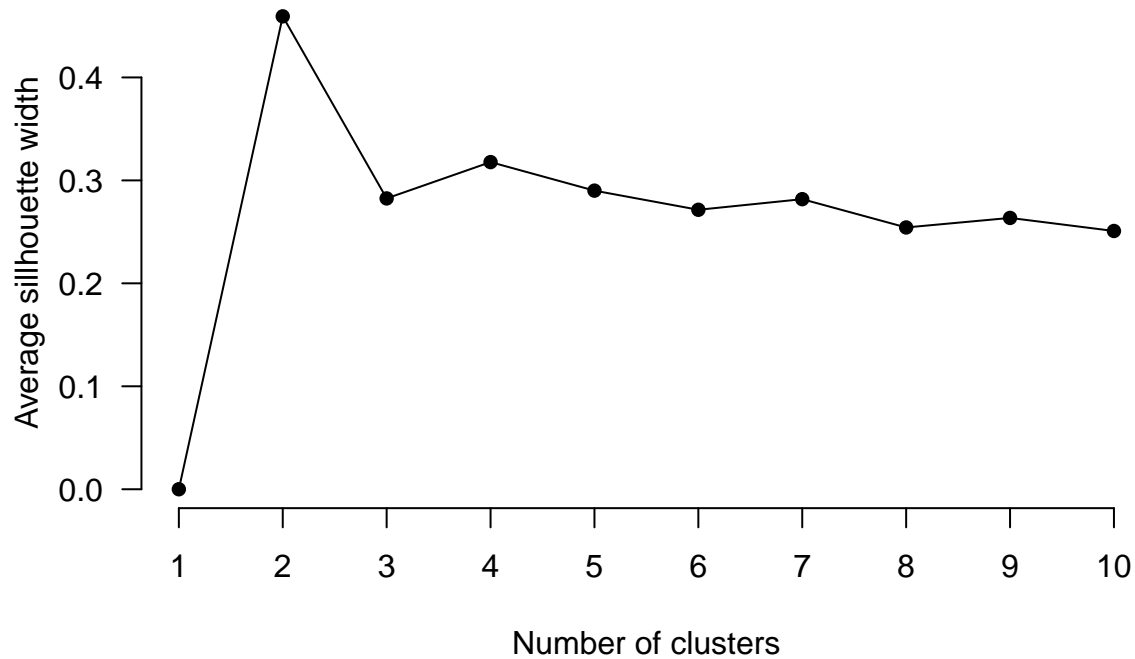
Run the cluster analysis

```
df.split (training.set, ts.sp)      # split the data
dis <- vegdist(spec, "euclidean")    # set distance based on rule. Set this e.g. "bray" is bray curtis
clusters <- pamk(dis, krange = 1:10, criterion = "multiasw", critout = TRUE, metric = "euclidean") #
```

```
## 1 clusters 0
## 2 clusters 0.4593
## 3 clusters 0.2825
## 4 clusters 0.3178
## 5 clusters 0.29
## 6 clusters 0.2714
## 7 clusters 0.2818
## 8 clusters 0.2543
## 9 clusters 0.2636
## 10 clusters 0.2509
```

Plot the clusters in a broken hockey stick using grahams function 'pam_hockey_stick.R'

```
pam_hockey_stick()      # uses grahams functions in pam_hockey_stick to plot broken stick graph to asses
```



Set to the desired number of clusters and plot the clusters using graham's functions in 'plot_pam.R'. Four plots are produced: 1. A silhouette plot, 2. The samples grouped by cluster, plotted against SWLI and coloured by SWLI, 3. The samples grouped by cluster, plotted against SWLI and coloured by site. 4. Boxplot of the clusters against SWLI.

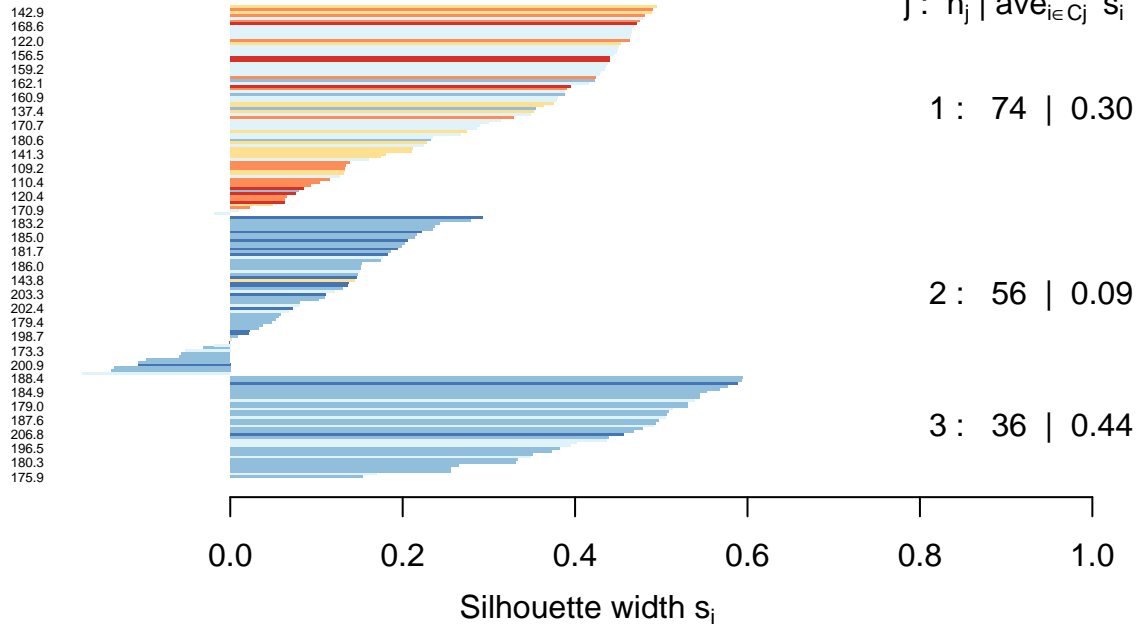
```
cluster <- pamk(dis, krange = 3, criterion = "multiasw", critout = TRUE, metric = "euclidean") # set k
pt <- plot.pamk(k = 3, p2 = TRUE, p3 = TRUE, boxplot = TRUE) # plot the clusters
```

Silhouette plot of pam(x = sdata, k = k, diss = diss, metric = "e

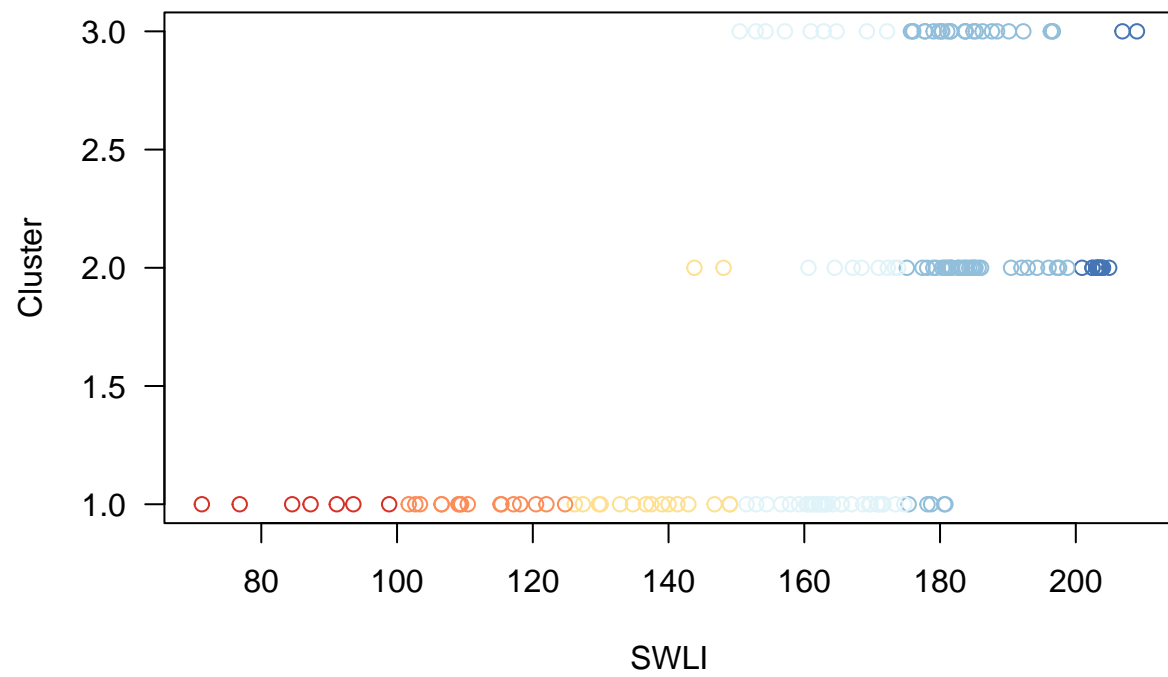
n = 166

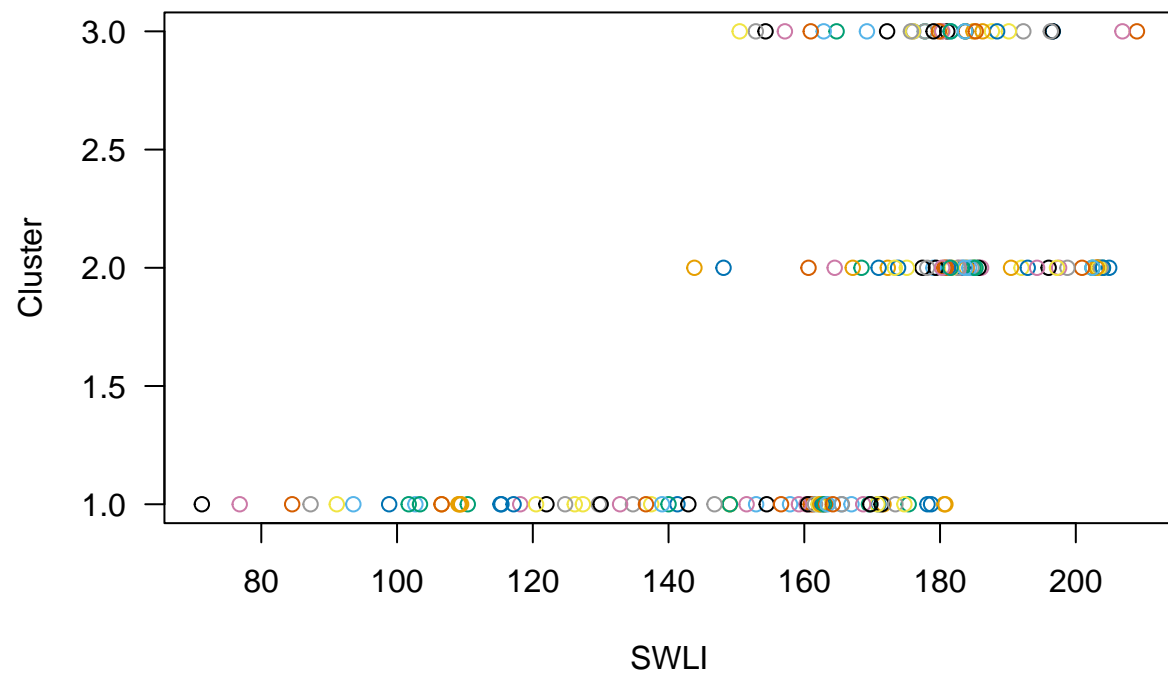
3 clusters C_j

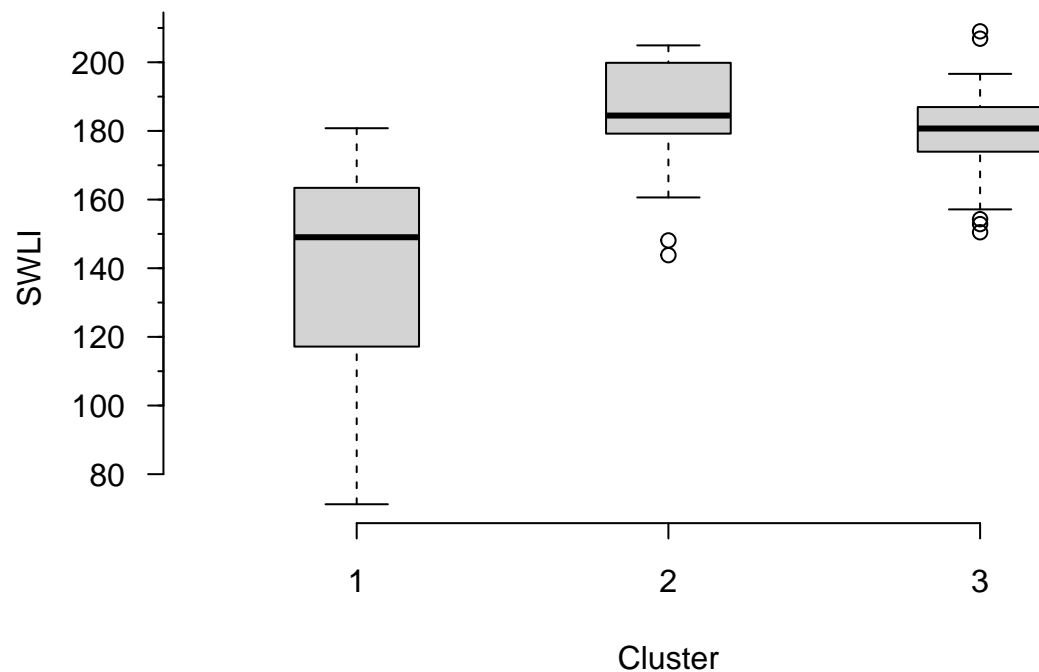
$j : n_j \mid \text{ave}_{i \in C_j} s_i$



Average silhouette width : 0.26







Create a table of the data

```
clustering <- as.data.frame(pt)
clustering
```

```
##   cluster size av.widths max_diss av_diss med_swli min_swli max_swli
## 1      1   74     0.30   78.43   35.31    93.56    71.24   180.8
## 2      2   56     0.09  105.33   33.18   203.08   143.81   204.9
## 3      3   36     0.44   44.61   20.90   181.55   150.48   209.0
```

CCA & DCA

Run correlation analysis to understand the relationships.

```
pcca <- cca(spec, env$SWLI)      # run CCA
w.cca <- round((pcca$CCA$eig / pcca$tot.chi) * 100, 2)  # extract the proportion of variance explained
w.cca      # show the value
```

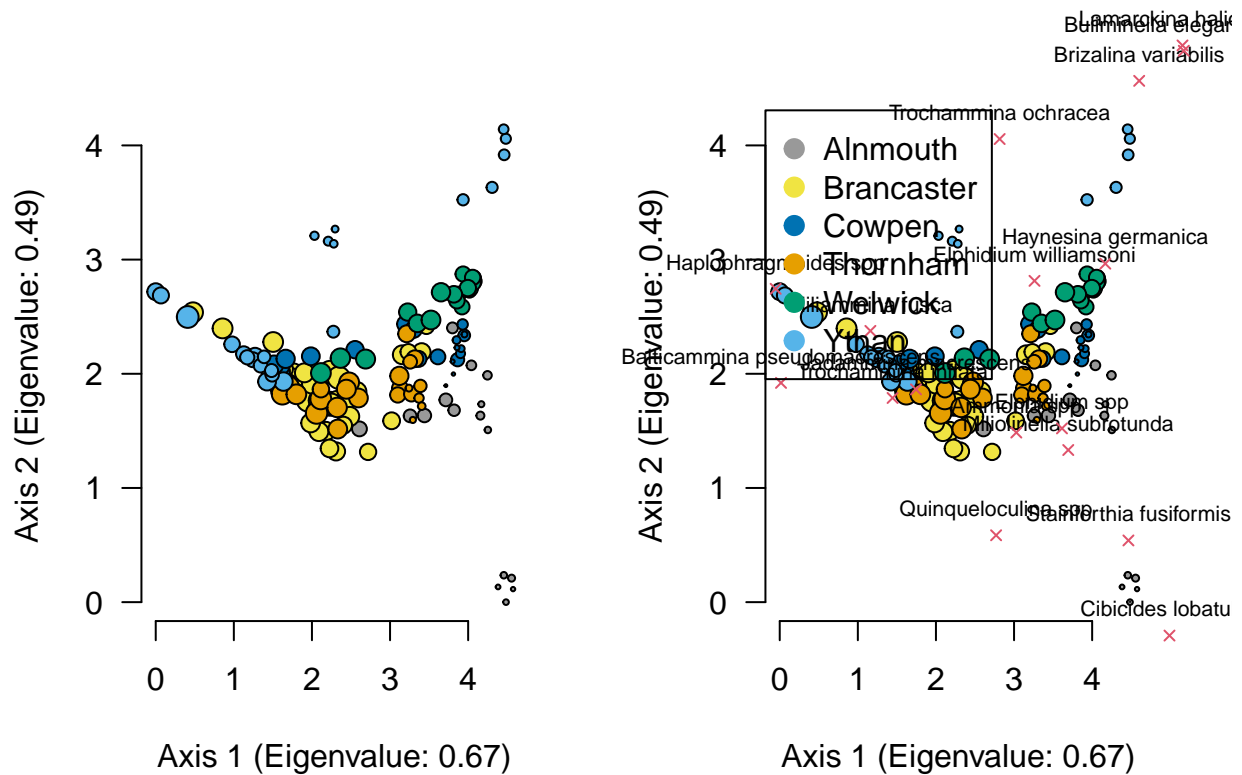
```
## CCA1
## 10.73
```

```
ns.dca <- decorana(veg=spec)     # run dca
ns.dca
```



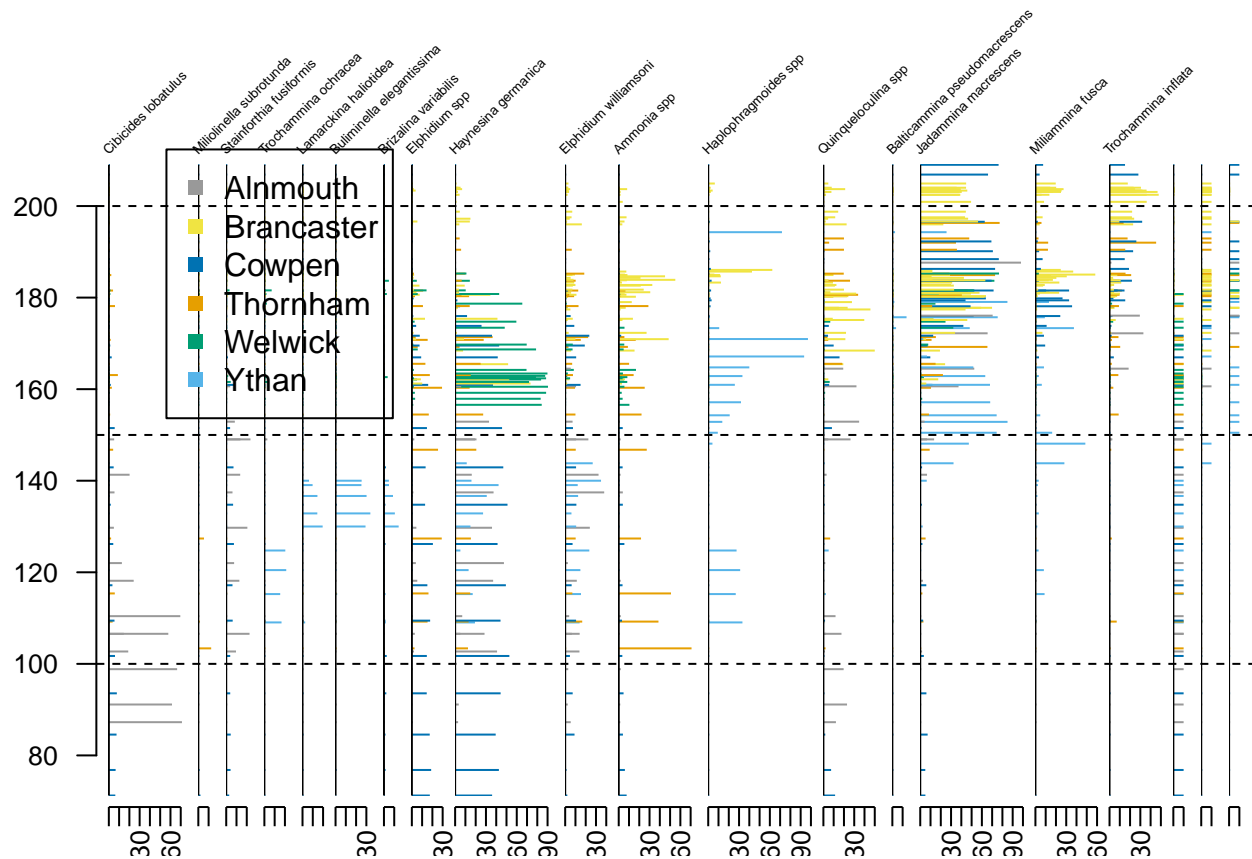
```
##
## Call:
## decorana(veg = spec)
##
## Detrended correspondence analysis with 26 segments.
## Rescaling of axes with 4 iterations.
##
##           DCA1  DCA2  DCA3  DCA4
## Eigenvalues  0.663 0.421 0.239 0.209
## Decorana values 0.670 0.488 0.218 0.127
## Axis lengths  4.575 4.141 2.747 1.821
```

```
plot.new()
plot_dca(origin = T)
```



plot the foram species diagram using grahams function in 'plot_foram_diagram.R'

```
plot_foram_diagram(data = training.set, min.species = 10, clusters = 3, method = "euclidean", plot_zones = T)
```

Perform the transfer functions

WA

```
df.split (training.set, ts.sp)      # split the data
env$colour <- training_sets$cols$northsea[env$Site]

fit.wa <- WA(spec,env$SWLI, toldW = T)      # run the WA transfer function
cv <- crossval(fit.wa, cv.method = "boot", nboot = 1000)      # perform cross-validation using bootstrapping
cv.wa.loso <- crossval(fit.wa, cv.method = "lgo", ngroups = env$Site)      # perform cross-validation using
test.wa <- as.data.frame(rand.t.test(cv))
```

```
test.wa      # show results
```

##		RMSE	R2	Avg.Bias	Max.Bias	Skill	delta.RMSE	p
##	WA.inv	18.74	0.6324	-0.028159	62.68	63.24	NA	NA
##	WA.cla	22.66	0.6344	0.007916	50.72	47.25	NA	NA
##	WA.inv.tol	17.78	0.6745	-0.340427	64.37	67.42	-5.120	0
##	WA.cla.tol	20.73	0.6757	-0.402279	55.15	56.85	-8.537	0

WAPLS

```
fit.wapls <- WAPLS(spec,env$SWLI)      # run the WAPLS transfer function
cv.loo <- crossval(fit.wapls, cv.method= "boot", nboot = 1000)  # perform cross-validation using boots
cv.loso <- crossval(fit.wapls, cv.method= "lgo", ngroups = env$Site)  # perform cross-validation usin
test.wapls.loo <- as.data.frame(rand.t.test(cv.loo))
test.wapls.loso <- as.data.frame(rand.t.test(cv.loso))
```

```
test.wapls.loo      # show results
```

```
##           RMSE      R2 Avg.Bias Max.Bias Skill delta.RMSE      p
## Comp01 18.74 0.6323 -0.03585   62.60 63.23   -38.489 0.001
## Comp02 17.79 0.6844  0.20010   62.00 68.32    -5.099 0.020
## Comp03 17.32 0.7309  0.32536   53.48 72.92    -2.605 0.018
## Comp04 17.65 0.7387  0.41108   47.78 73.60     1.915 0.291
## Comp05 18.52 0.7359  0.82169   43.04 72.86     4.886 0.758
```

LW

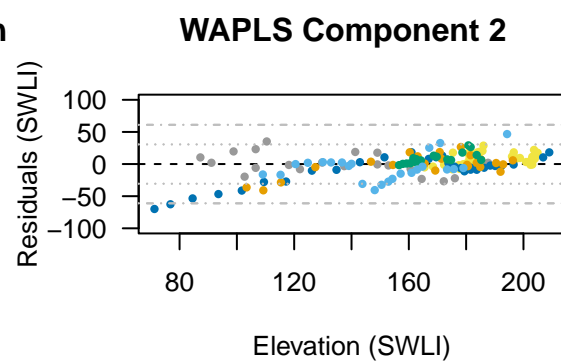
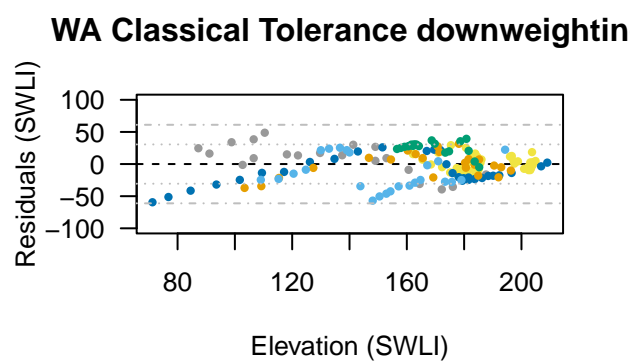
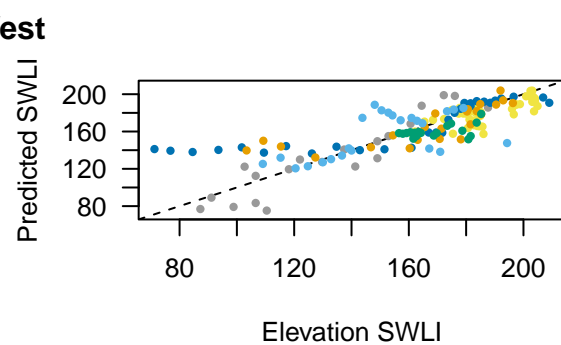
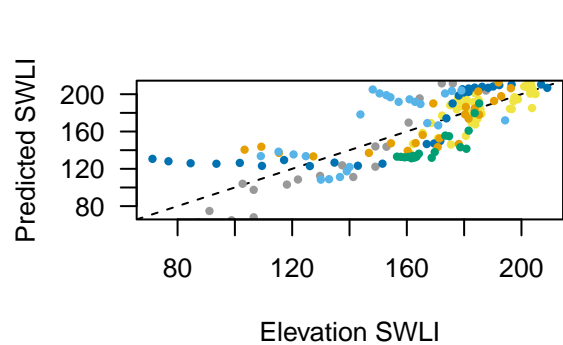
```
fit.lw <- LWR(spec, env$SWLI, FUN=WAPLS, dist.method="sq.chord", k=50)  # run the locally weighted tr
cv.lw <- crossval(fit.lw, cv.method="boot", nboot = 100)  # cross validate the results using bootstra
```

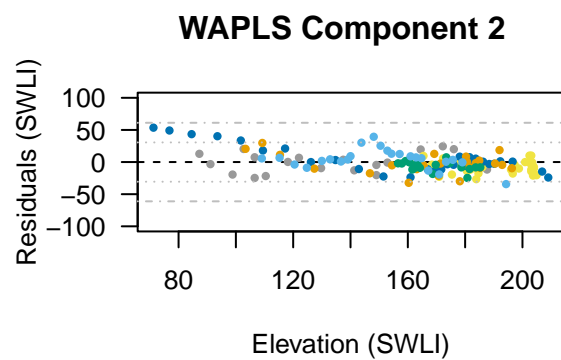
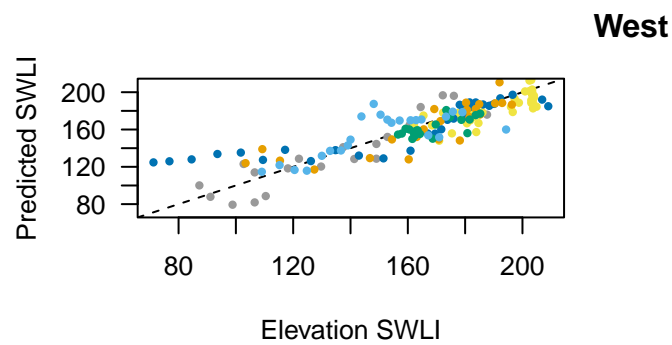
```
cv.lw      # show the results
```

```
##
## Method : Locally Weighted Regression
## Call    : LWR(y = y, x = x, FUN = WAPLS, dist.method = "sq.chord", k = 50,
##      lean = TRUE)
## Distance      : sq.chord
## No. samples   : 166
## No. species   : 42
## No. local     : 50
##
## Performance:
##           RMSE      R2 Avg.Bias Max.Bias Skill
## Comp01      16.16 0.7201  0.3628   56.27 71.87
## Comp02      13.70 0.8013  1.5608   43.15 79.77
## Comp03      13.64 0.8011  1.1919   37.77 79.95
## Comp04      14.36 0.7790  0.6328   37.41 77.78
## Comp05      16.13 0.7297  0.6771   39.03 71.97
## Comp01_XVal 17.63 0.6674  1.4233   60.28 66.51
## Comp02_XVal 14.77 0.7680  1.6195   48.69 76.52
## Comp03_XVal 13.77 0.7966  0.6810   37.83 79.58
## Comp04_XVal 14.02 0.7894  0.7923   34.97 78.83
## Comp05_XVal 14.37 0.7786 -0.0464   33.43 77.77
```

Plot the residuals and predictions against the true value with 1 and 2 standard deviations shown using grahams functions in 'plot_cross_validation.R'

```
plot_residuals(wa.mod = 2, zoom = TRUE)  # set to the desired wa deshrinking method. 2 = classical
plot_residuals_lw(model = 2, zoom = TRUE)
```





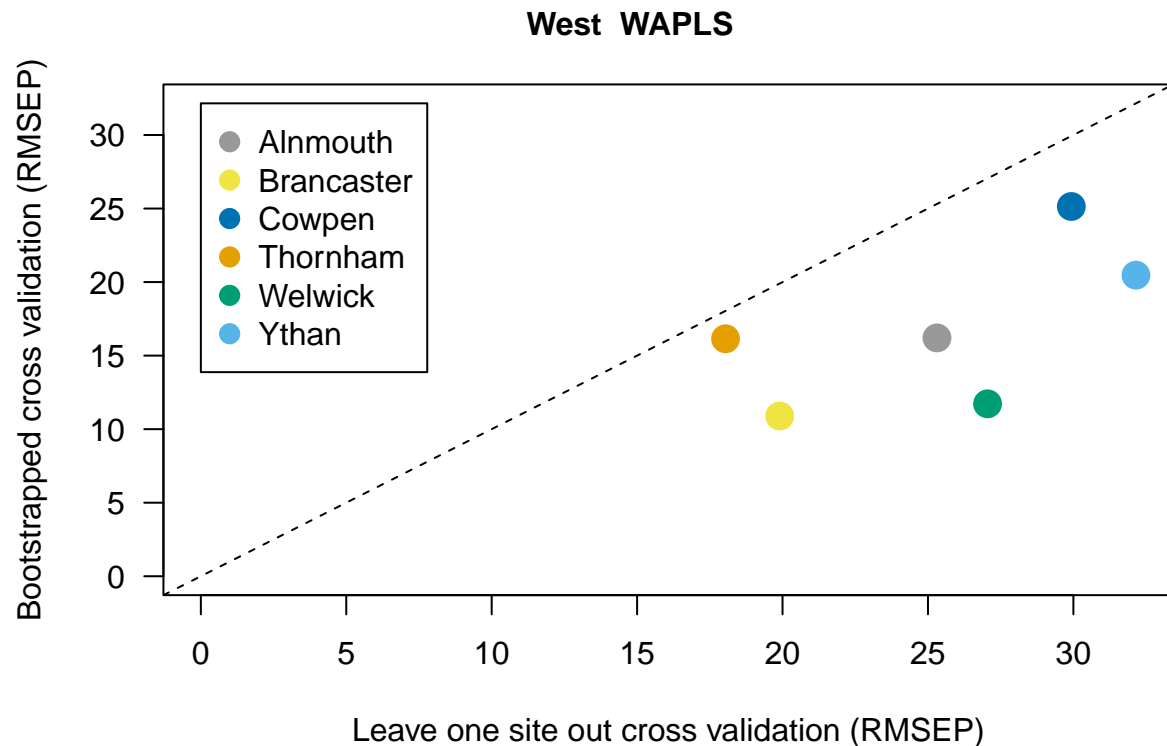
Compare cross-validation using leave-one-site-out using Grahams function in 'loso.R'

```
compare <- loso(wapls.mod, name)
```

```
##           L00  LOS0      Site
## Alnmouth  16.20 25.31  Alnmouth
## Brancaster 10.89 19.90 Brancaster
## Cowpen    25.14 29.93   Cowpen
## Thornham   16.15 18.04  Thornham
## Welwick   11.72 27.05   Welwick
## Ythan     20.47 32.15   Ythan
```

Plot the bootstrapping and loso cross-validation

```
plot_loso (zoom = TRUE, text = FALSE)
```



Save the results using Grahams function 'saver.R'

```
results <- saved(region = reg, method = paste("WAPLS-C", wapls.mod))
file_name <- paste("results/", "tf_", reg, ".csv", sep = "")
write.csv(results, file_name)
file_name <- paste("results/", "WAPLS-C", wapls.mod, "-compare-", reg, ".csv", sep = "")
write.csv(compare, file = file_name)
```

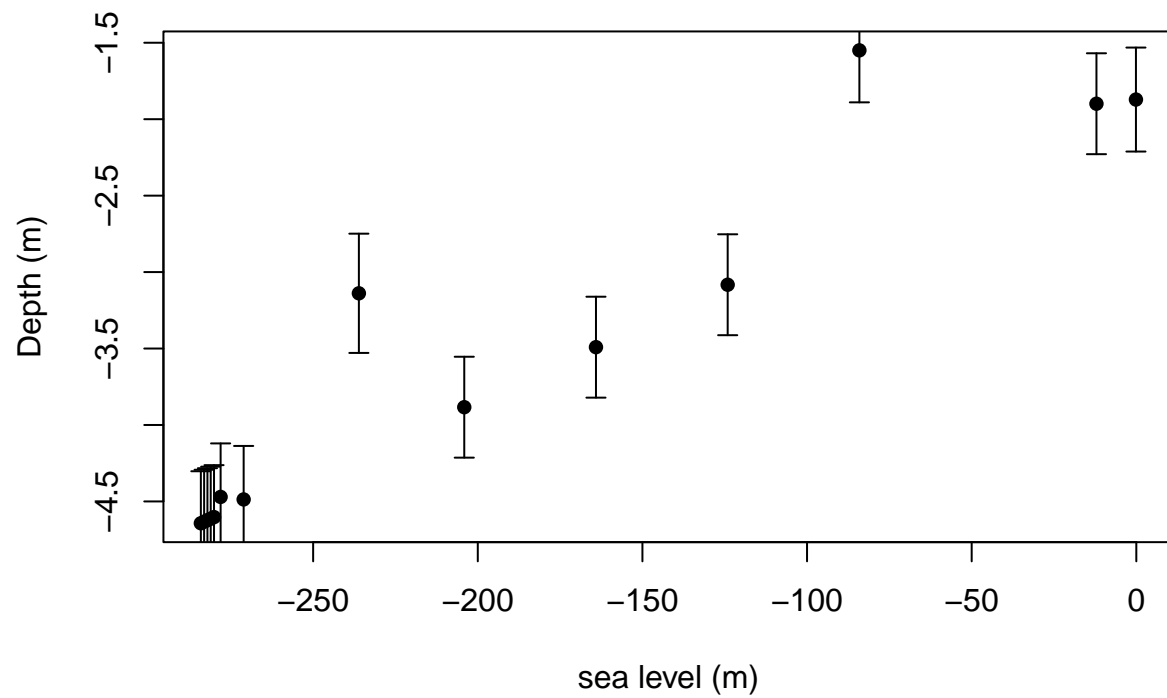
Perform the reconstructions

Clean the core using grahams function in 'cleaning.R'

```
core_clean <- clean_core(core = core_data, s = 15, td = 1, rare = F, f = F)
core <- c.split (core_clean, s = 9) # split the core to species and environmental data. 15 is the last
```

Predict the SWLI for core samples using WA using grahams function in 'Reconstructions.R' Change the components to match the deshrinking method

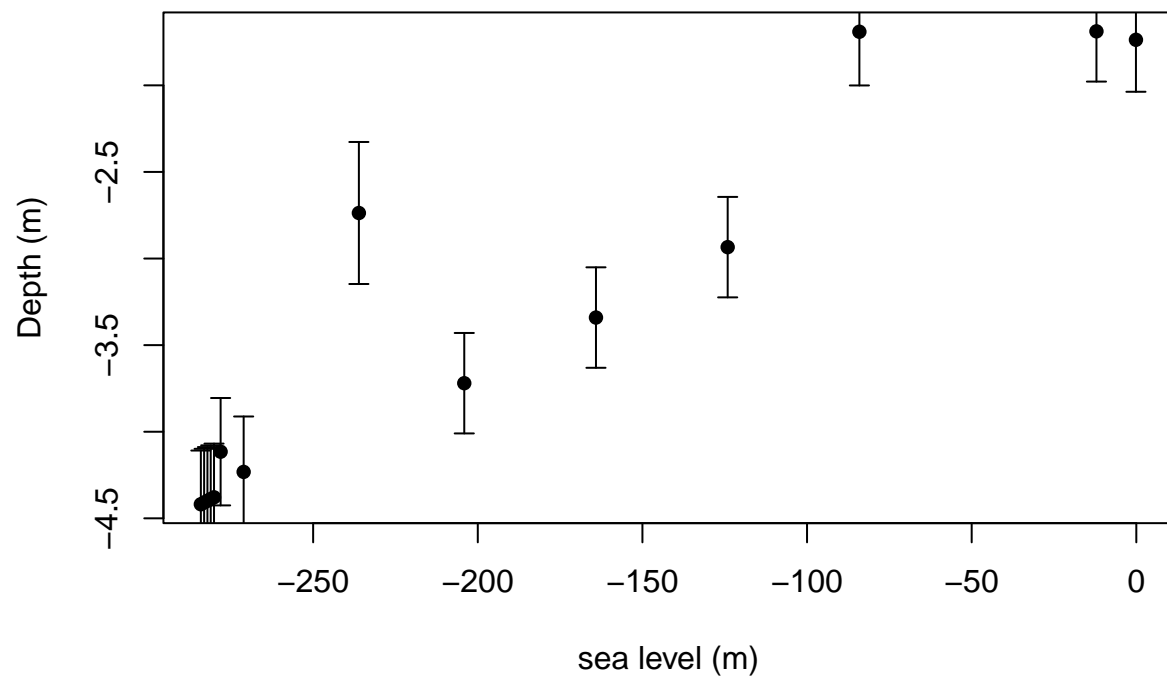
```
prediction_wa <- reconstruct_core(core = core, tf = fit.wa, components = 4, species = 9, mhhw = 1.95, m
```



```
core_clean <- cbind(core_clean, prediction_wa) # add to the data
```

Predict the SWLI for core samples using WAPLS using grahams function in 'Reconstructions.R' Change the components to match the components

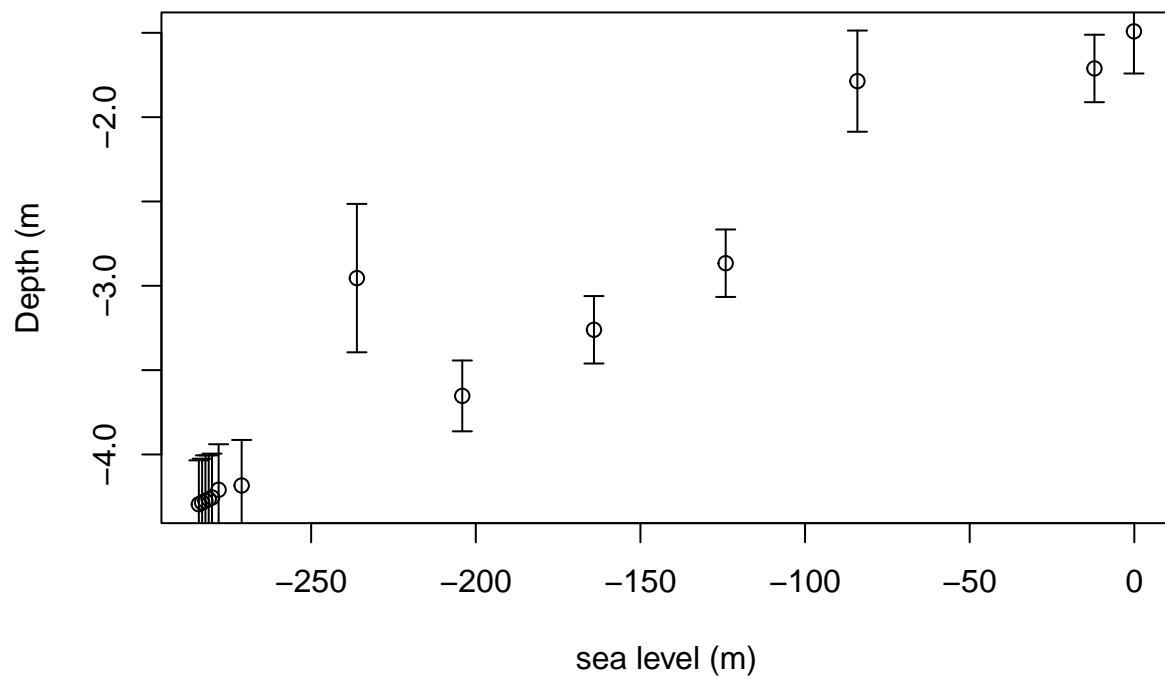
```
prediction_wapls <- reconstruct_core(core = core, tf = fit.wapls, components = 2, species = 9, mhhw = 1
```

```
core_clean <- cbind(core_clean, prediction_wapls) # add to data for exporting and comparison
```

Predict the SWLI for core samples using Locally weighted - WAPLS

```
prediction_lw <- run_lw_tf(n_analogues = 30, components = 2, tf = WAPLS, species = 9, mhhw = 1.95, mtl = 1.95)
```

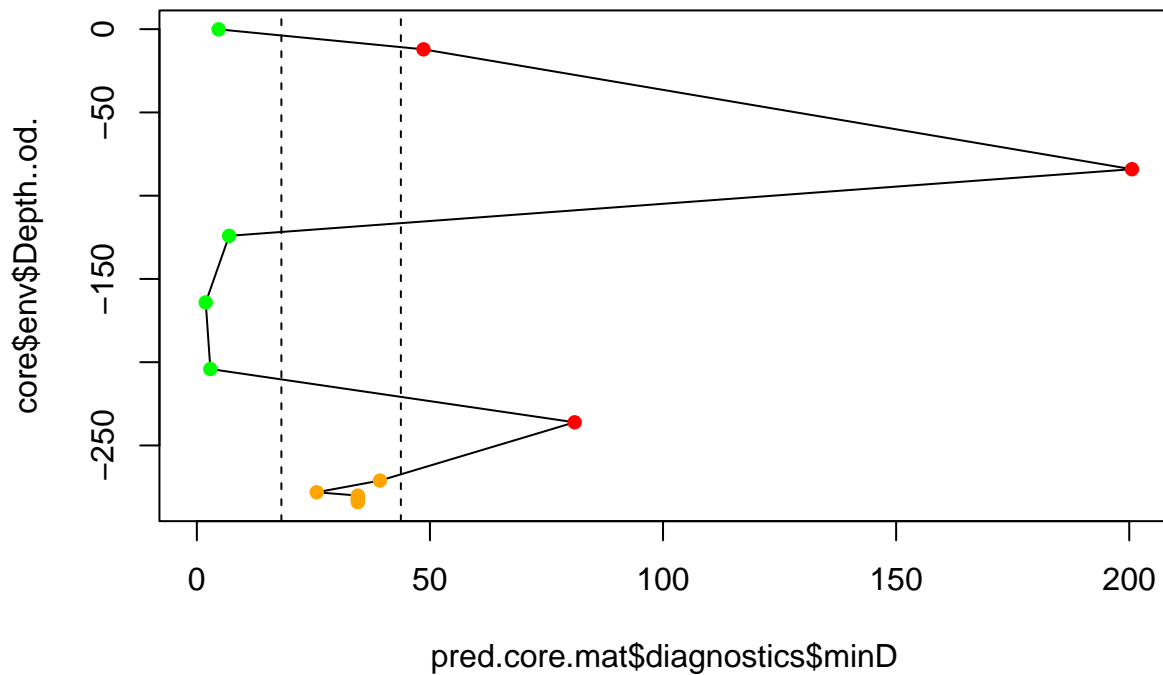


```
core_clean <- cbind(core_clean, prediction_lw$sea_level)    # add to the data -->
```

-> ->

Test the analogues. using MAT or goodness of fit using grahams functions in 'test-mat.R'

```
mat <- run.mat(z = 50, d = "sq.chord", plot = TRUE)    # run the mat.
```



```
core_clean <- cbind(core_clean, mat$mat)      # add to the data
# gof <- goodness_of_fit(plot = TRUE)        # run the goodness of fit
# core_clean <- cbind(core_clean, gof)        # add to the data
```

Save the results for each region

```
file_name <- paste("results/", "reconstructions_", reg, ".csv", sep = "")
write.csv(core_clean, file_name)
```

Test whether the reconstructions are significant

```
ralgh <- randomTF(spp = spec, env = env$SWLI, fos = core$spec, n = 99, fun = WAPLS, col = 2)
ralgh.wa <- randomTF(spp = spec, env = env$SWLI, fos = core$spec, n = 99, fun = WA, col = 2)
ralgh$sig      # show the data
```

```
## env
## 0.77
```

```
ralgh.wa$sig    # show the data
```

```
## env
## 0.72
```