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##### R-Script explaining manual forward selection #####

# The manual forward selection has the objective to identify environmental parameters where each
# explains a separate dimension of variance in the taxa data (i.e. that show no collinearity between
# each other). By following this procedure, we will obtain a set of independent forcing variables that
# drive the taxa assemblage.

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# Ranking the 6 parameters by eigenvalue (the amount of taxa variance they explain):

rda(TAXA ~ PARAMETER.X, data=ENVI)

# Result: SSTsummer (12.7%), Sealce (9.7%), SSSsummer (6.9%), PPsummer (4.6%), PPannual
# (4.2%), PPspring (2.5%)

# Evaluating the independence between all 6 parameters:
# To this end we calculated Variance Inflation Factors (VIF), expressing how much of the taxa
# variance explained by one environmental variable is already explained by another parameter. The
# VIF of a variable is calculated from the multiple correlations (r) among the environmental variables
# (ter Braak and Smilauer 2002), using the equation  $VIF = 1/(1-r^2)$ . We chose a cut-off value of  $VIF \leq 2$ 
# for all parameters as also suggested in other studies (e.g., Lopes et al. 2010). Such a VIF value only
# allows collinearities of  $r^2 \leq 0.5$  and thus not more than half of the variance in the taxa data explained
# by one variable to also be explained by another variable.

# Now we start with the actual forward selection:
# After ranking the 6 variables by their eigenvalue we start with the first one and add step-by-step
# another variable and check if the VIF's < 2.

n.rda <- rda(TAXA ~ SSTsummer+Sealce, data=ENVI)
vif.cca(n.rda)

# VIF < 2? YES
# Result:      SSTsummer   Sealce
#           1.78         1.78
# Taxa variance explained: 18.7%

# Proceede with the above model and add the next parameter:

n.rda <- rda(TAXA ~ SSTsummer+Sealce+SSSsummer, data=ENVI)
vif.cca(n.rda)

# VIF < 2? NO
# Result:      SSTsummer   Sealce      SSSsummer
#           2.13         2.60         1.46
# We find that two parameters show too much collinearity. To decide which parameters to keep and
# which to exclude from the set of independent forcing variables, we check which model explains more
# taxa variance and how large the VIFs are:

n.rda<-rda(TAXA ~ SSTsummer+Sealce, data=ENVI)
# Taxa variance explained: 18.7%   VIFs: SSTsummer 1.78 Sealce 1.78

n.rda<-rda(TAXA ~ SSSsummer+Sealce, data=ENVI)
# Taxa variance explained: 17.5%   VIFs: SSSsummer 1.23 Sealce 1.23

n.rda<-rda(TAXA ~ SSSsummer+SSTsummer, data=ENVI)
# Taxa variance explained: 19.6% VIFs: SSTsummer 1.00 SSSsummer 1.00

# The model including SSTsummer and SSSsummer (excluding Sealce) is the better model explaining
# the largest amount of taxa variance and showing the highest amount of independence.
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# Note:
# We exclude Sealce from our dataset because it does not explain a separate dimension of variance
# in taxa assemblages within the regional Baffin Bay dataset. This does not mean, that it cannot be
# reconstructed or does not explain taxa variance! However, our analysis suggests that SSTsummer
# and Sealce "play the same part" in driving assemblage compositions, meaning that by
# reconstructing one we actually reconstruct a "mixture" of SSTsummer and Sealce. This is
# strengthened by the result of the MFA where we detected SST on the one end of the first dimension
# and Sealce on the other end. However, to calibrate an independent dataset, we need to decide
# between SSTsummer and Sealce. Statistics favour SSTsummer. But, we have to bear in mind when
# applying the independent calibration dataset that the SSTsummer parameter is a place holder for
# several temperature parameters like SSTsummer, Sealce and presumably others.
```

```
# Proceede with the best performing model and add the next variable
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```
n.rda <- rda(TAXA ~ SSTsummer+SSSummer+Ppsummer, data=ENVI)
vif.cca(n.rda)
```

```
# VIF < 2? NO
```

```
# Result:      SSTsummer   SSSsummer   Ppsummer
#             1.87         1.22         2.08
```

```
# We follow the same procedure as above: Which model explains more variance and how large are
# the VIFs?
```

```
n.rda <- rda(TAXA ~ SSSsummer+Ppsummer, data=ENVI)
# Taxa variance explained: 10.2%   VIFs: SSSsummer 1.11 Ppsummer 1.11
```

```
n.rda <- rda(TAXA ~ SSTsummer+SSSummer, data=ENVI)
# Taxa variance explained: 19.6%   VIFs: SSTsummer 1.00 SSSsummer 1.00
```

```
n.rda <- rda(TAXA ~ SSTsummer+Ppsummer, data=ENVI)
# Taxa variance explained: 17.6%   VIFs: SSTsummer 1.71 Ppsummer 1.71
```

```
# Proceede with the best performing model and add the next variable
```

```
n.rda <- rda(TAXA ~ SSTsummer+SSSummer+Ppannual, data=ENVI)
vif.cca(n.rda)
```

```
# VIF < 2? NO
```

```
# Result:      SSTsummer   SSSsummer   Ppannual
#             2.11         1.09         2.19
```

```
# We follow the same procedure as above: Which model explains more variance and how large are
# the VIFs?
```

```
n.rda <- rda(TAXA ~ SSSsummer+Ppannual, data=ENVI)
# Taxa variance explained: 10.4%   VIFs: SSSsummer 1.04 Ppannual 1.04
```

```
n.rda <- rda(TAXA ~ SSTsummer+SSSummer, data=ENVI)
# Taxa variance explained: 19.6%   VIFs: SSTsummer 1.00 SSSsummer 1.00
```

```
n.rda <- rda(TAXA ~ SSTsummer+Ppannual, data=ENVI)
# Taxa variance explained: 17.7%   VIFs: SSTsummer 2.01 Ppsummer 2.01
```

```
# Proceede with the best performing model and add the next (last) variable
```

```
n.rda <- rda(TAXA ~ SSTsummer+SSSummer+Ppspring, data=ENVI)
vif.cca(n.rda)
```

```
# VIF < 2? YES
```

```
# Result:      SSTsummer   SSSsummer   Ppspring
#             1.81         1.00         1.81
```

```
# Taxa variance explained: 23.6%
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Final results:

- # - The final model is SSTsummer+SSSummer+PPspring
- # - Each of the three parameters explain an independent part of the variance in the assemblage composition, while together explaining 23.6% of the total taxa variance
- # - Sealce is excluded as it presumably explains the same part of the variance as SSTsummer
- # - SSTsummer reconstructions will reflect Sealce reconstructions (if we had decided to keep Sealce, Sealce reconstructions would reflect SSTsummer changes)
- # - PPannual and PPspring are excluded as they presumably explain the same part of the variance as PPspring does
- # - In the local calibration dataset we find three "signals" in the taxa variance regarding the 6 parameters we took into account.

References:

ter Braak, C.J.F., Smilauer, P., 2002. CANOCO Reference Manual and User's Guide to Canoco for Windows: Software for Canonical Community Ordination (Version 4.5), Microcomputer Power. Microcomputer Power, Ithaca, New York, U.S.A.

Lopes, C., Mix, A.C., Abrantes, F., 2010. Environmental controls of diatom species in northeast Pacific sediments. *Palaeogeogr. Palaeoclimatol. Palaeoecol.* 297, 188–200.
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