Transfer functions — Weighted averaging and all that

Gavin Simpson
(gavin.simpson@ucl.ac.uk)

Environmental Change Research Centre, UCL

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Outline

1. Motivating Examples
2. Introduction
3. Weighted Averaging
4. Modern Analogue Technique
5. Model performance and diagnostics

Example 1: Was acid rain to blame for acid lakes?

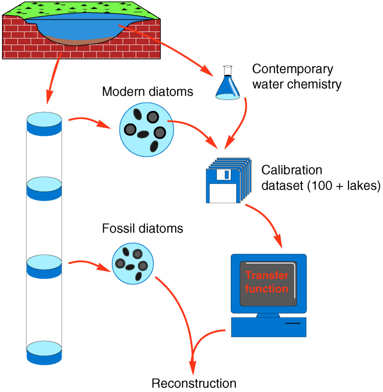
- In the 1970s and early 1980s there was a great deal of concern about acid lakes and rivers in northern Europe
- Driven mainly by losses of Salmon in Scandinavian rivers, this was a major political hot potato
- A vast amount of money was expended to determine the cause of the acidification — was it due to acid emissions from power stations or some other cause?
- Palaeolimnological data provided conclusive proof that acid deposition was the cause
- In Europe, the Surface Waters Acidification Project (SWAP) was a major contributor to the debate
- Diatoms collected from 167 lakes across UK, Norway, Sweden and associated water chemistry
- Can we predict lake-water pH from the diatom species assemblages?
- Apply to diatoms counted from a sediment core from the Round Loch of Glenhead (RLGH) covering most of the Holocene

Example 2: Reconstructing past sea surface temperatures

- Sea surface temperatures are related to global air temperatures
- An important arm of palaeoceanography is involved in reconstructing past climates from various proxies
- These past climates tell use how the world responded to previous climatic shifts and provide targets for climate modellers to try to model
- The data set here is the Imbrie & Kipp data set — the data set that started it all!
- 61 core-top samples from ocean cores, mainly from Atlantic
- 27 species of planktonic foraminifera were identified in the core-top samples
- Summer and Winter sea surface temperatures (SST) and sea water salinity values measured at each of the 61 core locations
- Applied to reconstruct SST and salinity for 110 samples from Core V12-133 from the Caribbean

Palaeoecological transfer functions

- Transfer functions
- Calibration
- Bioindication
- Aim is to predict the environment from observations on species environment
- The reverse of constrained ordination from yesterday
- ter Braak (1995) *Chemometrics and Intelligent Laboratory Systems* **28**: 165–180


Contemporary water chemistry
Modern diatoms
Calibration dataset (100 + lakes)
Fossil diatoms
Transfer function
Reconstruction

Palaeoecological transfer functions

- More formally we have
  - Matrix of species abundances, $\mathbf{Y}$
  - Vector of observations of an environmental variable, $\mathbf{x}$
- Assume $\mathbf{Y}$ is some function f of the environment plus an error term

$$\mathbf{Y} = f(\mathbf{x}) + \varepsilon$$

- In the classical approach f is estimated via regression of $\mathbf{Y}$ on $\mathbf{x}$
- Then invert f, (f^{-1}) to yield estimate of environment $\mathbf{x_0}$ from fossil species assemblage $\mathbf{y_0}$

$$\hat{\mathbf{x}}_\mathbf{0} = f(\mathbf{y_0})^{-1}$$

- In all but simplest cases f^{-1} doesn't exist and must be estimated via optimisation

Palaeoecological transfer functions

- To avoid problems of inverting f, the indirect approach directly estimates the inverse of f, here g, from the data by regression $\mathbf{x}$ on $\mathbf{Y}$

$$\mathbf{x} = g(\mathbf{Y}) + \varepsilon$$

- We do not believe that the species influence their environment!
- This is just a trick to avoid having to estimate f
- The predicted environment for a fossil sample $\mathbf{y_0}$ is

$$\hat{\mathbf{x}}_\mathbf{0} = g(\mathbf{y_0})$$

Assumptions of palaeoecological transfer functions

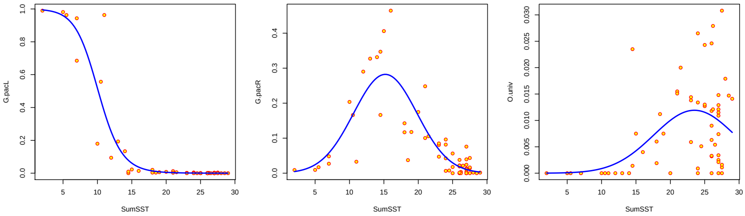
- Taxa in training set are systematically related to the environment in which they live
- Environmental variable to be reconstructed is, or is linearly related to, an ecologically important variable in the ecosystem
- Taxa in the training set are the same as in the fossil data and their ecological responses have not changed significantly over the timespan represented by the fossil assemblages
- Mathematical methods used in regression and calibration adequately model the biological responses to the environment
- Other environmental variables have negligible influence, or their joint distribution with the environmental variable of interest is the same as in the training set
- In model evaluation by cross-validation, the test data are independent of the training data — the secret assumption until Telford & Birks (2005)

Different types of transfer functions

- There are a large number of transfer function models
- Many motivated from chemometrics, but modified to deal with non-linear species responses
- Partial least squares (PLS) and WA-PLS
- Mutual Climate Range method
- So-called maximum likelihood method (Multivariate Gaussian logistic regression)
- Two of the most used (except WA-PLS) are
  - Weighted Averaging (WA)
  - Modern Analogue Technique (MAT)
  - These are the two techniques we will investigate today
- Large number of potential techniques from machine learning, bioinformatics, that have yet to be investigated

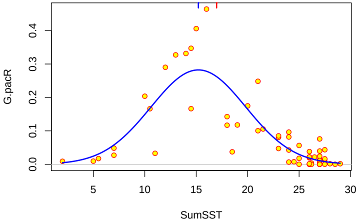
Weighted averaging

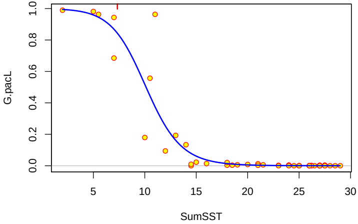
- Species don't respond in simple ways to *environmental gradients*
- Maximum likelihood method fitted Gaussian curves to each species and then numerical optimisation used to predict for fossil samples
- Computationally very intensive, especially when doing cross-validation
- Weighted averaging is an approximation to this maximum likelihood approach



Weighted averaging

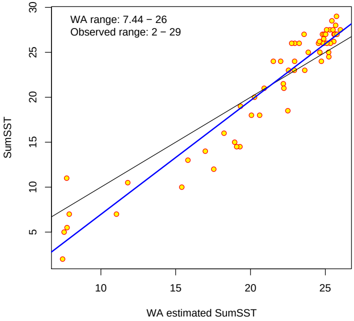
- A very simple idea
- In a lake, with a certain pH, a species with their pH optima close to the pH of the lake will tend to be the most abundant species present
- A simple estimate of the a species' pH optimum is an average of all the pH values for lakes in which that species occurs, weighted by their abundance
- An estimate of a lake's pH is the weighted average of the pH optima of all the species present, again weighted by species abundance





Deshrinking

- By taking averages twice, the range of predicted values is smaller than the observed range
- Deshrinking regressions stretch the weighted averages back out to the observed range
- Can do inverse or classical regressions
  - inverse: regress gradient values on WA's
  - classical: regress WA's on gradient values
  - Vegan also allows to just make variances equal
- Inverse and classical regression remove both bias and error, equalising variances deshrinks without adjusting the bias



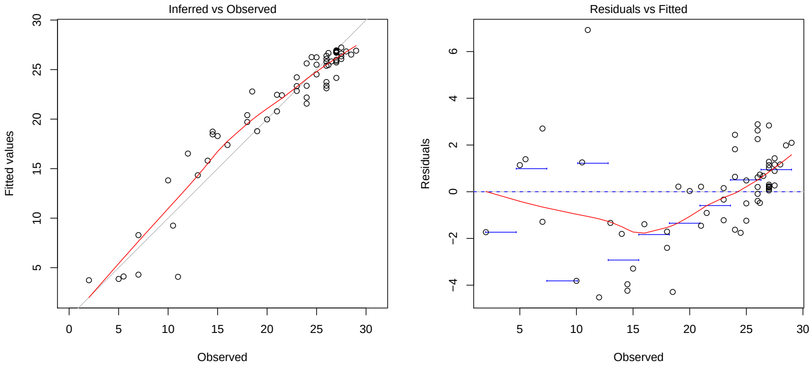
WA in analogue

- **analogue** contains R code for fitting WA transfer functions and associated helper functions

```
> #SumSST <- imbrie.env$SumSST #$
> mod <- wa(SumSST ~ ., data = ImbrieKipp, deshrink = "inverse")
> mod

Weighted Averaging Transfer Function

Call:
wa(formula = SumSST ~ ., data = ImbrieKipp, deshrink = "inverse")

Deshrinking  : Inverse
Tolerance DW : No
No. samples  : 61
No. species  : 27

Performance:
     RMSE  R-squared  Avg. Bias  Max. Bias
   2.0188     0.9173     0.0000    -3.8155
```

WA — diagnostic plots

```
> opar <- par(mfrow = c(1,2))
> plot(mod)
> par(opar)
```



WA — predictions I

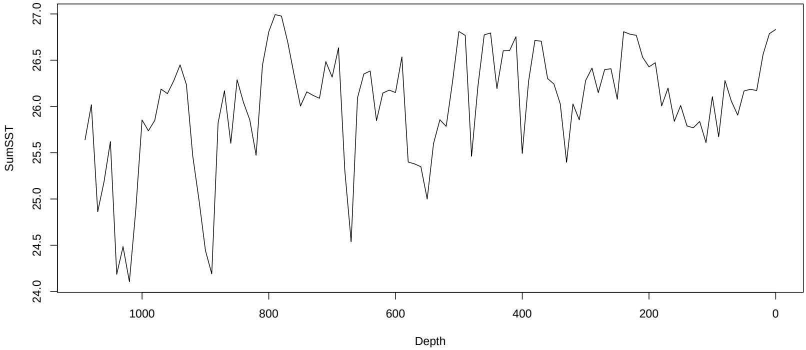
```
> pred <- predict(mod, V12.122)
> pred

Weighted Averaging Predictions

Call:
predict(object = mod, newdata = V12.122)

Deshrinking     : Inverse
Crossvalidation : none
Tolerance DW    : No

Performance:
   RMSEP        R2  Avg.Bias  Max.Bias
  2.0188    0.9173    0.0000   -3.8155

Predictions:
      0      10      20      30      40      50      60      70      80      90
26.8321 26.7870 26.5611 26.1722 26.1857 26.1670 25.9064 26.0574 26.2797 25.6723
    100     110     120     130     140     150     160     170     180     190
26.1054 25.6092 25.8379 25.7696 25.7891 26.0105 25.8400 26.1986 26.0054 26.4729
    200     210     220     230     240     250     260     270     280     290
26.4282 26.5318 26.7689 26.7812 26.8077 26.0786 26.4078 26.3981 26.1494 26.4148
    300     310     320     330     340     350     360     370     380     390
26.2799 25.8553 26.0269 25.3974 26.0271 26.2423 26.3020 26.7047 26.7140 26.2727
    400     410     420     430     440     450     460     470     480     490
25.4927 26.7538 26.6039 26.6019 26.1936 26.7939 26.7742 26.2152 25.4620 26.7682
    500     510     520     530     540     550     560     570     580     590
26.8107 26.2679 25.7851 25.8562 25.5992 25.0000 25.3488 25.3794 25.3995 26.5347
    600     610     620     630     640     650     660     670     680     690
```

WA — predictions II

```
26.1509 26.1765 26.1447 25.8472 26.3835 26.3507 26.0932 24.5383 25.3052 26.6331
    700     710     720     730     740     750     760     770     780     790
26.3173 26.4848 26.0882 26.1193 26.1579 26.0043 26.3400 26.6920 26.9768 26.9926
    800     810     820     830     840     850     860     870     880     890
26.8074 26.4448 25.4736 25.8549 26.0450 26.2881 25.6021 26.1688 25.8223 24.1910
    900     910     920     930     940     950     960     970     980     990
24.4447 24.9817 25.4642 26.2359 26.4497 26.2772 26.1387 26.1874 25.8485 25.7372
   1000    1010    1020    1030    1040    1050    1060    1070    1080    1090
25.8538 24.8725 24.1065 24.4843 24.1864 25.6200 25.1869 24.8619 26.0186 25.6395
```

Plotting reconstructions

```
> reconPlot(pred, use.labels = TRUE, ylab = "SumSST", xlab = "Depth")
```



Modern Analogue Technique

- WA take a species approach to reconstruction — each species in the fossil sample that is also in the training set contributes to the reconstructed values
- MAT takes a more holistic approach — we predict on basis of similar assemblages
- In MAT, only the most similar assemblages contribute to the fitted values
- MAT is steeped in the tradition of uniformitarianism — the present is the key to the past
- We take as our prediction of the environment of the past, the (possibly weighted) average of the environment of the k sites with the most similar assemblages
- Several things to define; k, (dis)similarity
- MAT is k nearest neighbours (k-NN) regression/calibration

Measuring association — binary data

		Object *j*	
		+	−
Object *i*	+	a	b
	−	c	d

- Dissimilarity based on the number of species present only in *i* (*b*), or *j* (*c*), or in present in both (*a*), or absent in both (*d*).

Jaccard similarity

$$s_{ij} = \frac{a}{a + b + c}$$

Simple matching coefficient

$$s_{ij} = \frac{a + d}{a + b + c + d}$$

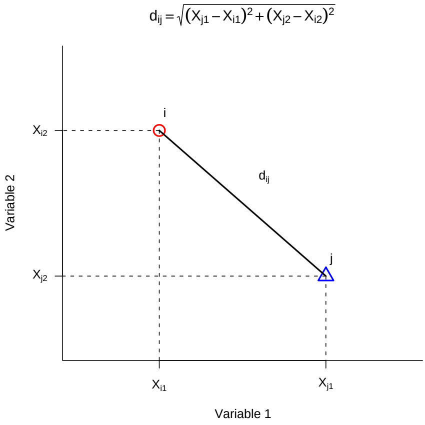
Jaccard dissimilarity

$$d_{ij} = \frac{b + c}{a + b + c}$$

Simple matching coefficient

$$d_{ij} = \frac{b + c}{a + b + c + d}$$

Measuring association — quantitative data



Euclidean distance

$$d_{ij} = \sqrt{\sum_{k=1}^{m} (x_{ik} - x_{jk})^2}$$

Manhattan distance

$$d_{ij} = \sum_{k=1}^{m} |x_{ik} - x_{jk}|$$

Bray-Curtis

$$d_{ij} = \frac{\sum_{k=1}^{m} |x_{ik} - x_{jk}|}{\sum_{k=1}^{m} (x_{ik} + x_{jk})}$$

Measuring association — quantitative data

- Euclidean distance dominated by large values.
- Manhattan distance less affected by large values.
- Bray-Curtis sensitive to extreme values.
- Similarity ratio (Steinhaus-Marczewski $\equiv$ Jaccard) less dominated by extremes.
- Chord distance, used for proportional data; signal-to-noise measure.

Similarity ratio

$$d_{ij} = \frac{\sum\limits_{k=1}^{m} x_{ik}x_{jk}}{\left(\sum\limits_{k=1}^{m} x_{ik}^2 + \sum\limits_{k=1}^{m} x_{jk}^2 - \sum\limits_{k=1}^{m} x_{ik}x_{jk}\right)^2}$$

Chord distance

$$d_{ij} = \sqrt{\sum_{k=1}^{m} (\sqrt{p_{ik}} - \sqrt{p_{jk}})^2}$$

Measuring association — mixed data

Gower's coefficient

$$s_{ij} = \frac{\sum_{i=1}^{m} w_{ijk} s_{ijk}}{\sum_{i=1}^{m} w_{ijk}}$$

- s_{ijk} is similarity between sites i and j for the kth variable.
- Weights w_{ijk} are typically 0 or 1 depending on whether the comparison is valid for variable k. Can also use variable weighting with w_{ijk} between 0 and 1.
- w_{ijk} is zero if the kth variable is missing for one or both of i or j.
- For binary variables s_{ijk} is the Jaccard coefficient.
- For categorical data s_{ijk} is 1 of i and k have same category, 0 otherwise.
- For quantitative data $s_{ijk} = (1 - |x_{ik} - x_{jk}|)/R_k$

MAT

- Once you have chosen a suitable dissimilarity coefficient, MAT begins
- We calculate the dissimilarity between each training set sample and every other
- For each site in turn, we order the training set samples in terms of increasing dissimilarity to the target training set sample
- Calculate the (weighted) average of the environment for the closest site, then the two closest sites, then the three closest sites, ... and so on
- The weights, if used, are the inverse of the dissimilarity $w_{jk} = 1/d_{jk}$
- For each model of size k we calculate some performance statistics
- Choose as our model, the k that achieves the lowest RMSEP across the whole training set
- Very simple!

MAT in analogue I

```
> data(swapdiat, swappH, rlgh)
> dat <- join(swapdiat, rlgh, verbose = TRUE)

Summary:

            Rows Cols
Data set 1:  167  277
Data set 2:  101  139
Merged:      268  277

> swapdiat <- with(dat, swapdiat / 100)
> rlgh <- with(dat, rlgh / 100)
> swap.mat <- mat(swappH ~ ., data = swapdiat, method = "SQchord")
> swap.mat

Modern Analogue Technique

Call:
mat(formula = swappH ~ ., data = swapdiat, method = "SQchord")

Percentiles of the dissimilarities for the training set:

   1%    2%    5%   10%   20%
0.416 0.476 0.574 0.668 0.815

Inferences based on the mean of k-closest analogues:

  k   RMSEP      R2 Avg Bias Max Bias
  1  0.4227  0.7139  -0.0254  -0.3973
  2  0.3741  0.7702  -0.0493  -0.4689
```

MAT in analogue II

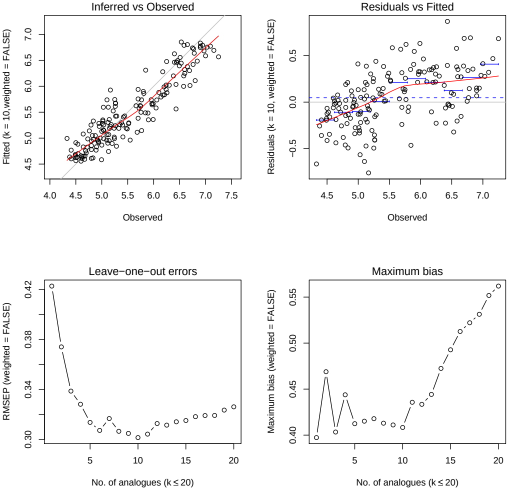
```
  3  0.3387  0.8088  -0.0379  -0.4034
  4  0.3282  0.8200  -0.0335  -0.4438
  5  0.3136  0.8356  -0.0287  -0.4124
  6  0.3072  0.8444  -0.0386  -0.4152
  7  0.3167  0.8364  -0.0481  -0.4179
  8  0.3065  0.8474  -0.0433  -0.4130
  9  0.3049  0.8495  -0.0436  -0.4111
 10  0.3015  0.8548  -0.0473  -0.4083

Inferences based on the weighted mean of k-closest analogues:

  k   RMSEP      R2 Avg Bias Max Bias
  1  0.4227  0.7139  -0.0254  -0.3973
  2  0.3711  0.7734  -0.0476  -0.4614
  3  0.3375  0.8102  -0.0385  -0.4088
  4  0.3272  0.8213  -0.0346  -0.4433
  5  0.3144  0.8348  -0.0298  -0.4205
  6  0.3077  0.8435  -0.0371  -0.4253
  7  0.3148  0.8377  -0.0451  -0.4250
  8  0.3049  0.8483  -0.0407  -0.4206
  9  0.3035  0.8500  -0.0408  -0.4205
 10  0.3005  0.8546  -0.0442  -0.4180
```

MAT in analogue

- The RMSEP here is a leave-one-out RMSEP
- Each prediction for training set sample *i* is produced on the basis of using all sites other than *i*
- **analogue** is unique (as far as I know) as it evaluates all *k* models at once
- This means it is slow at times...
- ...But you only need to do the fitting once to determine the model with lowest RMSEP

MAT diagnostic plots

```
> opar <- par(mfrow = c(2,2))
> plot(swap.mat)
> par(opar)
```



MAT predictions I

- To make a prediction for a fossil sample using MAT:
- Calculate dissimilarity between each fossil sample and each training set sample
- Take the *k* closest training set samples for each fossil sample
- The prediction for a fossil sample is the (weighted) average of these *k* closest training set samples

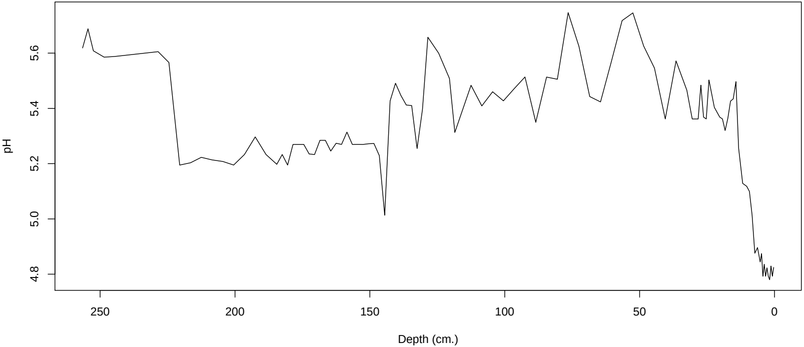
```
> rlgh.mat <- predict(swap.mat, rlgh, k = 10)
> rlgh.mat

Modern Analogue Technique predictions

Dissimilarity: SQchord
k-closest analogues: 10, Chosen automatically? FALSE
Weighted mean: FALSE
Bootstrap estimates: FALSE

Model error estimates:
    RMSEP r.squared  avg.bias  max.bias
  0.30150   0.85478  -0.04729  -0.40833

Predicted values:
000.3 000.8 001.3 001.8 002.3 002.8 003.3 003.8 004.3 004.8 005.3 006.3 007.3
```

MAT predictions II

```
4.824 4.793 4.830 4.780 4.793 4.823 4.793 4.836 4.793 4.874 4.844 4.896 4.876
008.3 009.3 010.3 011.8 013.3 014.3 015.3 016.3 017.3 018.3 019.3 020.3 022.3
5.013 5.100 5.118 5.129 5.256 5.497 5.434 5.426 5.364 5.320 5.362 5.368 5.404
024.3 025.3 026.3 027.3 028.3 030.5 032.5 036.5 040.5 044.5 048.5 052.5 056.5
5.503 5.362 5.368 5.484 5.362 5.362 5.466 5.572 5.362 5.546 5.626 5.746 5.718
060.5 064.5 068.5 072.5 076.5 080.5 084.5 088.5 092.5 096.5 100.5 104.5 108.5
5.569 5.423 5.443 5.625 5.747 5.505 5.513 5.350 5.514 5.471 5.427 5.460 5.409
112.5 118.5 120.5 124.5 128.5 130.5 132.5 134.5 136.5 138.5 140.5 142.5 144.5
5.484 5.313 5.508 5.600 5.658 5.396 5.255 5.410 5.412 5.447 5.491 5.427 5.014
146.5 148.5 150.5 152.5 154.5 156.5 158.5 160.5 162.5 164.5 166.5 168.5 170.5
5.229 5.273 5.272 5.270 5.270 5.270 5.314 5.270 5.274 5.246 5.284 5.284 5.233
172.5 174.5 176.5 178.5 180.5 182.5 184.5 188.5 192.5 196.5 200.5 204.5 208.5
5.235 5.270 5.270 5.270 5.195 5.233 5.198 5.233 5.297 5.233 5.195 5.208 5.214
212.5 216.5 220.5 224.5 228.5 244.5 248.5 252.5 254.5 256.5
5.223 5.203 5.195 5.566 5.605 5.588 5.585 5.608 5.688 5.619
```

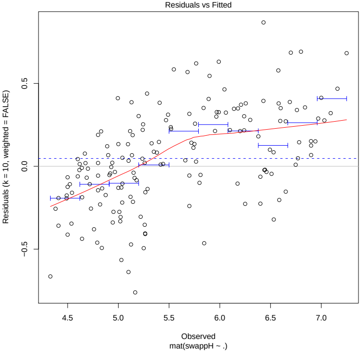
MAT reconstructions

```
> reconPlot(rlgh.mat, use.labels = TRUE, ylab = "pH", xlab = "Depth (cm.)")
```



Bias

- Bias is the tendency for the model to over or under predict
- Average bias is the mean of the residuals
- Maximum bias is found by breaking the range of the measured environment into *n* contiguous chunks ($n = 10$ usually)
- Within each chunk calculate the mean of the residuals for that chunk
- Take the maximum value of these as the maximum bias statistic



Cross-validation

- Without cross-validation, prediction errors, measured by RMSEP, will be biased, often badly so
- This is because we use the same data to both fit and test the model
- Ideally we'd have such a large training set that we can split this into a slightly smaller training set and a small test set
- Palaeoecological data is expensive to obtain — in money and person-hours!
- Also these ecosystems are complex, species rich, noisy etc., so we want to use all our data to produce a model
- One solution to this problem is to use cross-validation
- General idea is we perturb our training set in some way, build a new model on the perturbed training set and assess how well it performs
- If we repeat the perturbation several time we get an idea of the error in the model
- Several techniques; *n*-fold, leave-one-out, bootstrapping (aka bagging)

Cross-validation in **analogue**

- In **analogue**, several methods are available
- For MAT models, LOO is built into the procedure so only bootstrapping is available
- For WA models, both LOO and bootstrapping currently available
- *n*-fold CV will be available in a future version

LOO Cross-validation in **analogue**

- LOO CV is very simple
- In turn, leave out each sample from the training set
- Build a model on the remaining samples
- Predict for the left out sample
- Calculate the RMSEP of these predictions

```
> loo.pred <- predict(mod, V12.122, CV = "LOO", verbose = TRUE)

Leave one out sample 10
Leave one out sample 20
Leave one out sample 30
Leave one out sample 40
Leave one out sample 50
Leave one out sample 60

> performance(mod)

      RMSE          R2   Avg.Bias   Max.Bias
 2.019e+00  9.173e-01  2.228e-14 -3.815e+00

> performance(loo.pred)

   RMSEP       R2 Avg.Bias Max.Bias
 2.21791  0.90028 -0.01365 -4.59850
```

Bootstrap Cross-validation in **analogue**

- Bootstrapping used in machine learning to improve predictions
- Use bootstrapping to get more realistic RMSEP and bias statistics
- We draw a bootstrap sample (sampling with replacement) of the same size as our training set
- Build a model on the bootstrap samples
- Predict for the out-of-bag (OOB) samples
- Bootstrap prediction for each model sample is the mean of the OOB prediction for each sample
- Calculate the residuals and then the RMSEP

$$\mathrm{RMSEP}_{\mathrm{boot}} = \sqrt{s_1^2 + s_2^2}$$

- s_1^2 is the standard deviation of the OOB residuals
- s_2^2 is the mean of the OOB residuals
- We can also calculate the more usual RMSEP $\sqrt{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2/n}$

Bootstrap Cross-validation in **analogue**

```
> set.seed(1234)
> swap.boot <- bootstrap(swap.mat, n.boot = 200)
> swap.boot

Bootstrap results for palaeoecological models

Model type: MAT
Weighted mean: FALSE
Number of bootstrap cycles: 200

Leave-one-out and bootstrap-derived error estimates:

           k  RMSEP     S1     S2 r.squared avg.bias max.bias
LOO       10 0.3015      -      -    0.8548 -0.04729  -0.4083
Bootstrap 11 0.3278 0.1202 0.3049    0.9241 -0.05010  -0.4472

> RMSEP(swap.boot, type = "standard")

[1] 0.3049106
```

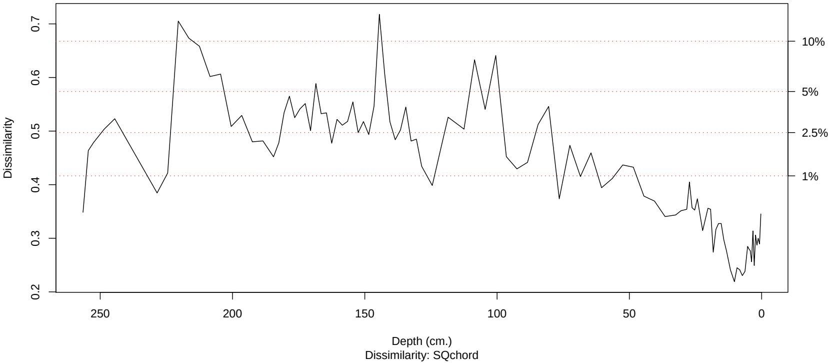
Minimum dissimilarity to a training set sample

- A measure of reliability for the reconstructed values can be determined from the distance between each fossil sample and the training set samples
- For a reconstructed value to be viewed as more reliable, it should have at least one close modern analogue in the training set
- Close modern analogues are defined as those modern training set samples that are as similar to a fossil sample as a low percentile of the observed distribution dissimilarities in the training set, say the 5th percentile

```
> rlgh.mdc <- minDC(rlgh.mat)
> plot(rlgh.mdc, use.labels = TRUE, xlab = "Depth (cm.)")
> quantile(as.dist(swap.mat$Dij), prob = c(0.01,0.025,0.05, 0.1))

       1%      2.5%        5%       10%
0.4164113 0.4972167 0.5738378 0.6676391
```

Minimum dissimilarity to a training set sample

```
> plot(rlgh.mdc, use.labels = TRUE, xlab = "Depth (cm.)")
> quantile(as.dist(swap.mat$Dij), prob = c(0.01,0.025,0.05, 0.1))

       1%      2.5%        5%       10%
0.4164113 0.4972167 0.5738378 0.6676391
```



Sample-specific error estimates

- We can use the bootstrap approach to generate sample specific errors for each fossil sample

$$\mathrm{RMSEP} = \sqrt{s^2_{1_{fossil}} + s^2_{2_{model}}}$$

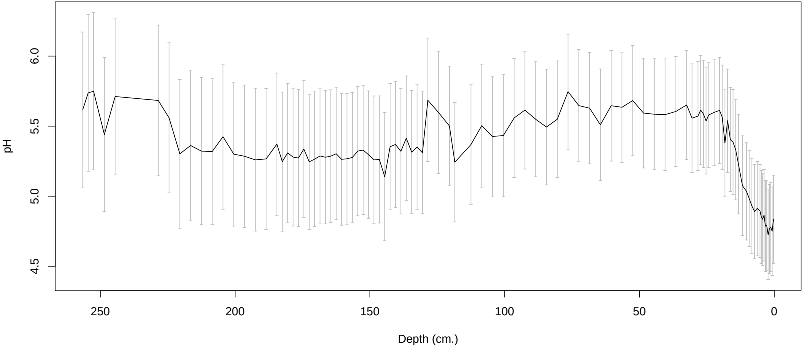
- $s^2_{1_{fossil}}$ is the standard deviation of the bootstrap estimates for the fossil samples
- $s^2_{2_{model}}$ is the average bias, the mean of the bootstrap OOB residuals from the model

Sample-specific error estimates

```
> swap.boot

Bootstrap results for palaeoecological models

Model type: MAT
Weighted mean: FALSE
Number of bootstrap cycles: 200

Leave-one-out and bootstrap-derived error estimates:

           k  RMSEP     S1     S2 r.squared avg.bias max.bias
LOO       10 0.3015      -      -    0.8548 -0.04729  -0.4083
Bootstrap 11 0.3278 0.1202 0.3049    0.9241 -0.05010  -0.4472

> set.seed(1234)
> rlgh.boot <- predict(swap.mat, rlgh, bootstrap = TRUE, n.boot = 200)
> reconPlot(rlgh.boot, use.labels = TRUE, ylab = "pH", xlab = "Depth (cm.)", display
```

Sample-specific error estimates

```
> reconPlot(rlgh.boot, use.labels = TRUE, ylab = "pH", xlab = "Depth (cm.)",
+           display.error = "bars", predictions = "bootstrap")
```


pH
Depth (cm.)