An Introduction to R for the Geosciences: Stratigraphic & Palaeoecological Data

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1. Transfer functions
2. Age-depth modelling
3. Summarising change in stratigraphic data
4. Rate of change analysis
5. Chronological clustering (zonation)

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

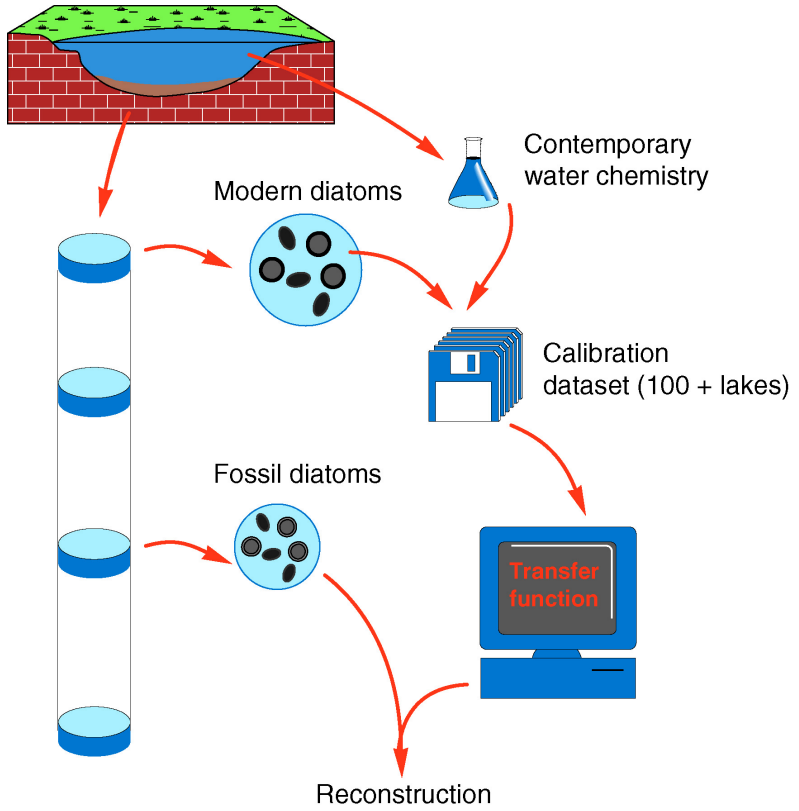
- In the 1970s and early 1980s there was a great deal of concern about acid lakes and rivers in northern Europe
- Driven mainly by losses of Salmon in Scandinavian rivers, this was a major political hot potato
- A vast amount of money was expended to determine the cause of the acidification — was it 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



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

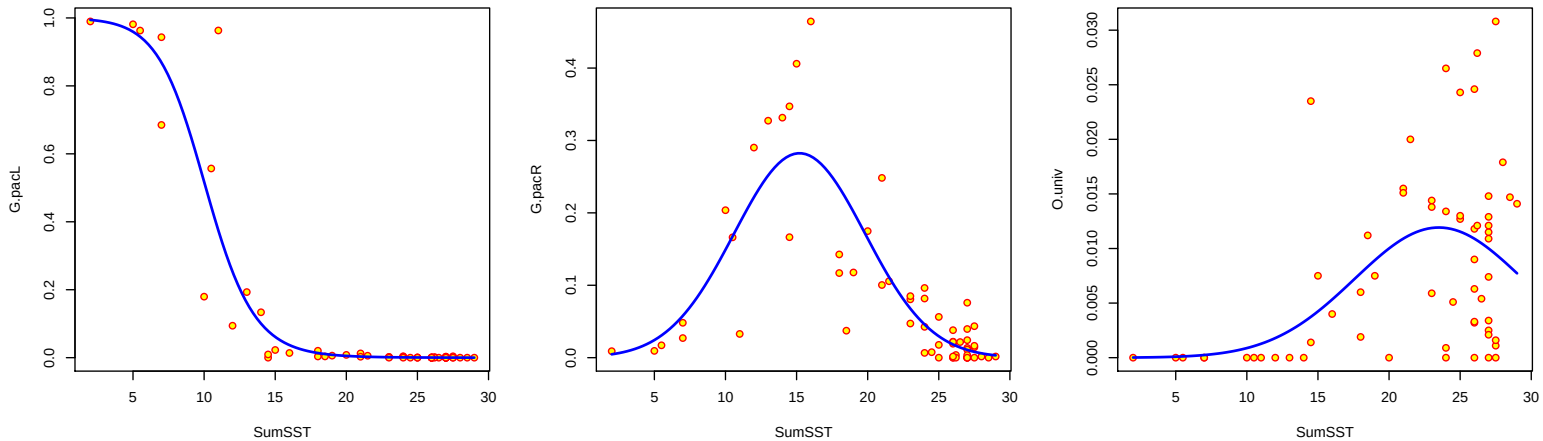
- Taxa in training set are systematically related to the environment in which they live
- Environmental variable to be reconstructed is, or is linearly related to, an ecologically important variable in the ecosystem
- Taxa in the training set are the same as in the fossil data and their ecological responses 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

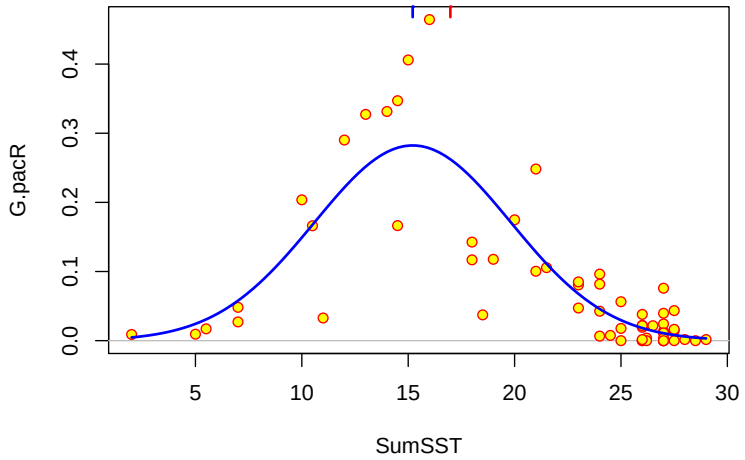
Weighted averaging

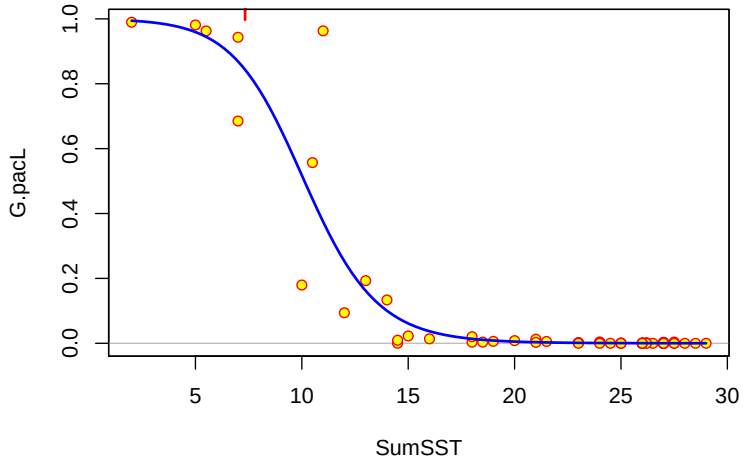
- Species don't respond in simple ways to *environmental gradients*
- Maximum likelihood method fitted Gaussian curves to each species and then numerical optimisation used to predict for fossil samples
- Computationally very intensive, especially when doing cross-validation
- Weighted averaging is an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



Weighted averaging

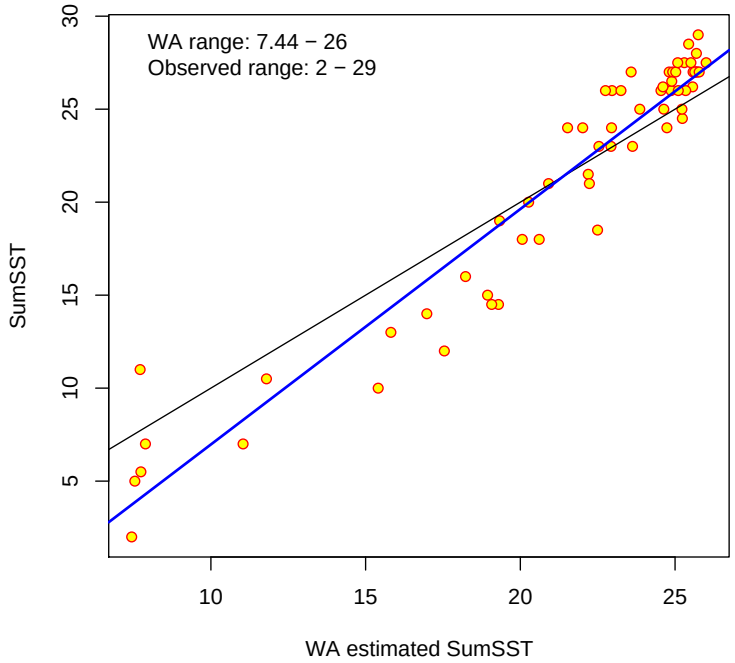
- A very simple idea
- In a lake, with a certain pH, a species with their pH optima close to the pH of the lake will tend to be the most abundant species present
- A simple estimate of the a species' pH optimum is an average of all the pH values for lakes in which that species occurs, weighted by their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



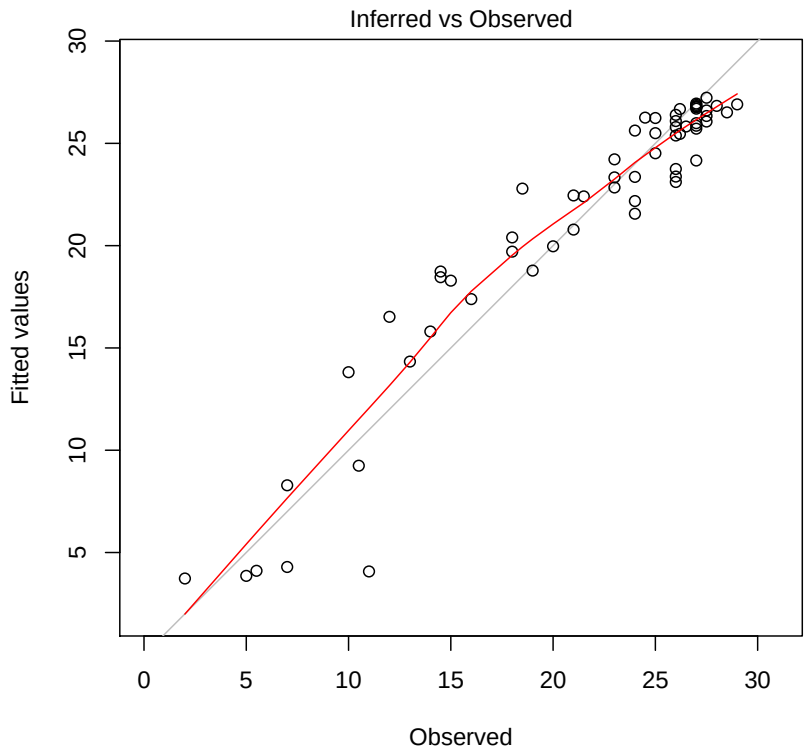
WA in analogue

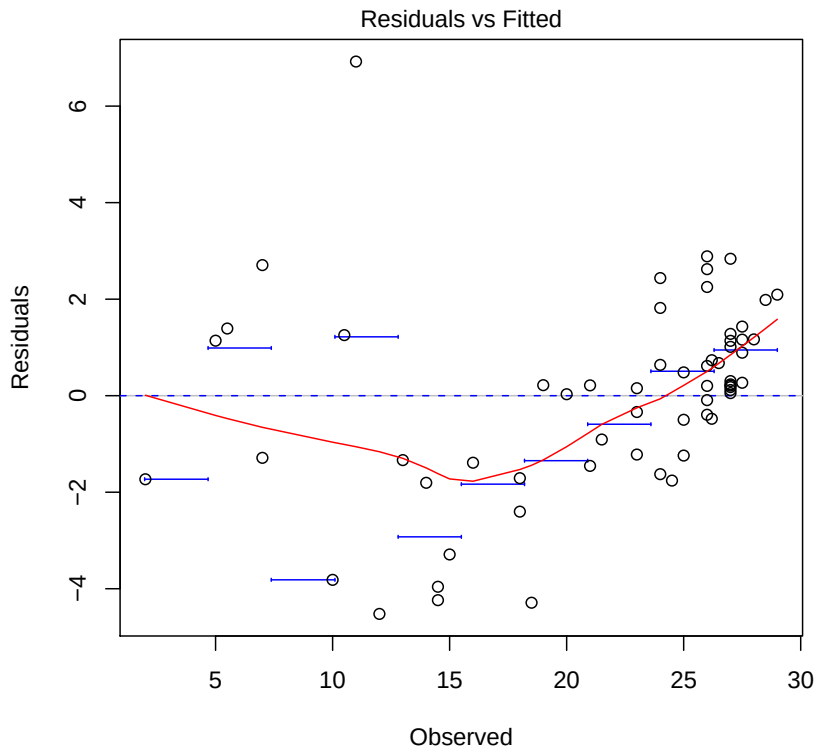
- **analogue** contains R code for fitting WA transfer functions and associated helper functions

```
> #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

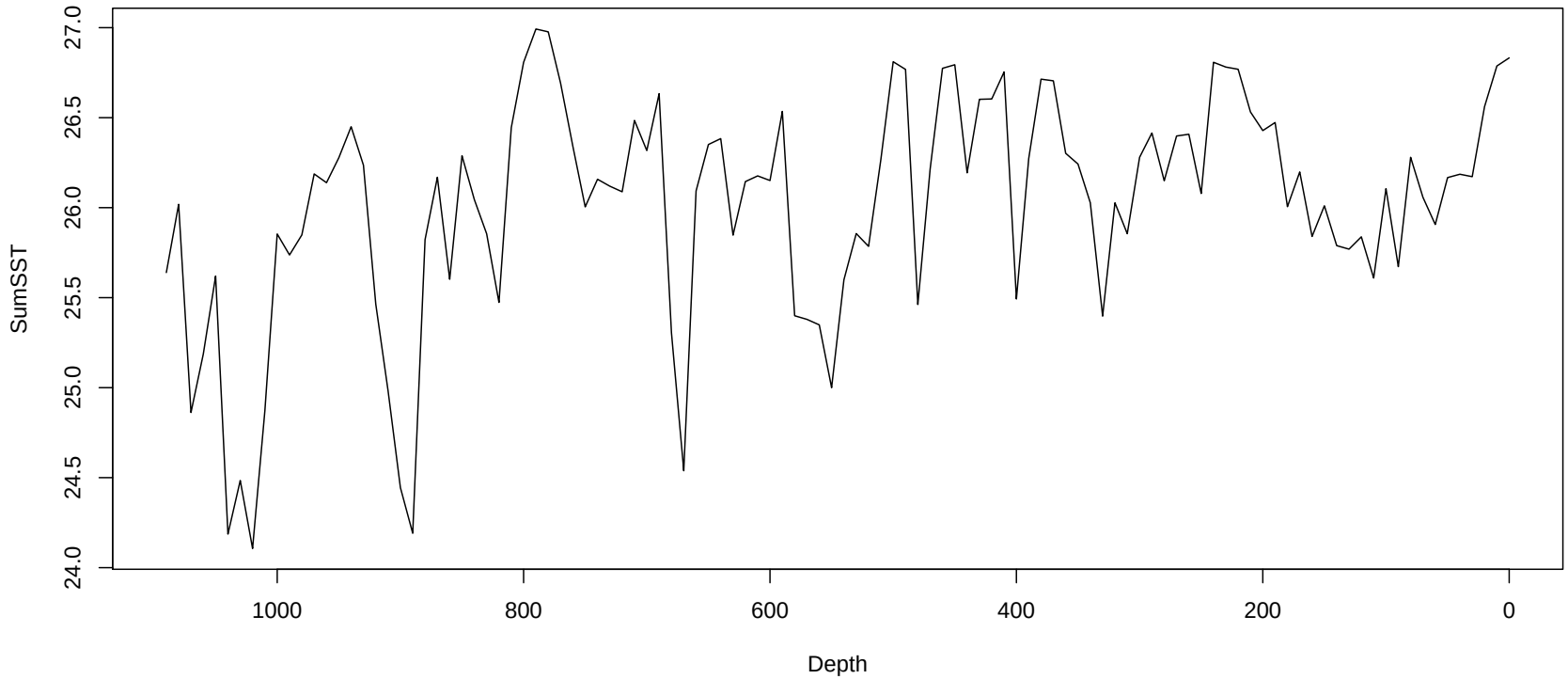
```
> pred <- predict(mod, V12.122)
> pred

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

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

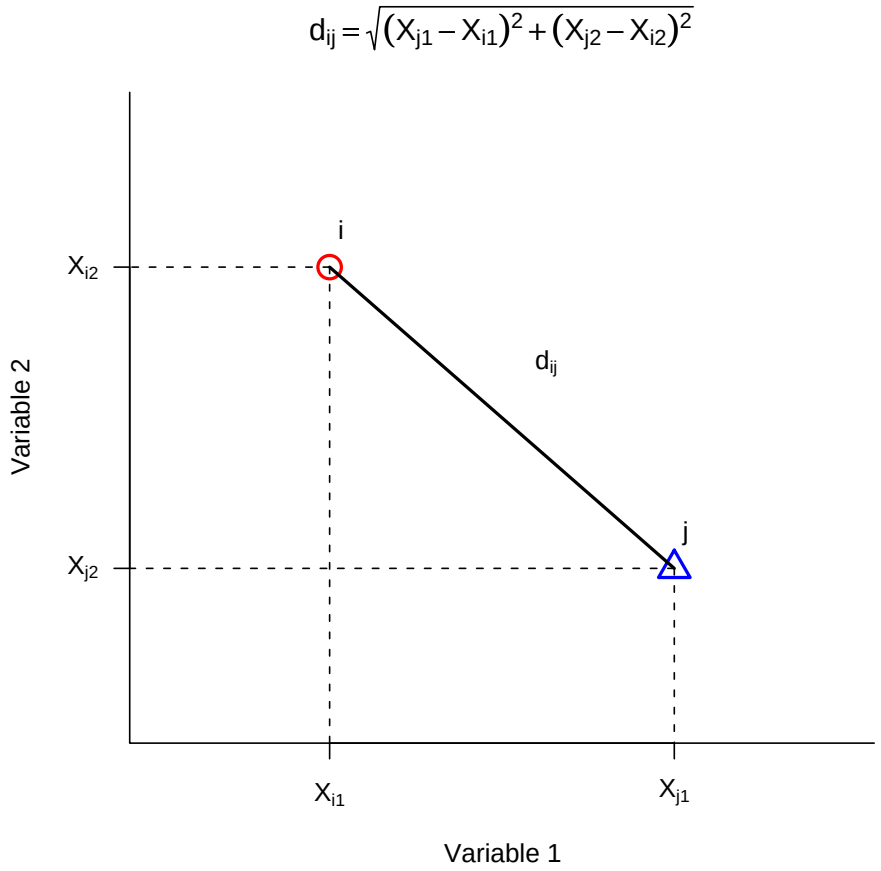
Jaccard dissimilarity

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

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

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

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

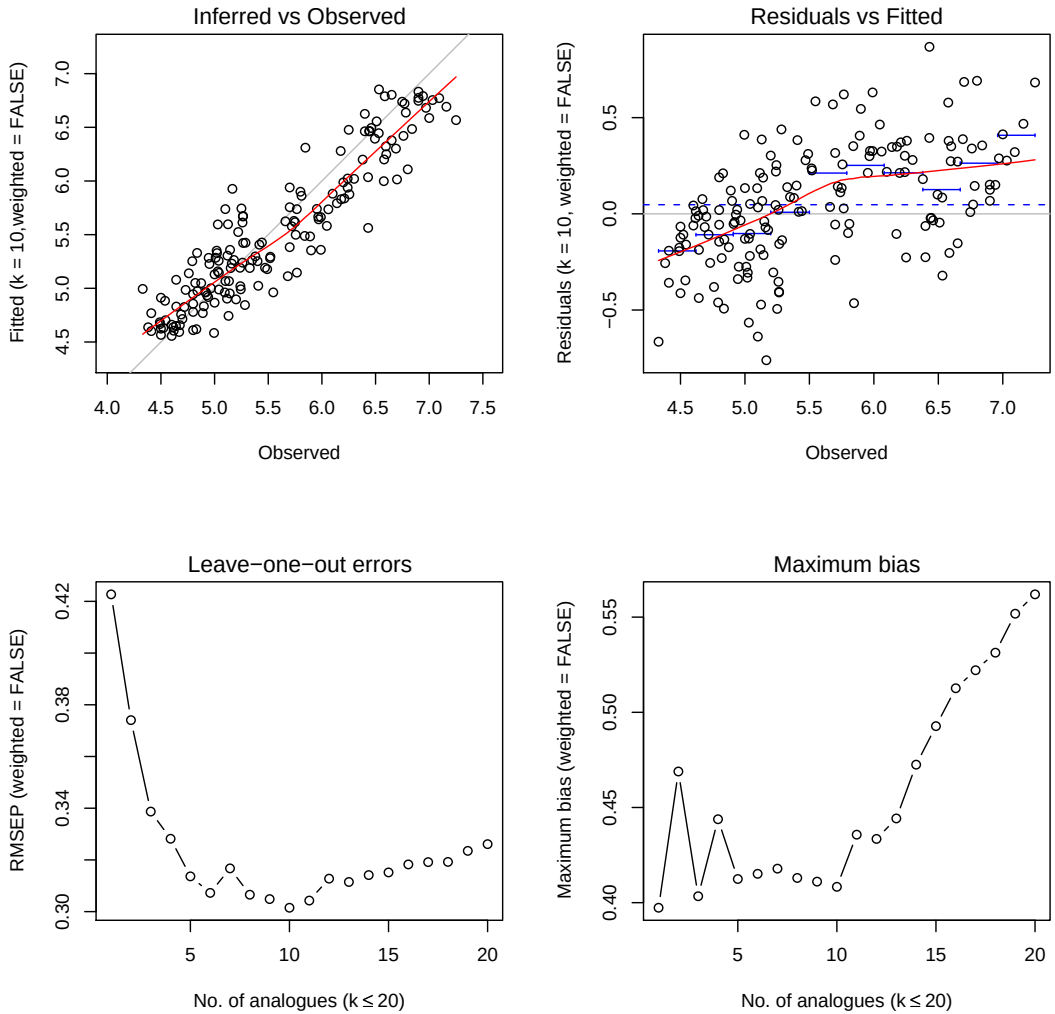
```
  3  0.3387  0.8088  -0.0379  -0.4034
  4  0.3282  0.8200  -0.0335  -0.4438
  5  0.3136  0.8356  -0.0287  -0.4124
  6  0.3072  0.8444  -0.0386  -0.4152
  7  0.3167  0.8364  -0.0481  -0.4179
  8  0.3065  0.8474  -0.0433  -0.4130
  9  0.3049  0.8495  -0.0436  -0.4111
 10  0.3015  0.8548  -0.0473  -0.4083

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

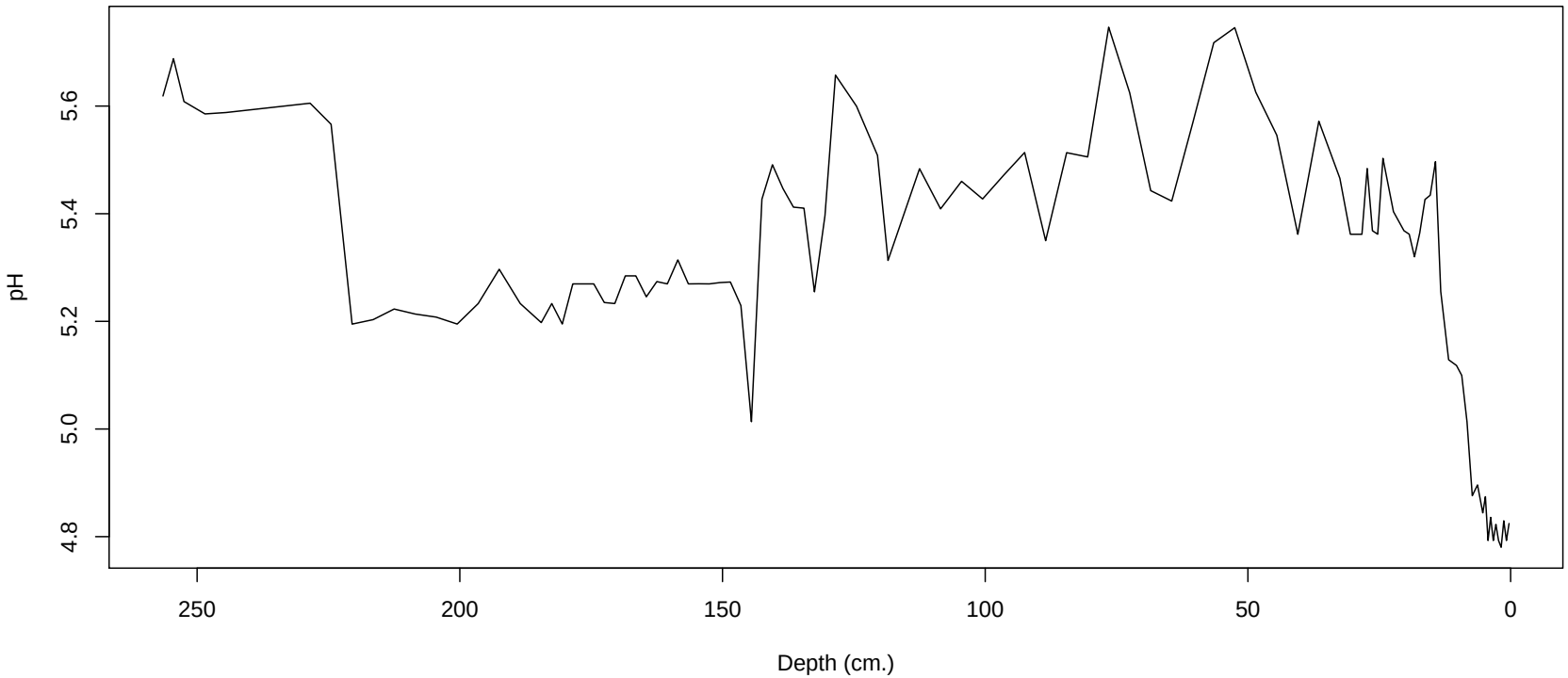
```
> rlgh.mat <- predict(swap.mat, rlgh, k = 10)
> rlgh.mat

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
```

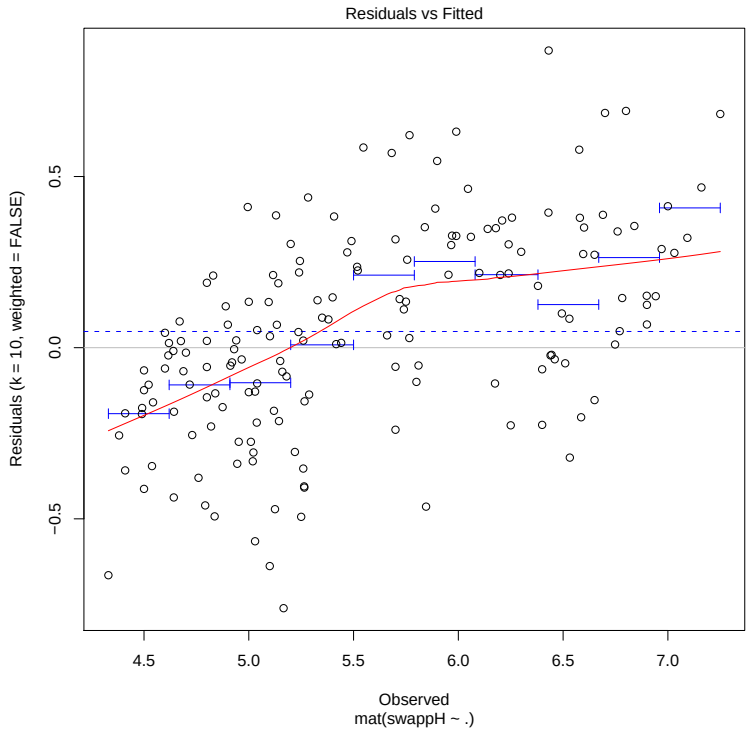
MAT reconstructions

```
> 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

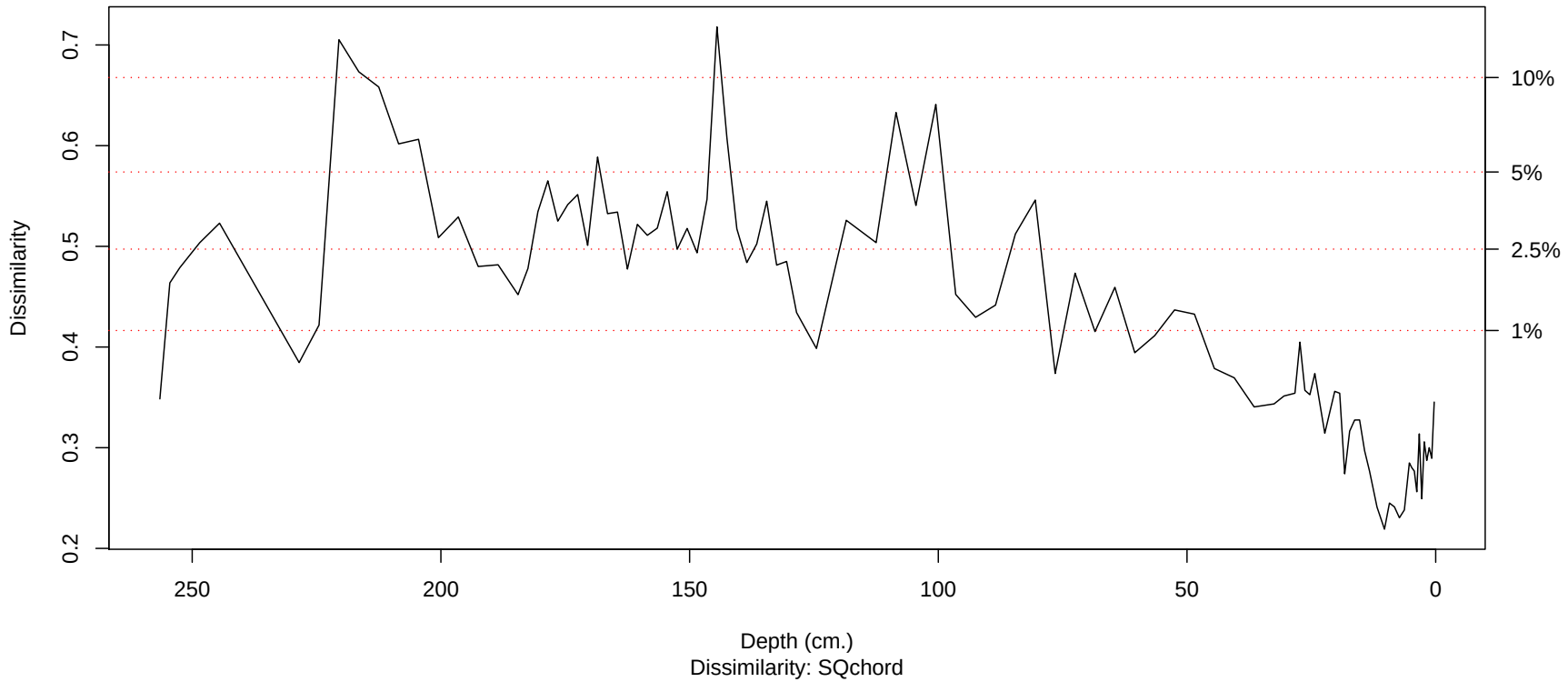
- A measure of reliability for the reconstructed values can be determined from the distance between each fossil sample and the training set samples
- For a reconstructed value to be viewed as more reliable, it should have at least one close modern analogue in the training set
- Close modern analogues 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 5^{th} 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

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

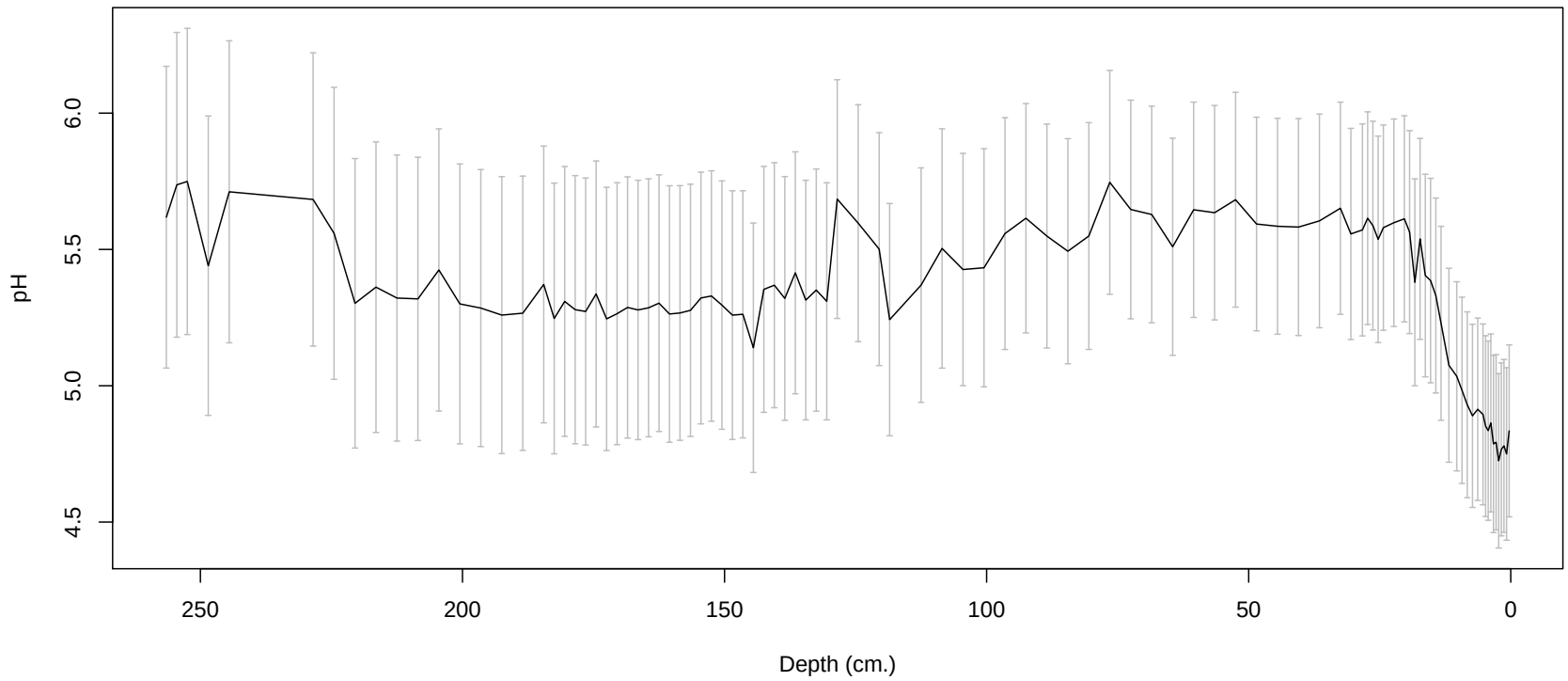
- $s^2_{1_{fossil}}$ is the standard deviation of the bootstrap estimates for the fossil samples
- $s^2_{2_{model}}$ is the average bias, the mean of the bootstrap OOB residuals from the model

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

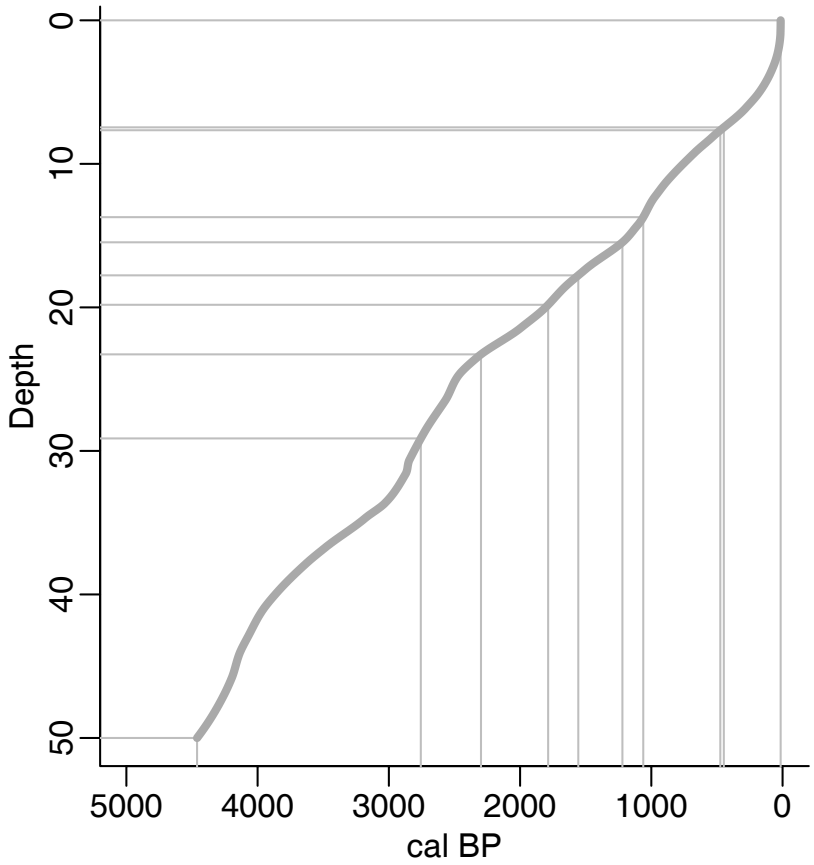
```
> reconPlot(rlgh.boot, use.labels = TRUE, ylab = "pH", xlab = "Depth (cm.)",
+           display.error = "bars", predictions = "bootstrap")
```

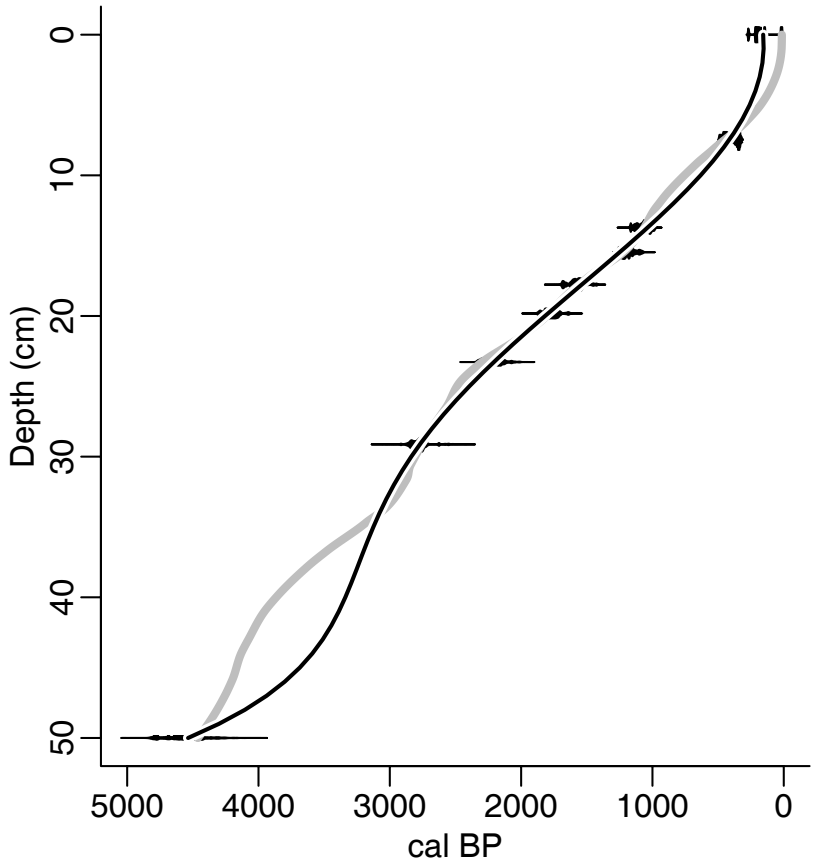


Age-depth modelling

- Accurate chronologies are essential component of a successful palaeoecological research
- Chronologies provide a time scale, the background upon which we interpret proxy records
- Allow us to correlate and compare events across multiple stratigraphic records
- Large number of techniques proposed for modelling age-depth relationships
  - Linear interpolation
  - Polynomial regression
  - Splines
  - Mixed effect models
  - Bayesian chronlogical ordering & Bayesian wiggle matching
- Use the modelled Age-depth relationship allows dates to be assigned to undated sediment samples

Age-depth modelling

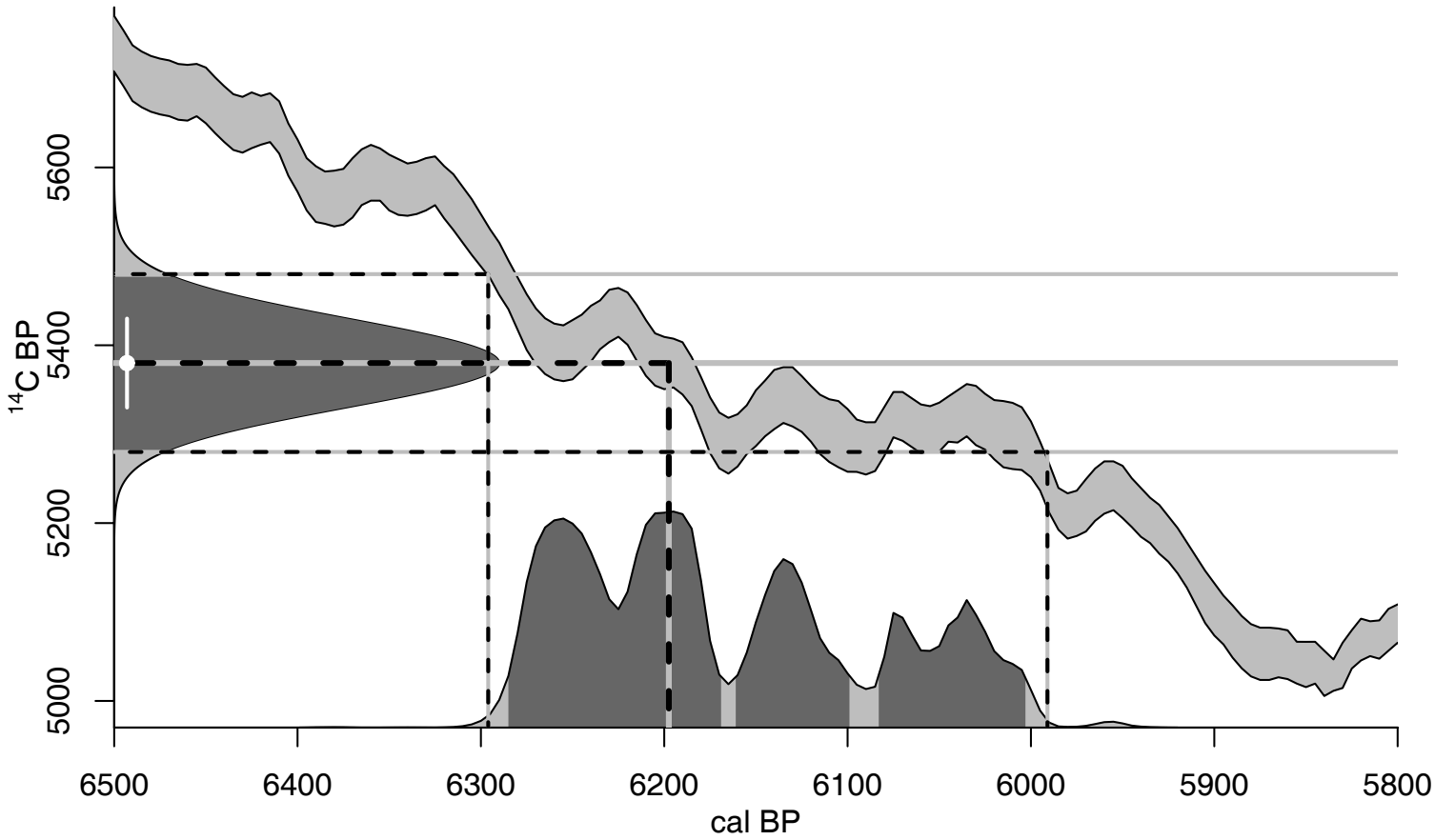




Blauuw & Heegaard (2012)

Age-depth modelling

Calibrating radiocarbon ages to calendar ages, leads to choice between analytical or Monte Carlo methods



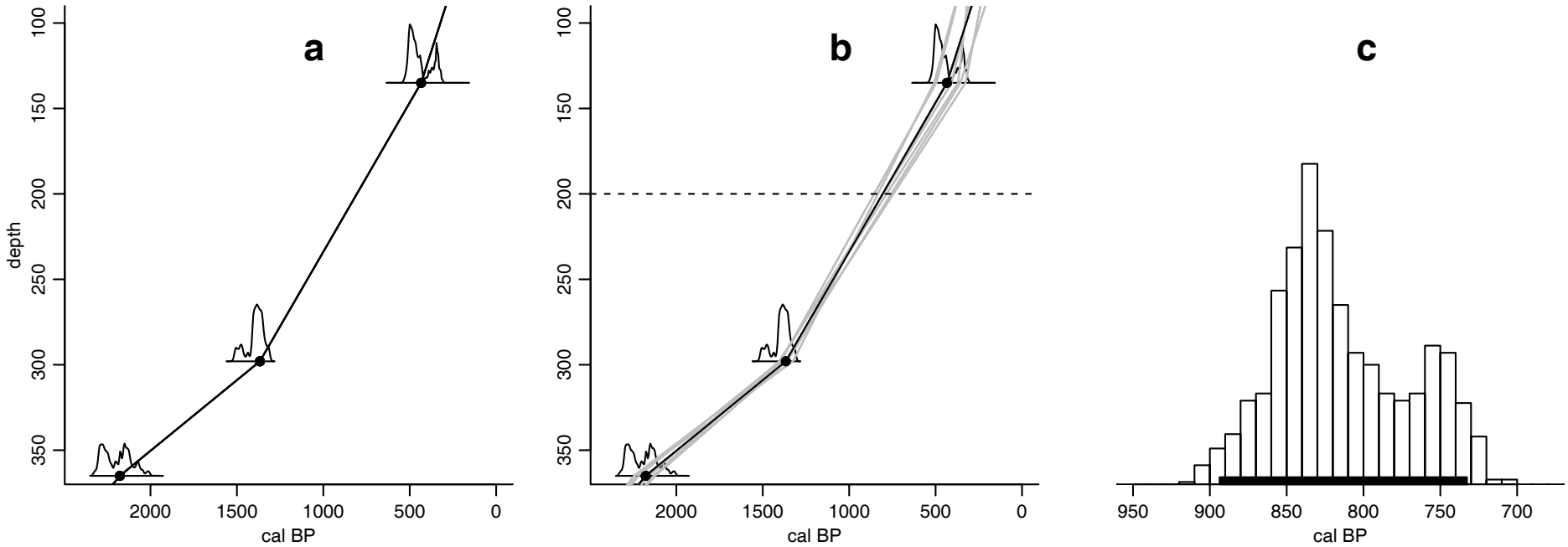
Blauuw & Heegaard (2012)

Analytical vs. Monte Carlo methods

- Analytical methods are those that have exact solutions; can be solved using a set of equations
- Least squares solution to linear regression is an example
- For other, possibly more complex, problems a closed-form solution may not exist
- Various resampling methods developed to tackle such problems
- Monte Carlo methods draw samples from a distribution at random and propogate them through equations
- In age-depth modelling
  1. Sample a calendar date from distribution; repeat for all dated levels
  2. Use the Monte Carlo sample to derive an age-depth relationship
  3. Record age from model for each sediment slice
  4. Repeat large number of times (e.g. 10000)
  5. Use distribution to obtain most likely date for each sample & use HPD for uncertainty

Monte Carlo resampling

- a) Linear interpolation model fitted to random draw from 3 calendar age distributions
- b) Repeated models fitted to random draws give different age-depth relationships
- c) Posterior distribution of age for indicated interval. Black bar is 95% HPD interval

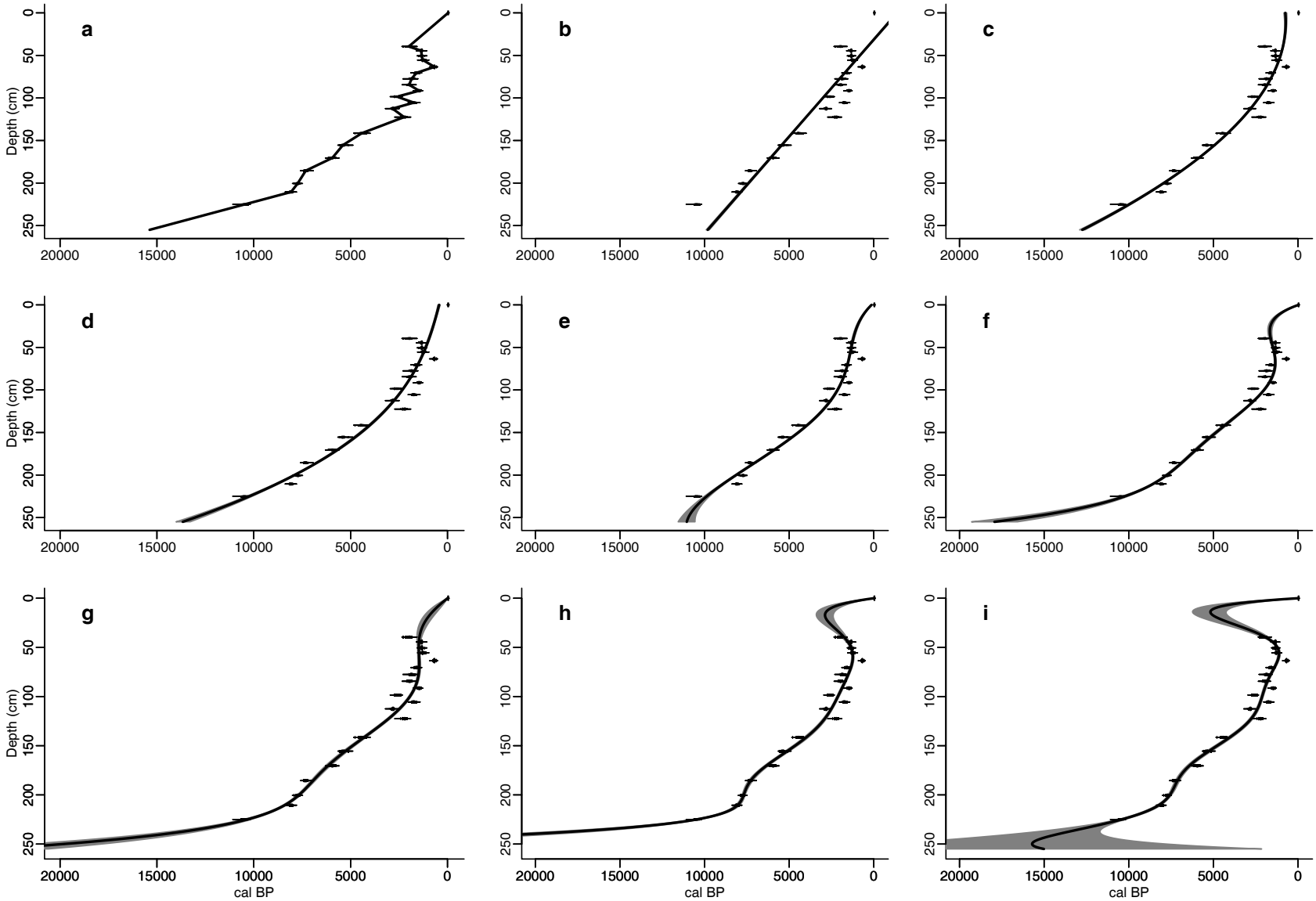


Blauuw & Heegaard (2012)

Basic Age-depth models

- Basic age-depth models consider only the uncertainties in the measured age estimates themselves
- Assume each measured age is independent of others
- Examples of such models include
  - Linear interpolation
  - Linear model (inc. polynomial fits)
  - Splines & smoothers
- Linear interpolation is simple & crude; join dated levels with straight lines
- Gives a piece-wise linear fit through all data points
- Assumes accumulation rate is constant between dated levels & only changes at dated levels
- Accumulation rates for intervals is the slope of the line between points
- May result in reversals
- Doesn't take into account uncertainty in age estimates

Basic Age-depth models



Blauuw & Heegaard (2012)

Linear models & Polynomials

- Polynomial have a general form

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \cdots + \beta_n x^n, n = N - 1$$

- A straight line has two terms and the equation

$$y = \beta_0 + \beta_1 x$$

- A quadratic relationship has three terms and the equation

$$y = \beta_0 + \beta_1 x + \beta_2 x^2$$

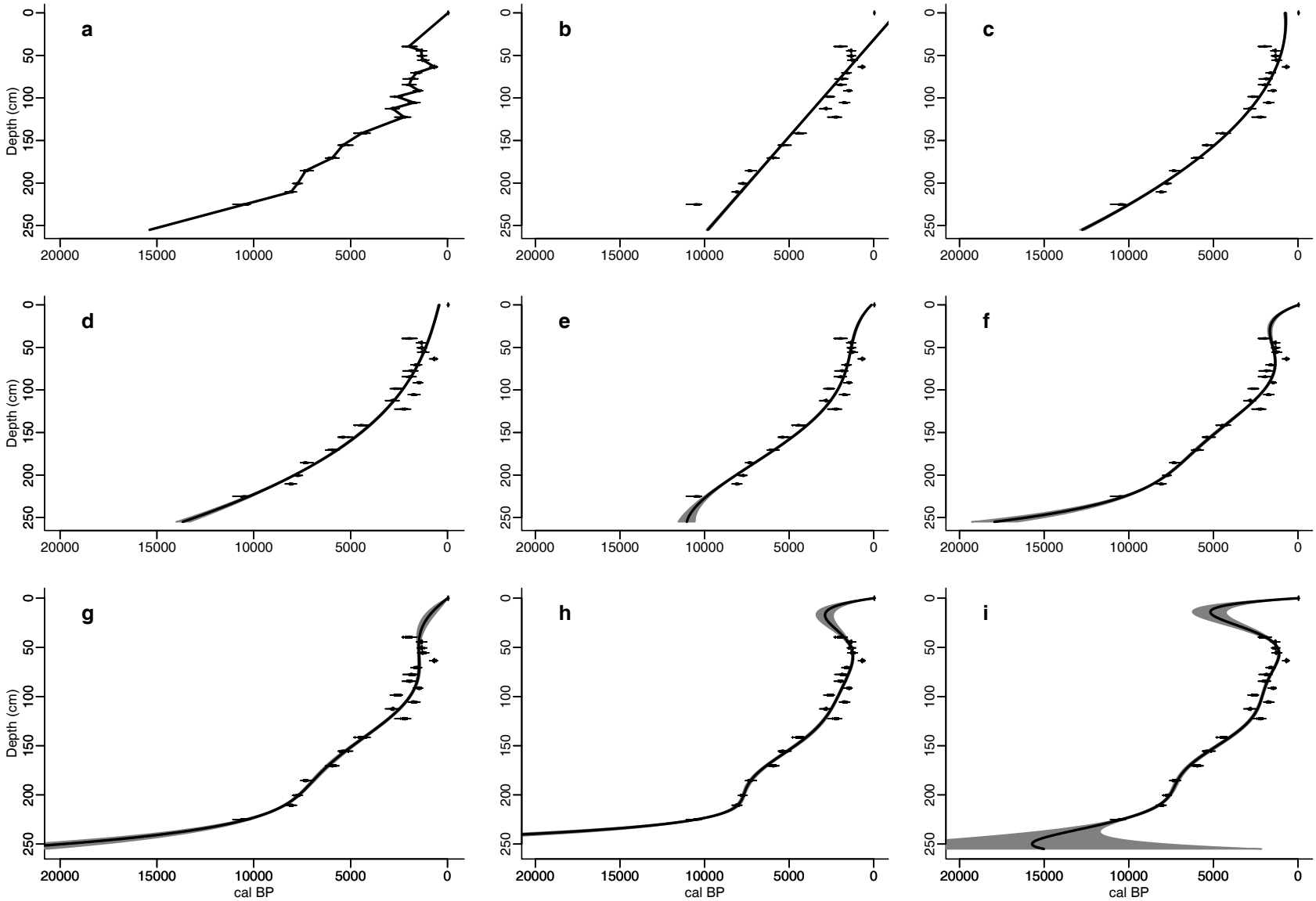
- A cubic relationship has four terms and the equation

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$$

Linear models & Polynomials

- Estimate coefficients β_j by minimising sum of squared errors
- Common to add an age for the core top (e.g. -60 $\pm$10 cal BP)
- As order of polynomial increases, fitted age-depth relationship becomes more flexible and more complex
- Aim to find a minimal yet adequate model that provides reasonable fit without reversals
- Use skills from regression lecture/practical
- Differentiation used to give accumulation rate at any point along fitted model
- Model fitting is done using least squares

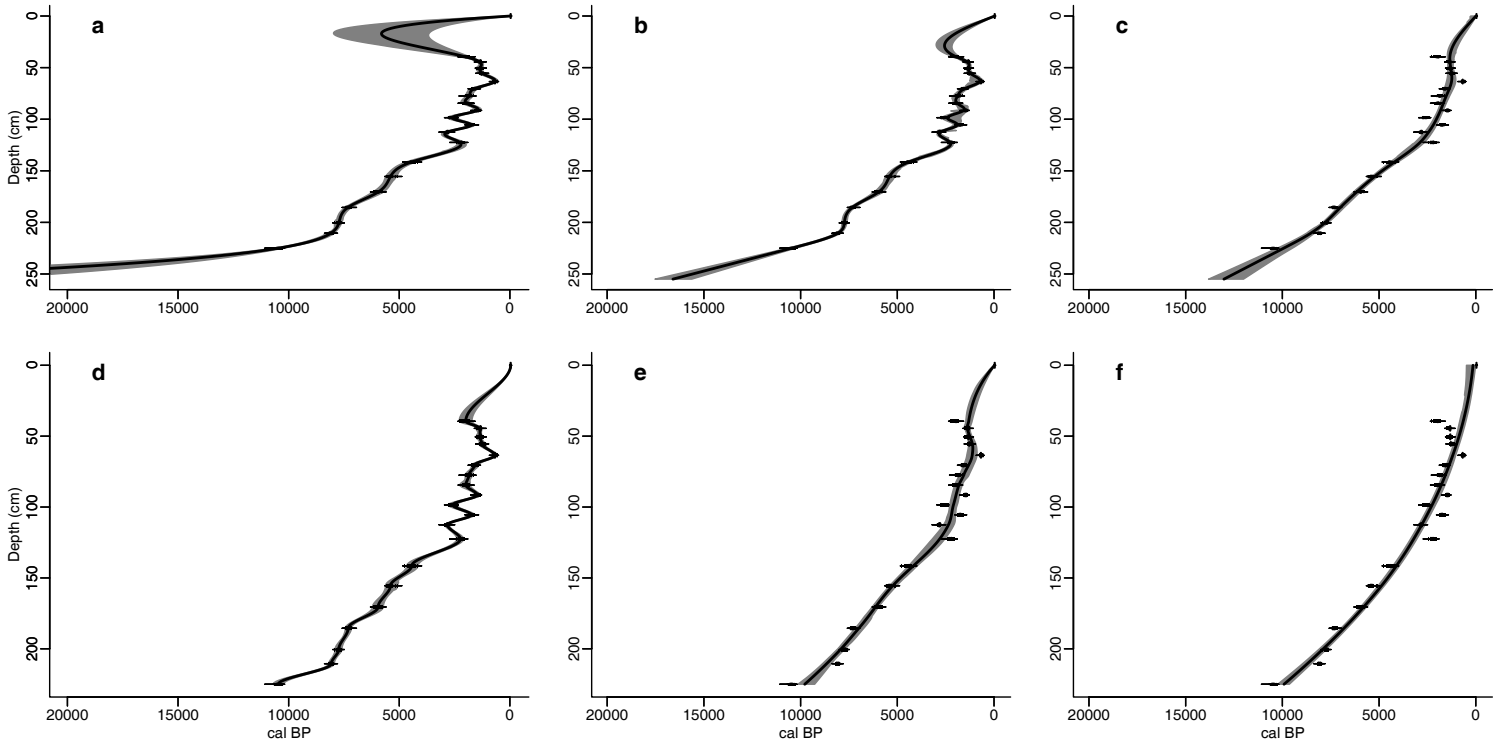
Basic Age-depth models



Blauuw & Heegaard (2012)

Splines & Smoother

- Smoothing spline (a–c) & LOESS smoothers (d–f)
- Simpler models better; unless constrained to be monotonic, reversals often occur
- Extrapolation not possible with LOESS & bad idea with most splines



Blauuw & Heegaard (2012)

Bayesian age-depth models

- Bayesian methods are increasingly popular in age-depth modelling
- Allow range of other information to be combined with the data in a single analysis
- The other information is the *prior* or *prior beliefs*
- Resulting model combines prior with likelihood to give the *posterior* distribution of the parameters of interest

Bayesian age-depth models; chronological ordering

- Use the stratigraphy as the prior by imposing ordering constraints on age estimates
- Usual to assume sediments get older as one moves down the sediment core; tend not to find older material above younger material
- Can use this and other constraints to form an age-depth model
- E.g. Ibbetson (2011) had three dates (104 ± 15; 193 ± 15; 146 ± 15) radiocarbon years
- First date from oldest sediments & last date from youngest, also know that all sediments are older than 1840s
- Radiocarbon in atmosphere fluctuated markedly during period
- Dates don't make sense at first

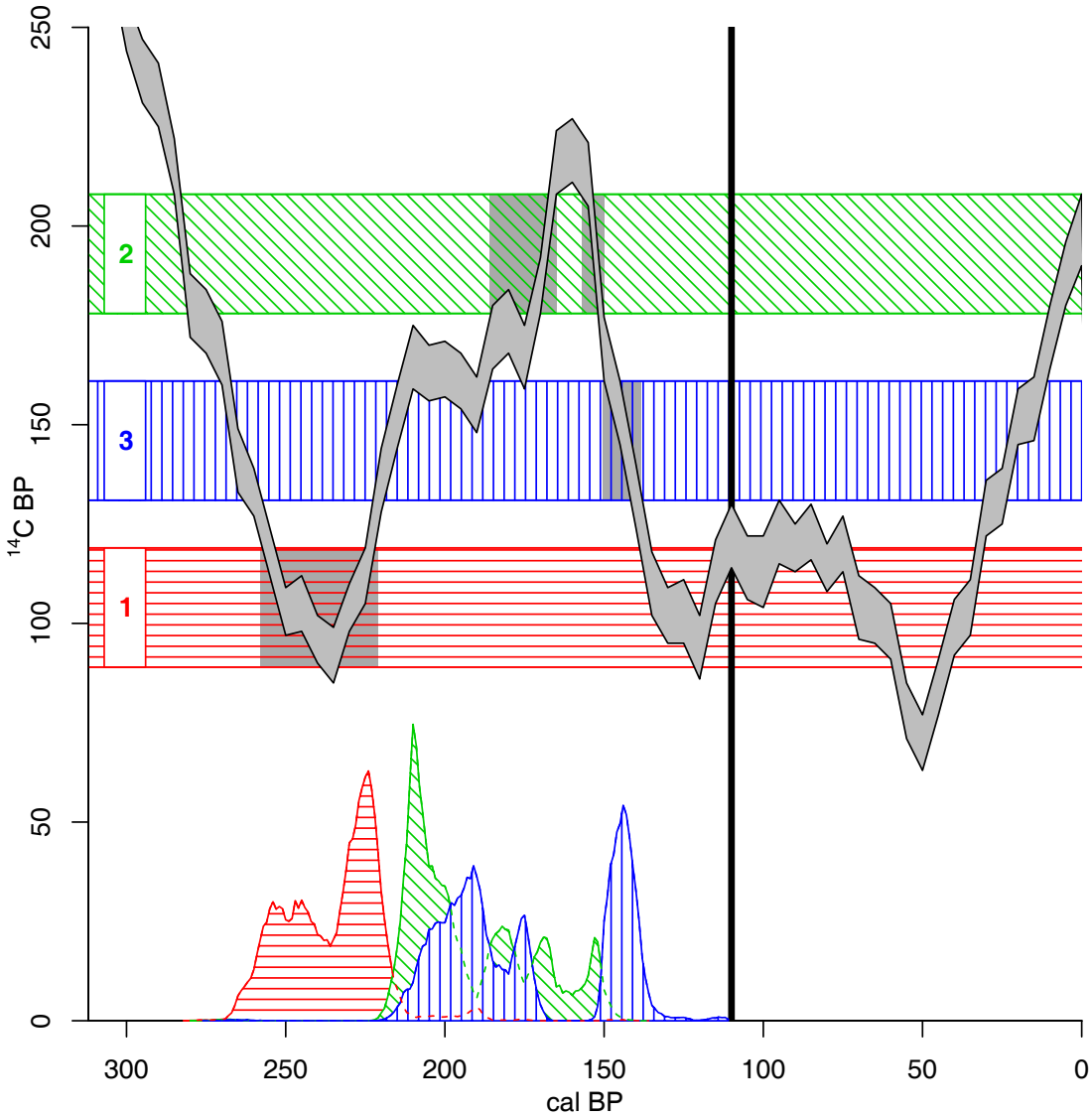
Bayesian age-depth models; chronological ordering

- More formally we express the prior information as (θ is calendar age)

$$\theta_1 > \theta_2 > \theta_3 \text{ and } \theta_{1,2,3} > 110 \text{ cal BP}$$

- Calculate posterior distribution of θ_i given this prior information
- Essentially, sample calendar ages $\hat{\theta}_i$ from calibrated distributions of 3 radiocarbon dates
- However only accept samples draws that meet the above criteria; reject draws that would give reversals or ages younger than 110 cal BP
- Resulting posterior includes information on ^{14}C dates, calibration process and the prior stratigraphic information
- Method doesn't give age estimates for undated levels

Bayesian age-depth models; chronological ordering

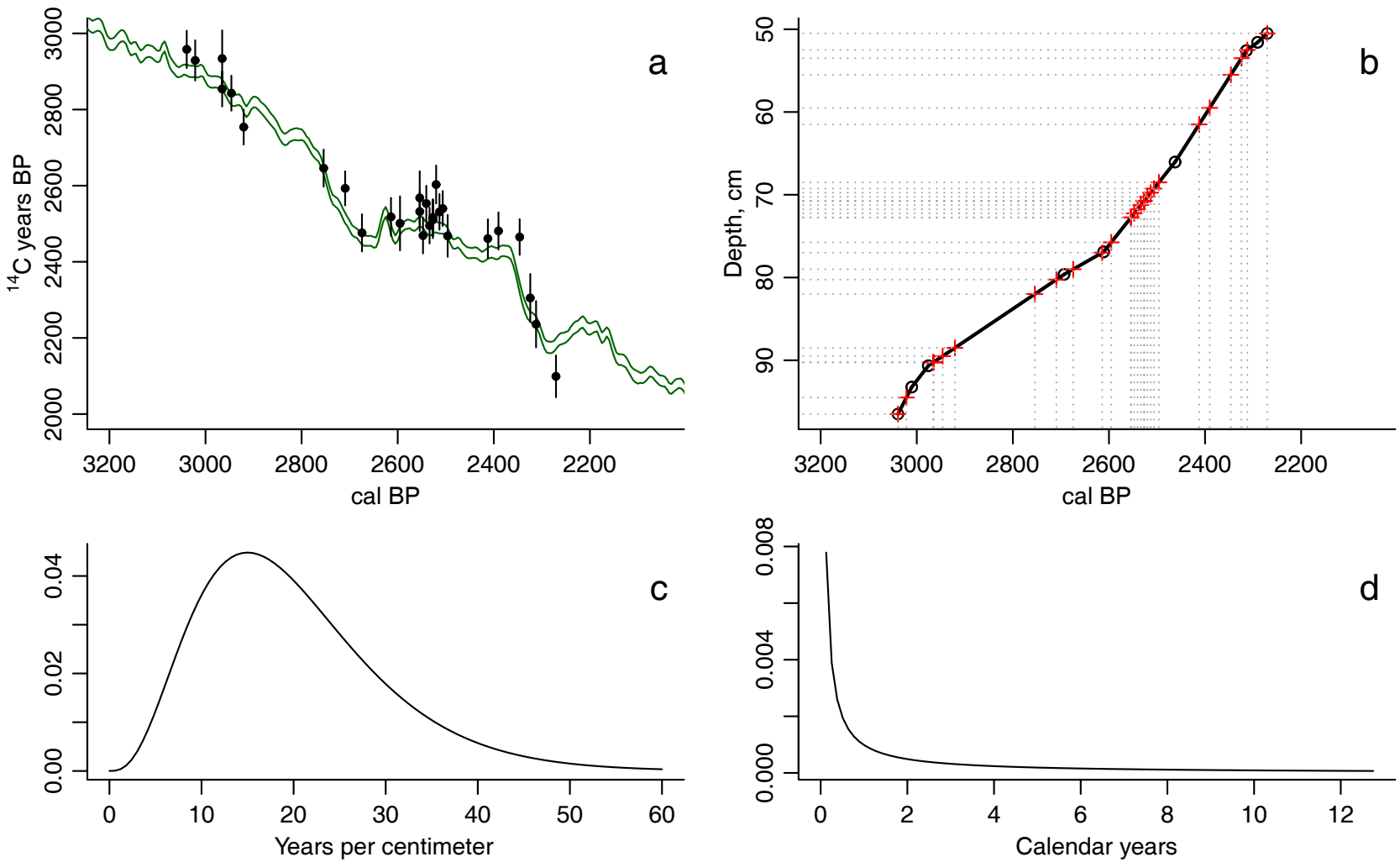


Blauuw & Heegaard (2012)

Bayesian age-depth models; wiggle-match dating

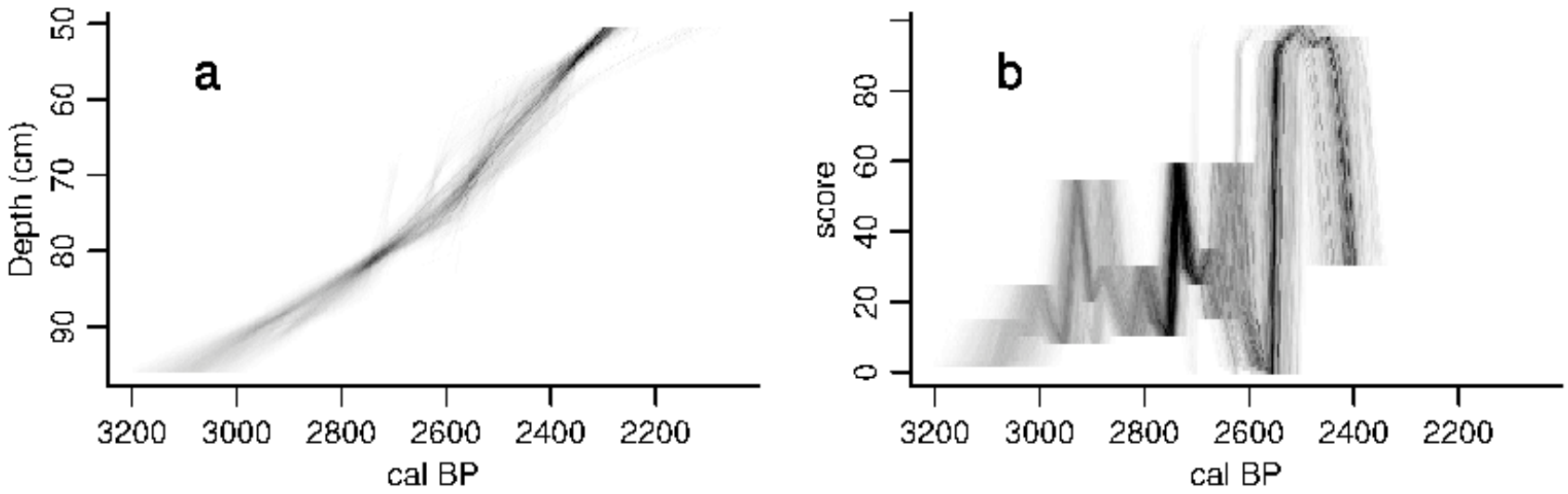
- Requires well-dated core with many dated levels close enough to reconstruct wiggles in ^{14}C calibration curve
- Assume constant sedimentation rate between dated levels
- Match wiggles in ^{14}C dates with wiggles in calibration curve
- Place constraints on how far curves can be moved
- Can't have negative accumulation rates& very high/low accumulation rates are unlikely
- Additional information can be incorporated (e.g. hiatuses, know accumulation rate changes)
- Priors are translated in gamma distributions (always positive)
- Sample repeatedly from the prior distributions & combine with likelihood of calendar age
- Markov Chain Monte Carlo (MCMC) used to generate posterior distribution

Bayesian age-depth models; wiggle-match dating



Blauuw & Heegaard (2012)

Bayesian age-depth models; wiggle-match dating



Blauuw & Heegaard (2012)

Bayesian age-depth models

- Bayesian chronological ordering; Bpeat (Blaauw & Christen 2005, Blaauw et al 2007)
- Piece-wise linear accumulation; Bacon (Blaauw & Christen 2011)
- Piece-wise linear accumulation rate may not be flexible enough
- OxCal (Bronk Ramsay, 2007) models accumulation rates as a Poisson process
- Bchron (Haslett & Parnell 2008) uses Poisson & gamma distributions to model accumulation

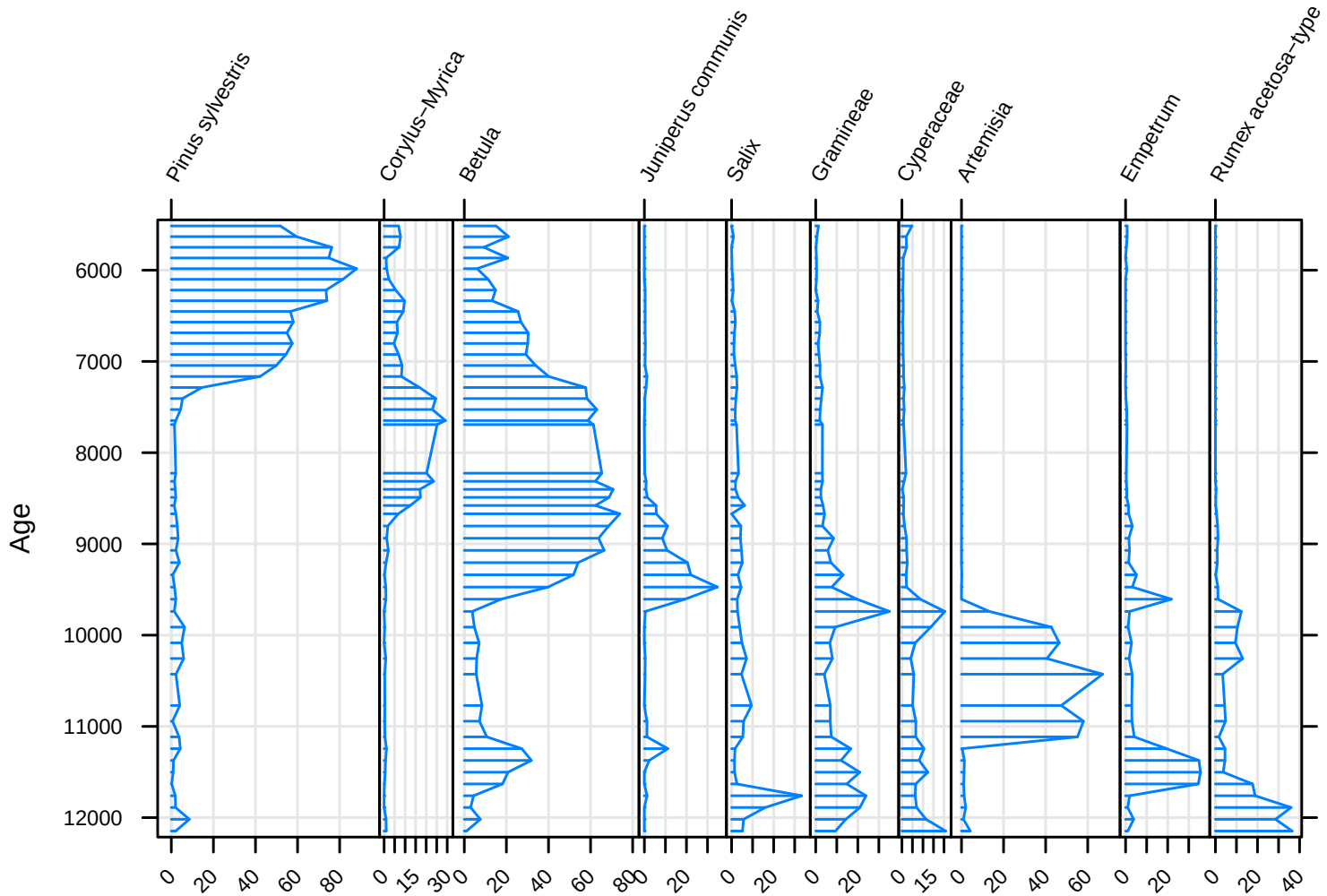
Summarising change in stratigraphic diagrams

- Ordination commonly used to describe patterns of change in multivariate sediment core data
- PCA, CA, or even DCA axis 1 and 2 scores commonly used
- These methods capture largest patterns of variation in underlying data under assumption of particular model
- Can be upset by data sets with a dominant gradient
- Can apply all techniques learned earlier in workshop to stratigraphic data
- Can we do any better than these methods?

Principal Curves

A single long or dominant gradient in an (palaeo)ecological data set poses particular problems for PCA and CA — horseshoe or arch

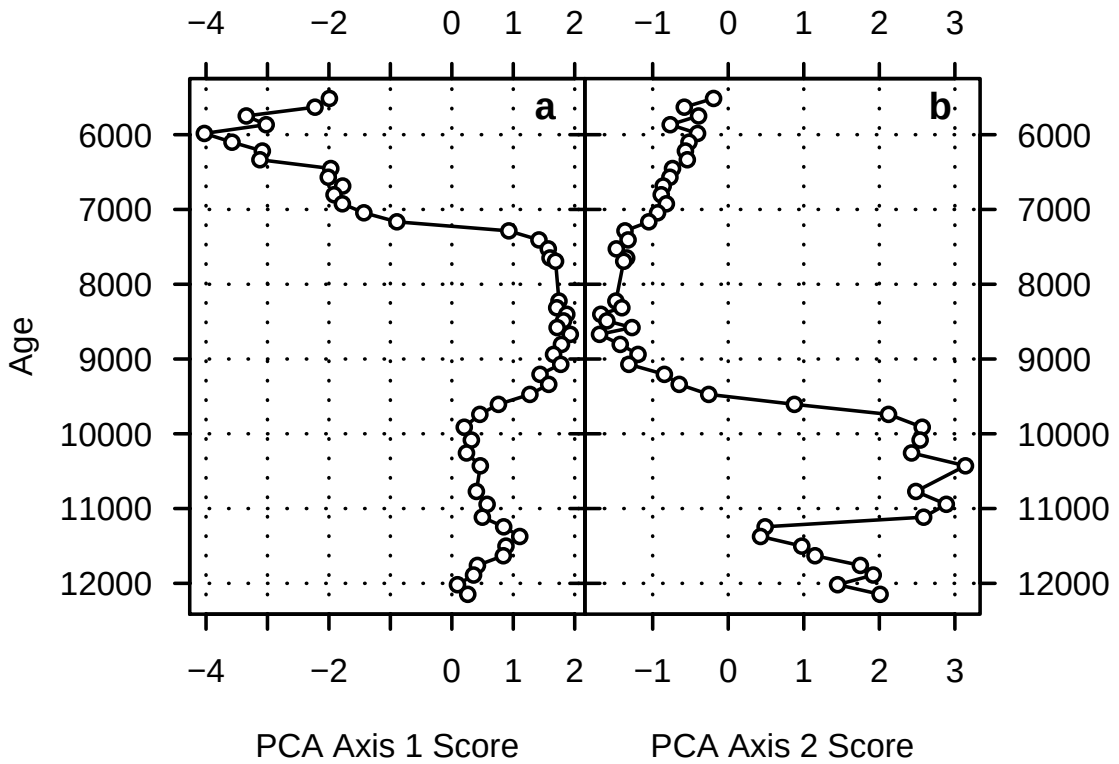
Abernethy Forest pollen data (Birks & Mathewes, 1978)

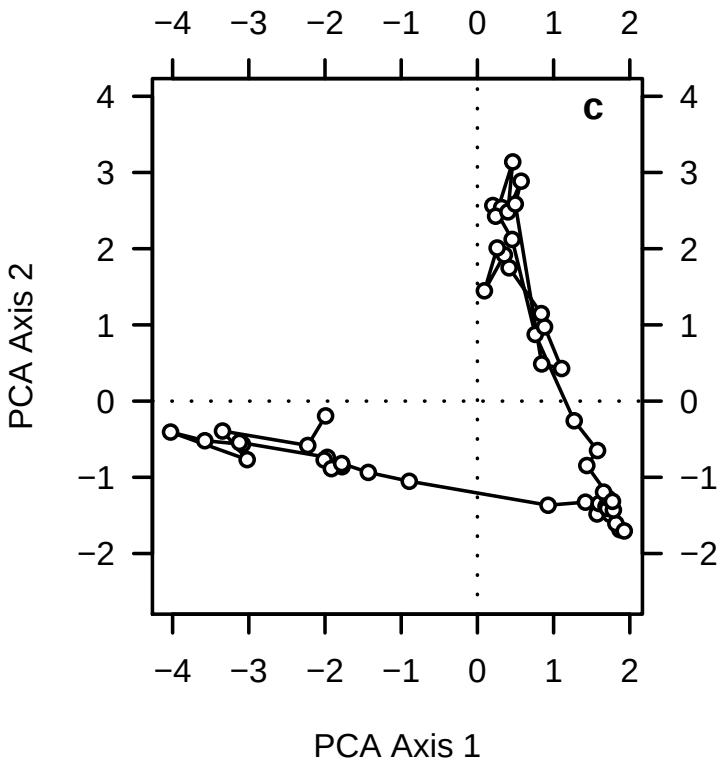


Principal Curves

A single long or dominant gradient in an (palaeo)ecological data set poses particular problems for PCA and CA — horseshoe or arch

Abernethy Forest pollen data (Birks & Mathewes, 1978)



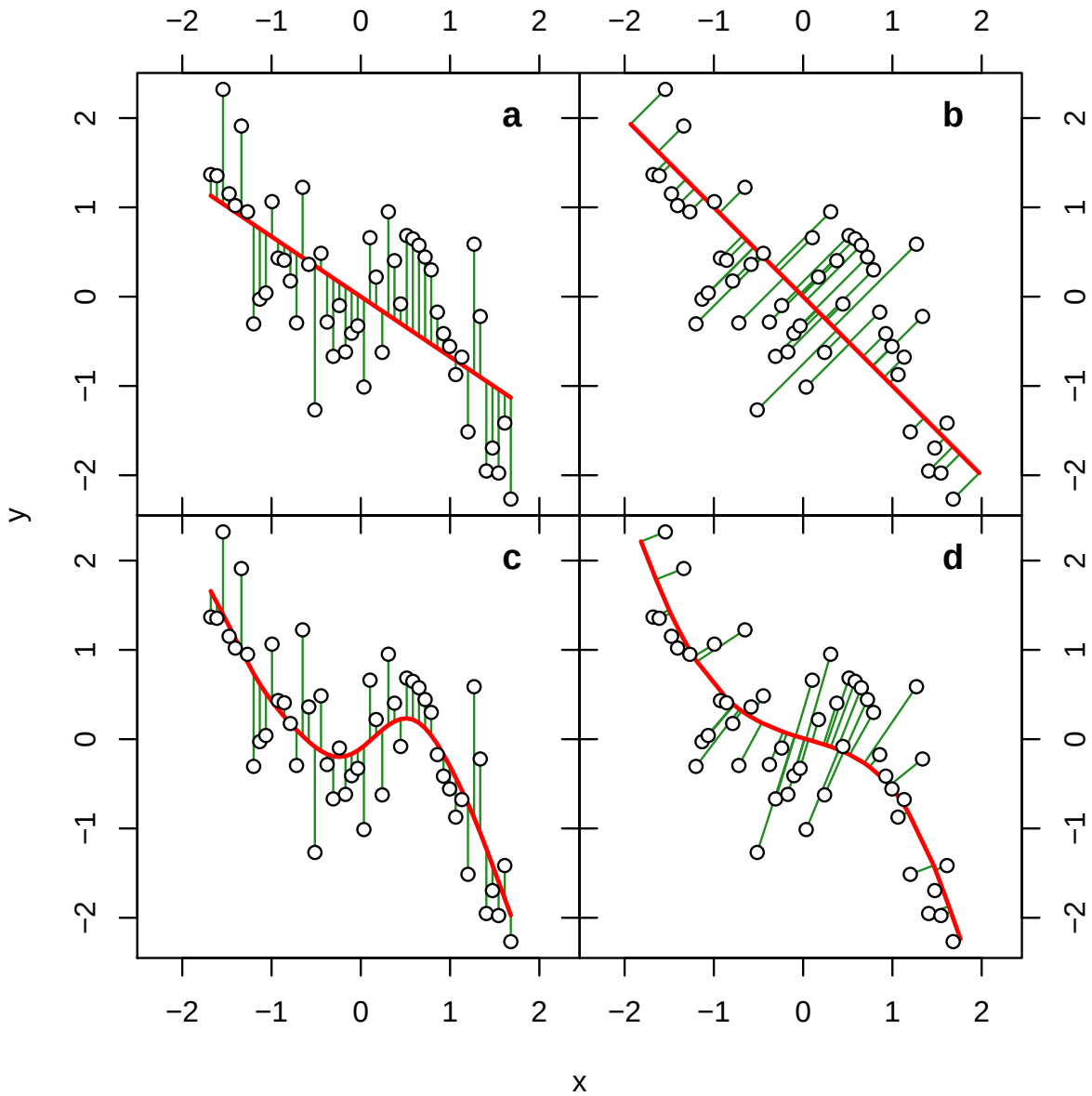


Can we generalise the PCA solution to be a smooth, non-linear surface?

Principal Curves — Comparison of estimation techniques

- In OLS regression, y is the response and x is assumed without error
- Errors are minimised in y only — sums of squared errors
- PCA can be seen as a regression of y on x where neither y nor x plays the role of response or predictor
- In PCA, errors in both x and y are minimised — sums of squared orthogonal errors

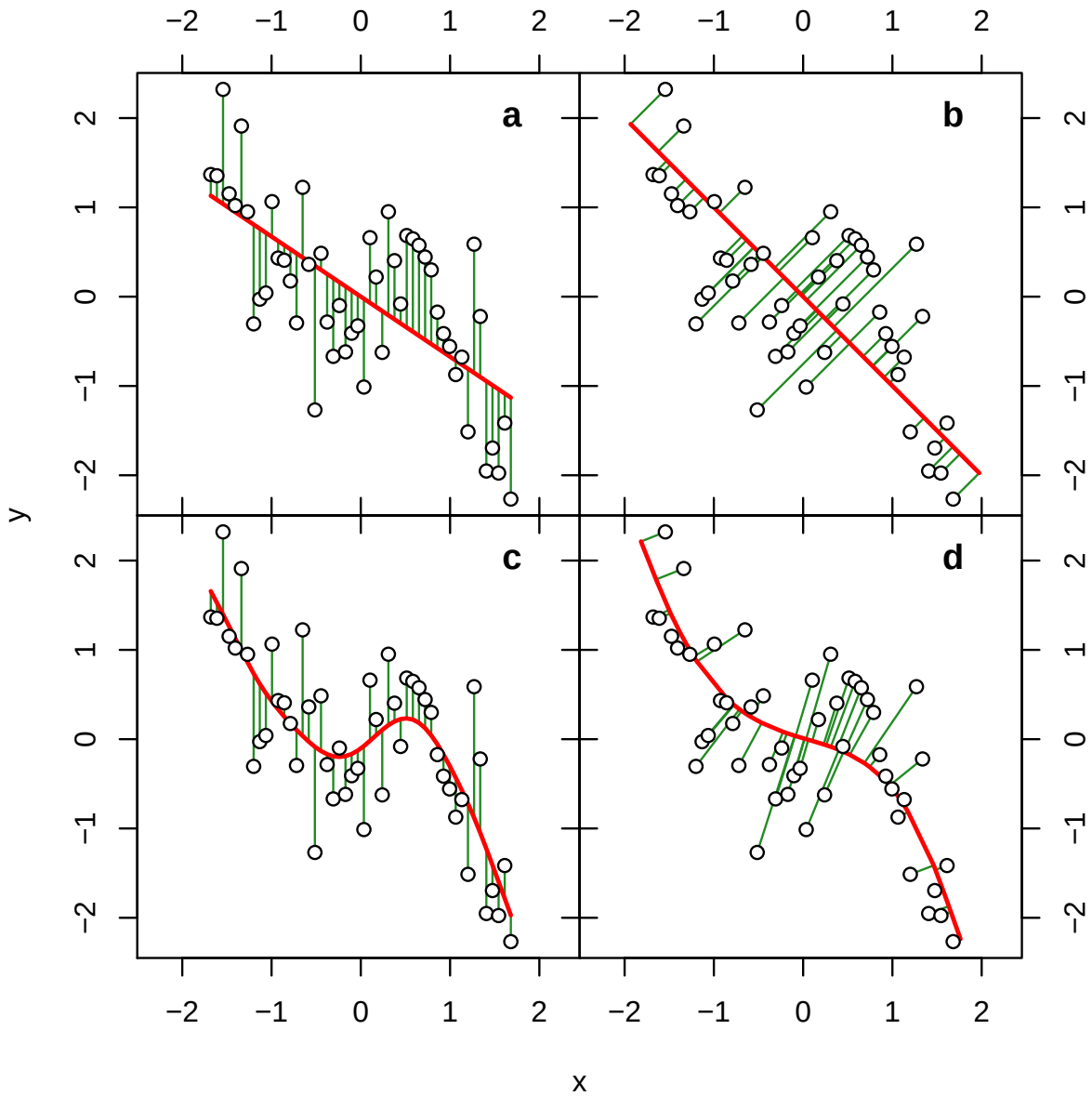
Principal Curves — Comparison of estimation techniques



Principal Curves — Comparison of estimation techniques

- We can generalise the OLS model to a regression of y on x using a smooth function of x ($f(x)$) as the predictor
- $f(x)$ can be estimated using a multitude of techniques
  - Loess smoother
  - Local-linear smooths
  - Smoothing splines
  - Regression splines
  - ...
- $f(x)$ is usually estimated from the data — smoothness determined by minimising a penalised sums of squares criterion under CV (or GCV)
- Errors are still assessed in y only

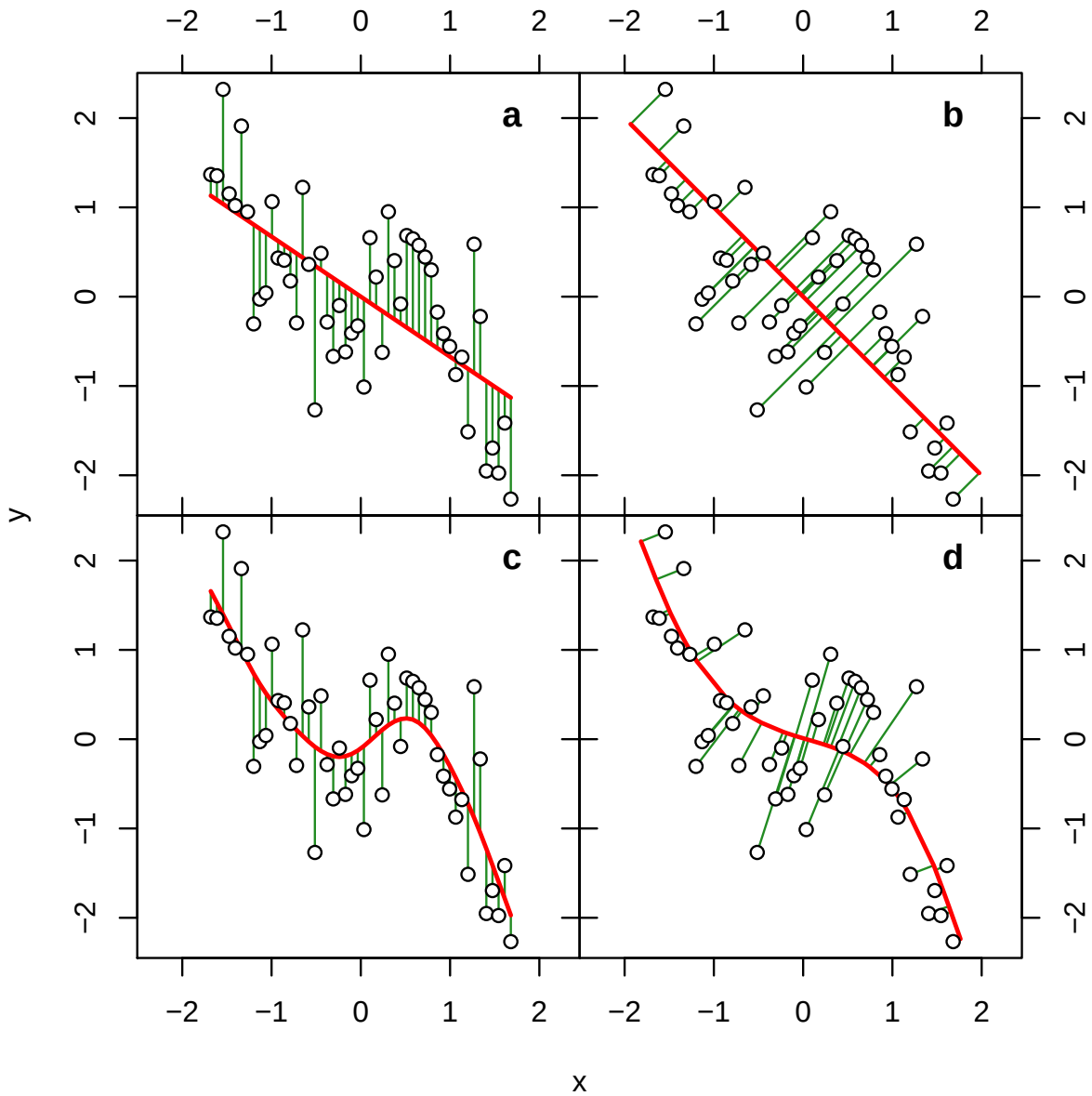
Principal Curves — Comparison of estimation techniques



Principal Curves — Comparison of estimation techniques

- Ideally we would generalise PCA to find non-linear manifolds in the same way as we went from OLS to semi-parametric regression using smoothers
- This is exactly what is done in the method of principal curves
- Our aim is to estimate as the principal curve, a 1-d manifold that passes through the data in high-dimensions that minimises the sum of squared orthogonal errors
- We bend the principal component (for example) towards the data to achieve a better fit to the data
- How far and how flexibly we can bend the curve towards the data is determined from the data to minimise a penalized criterion during fitting

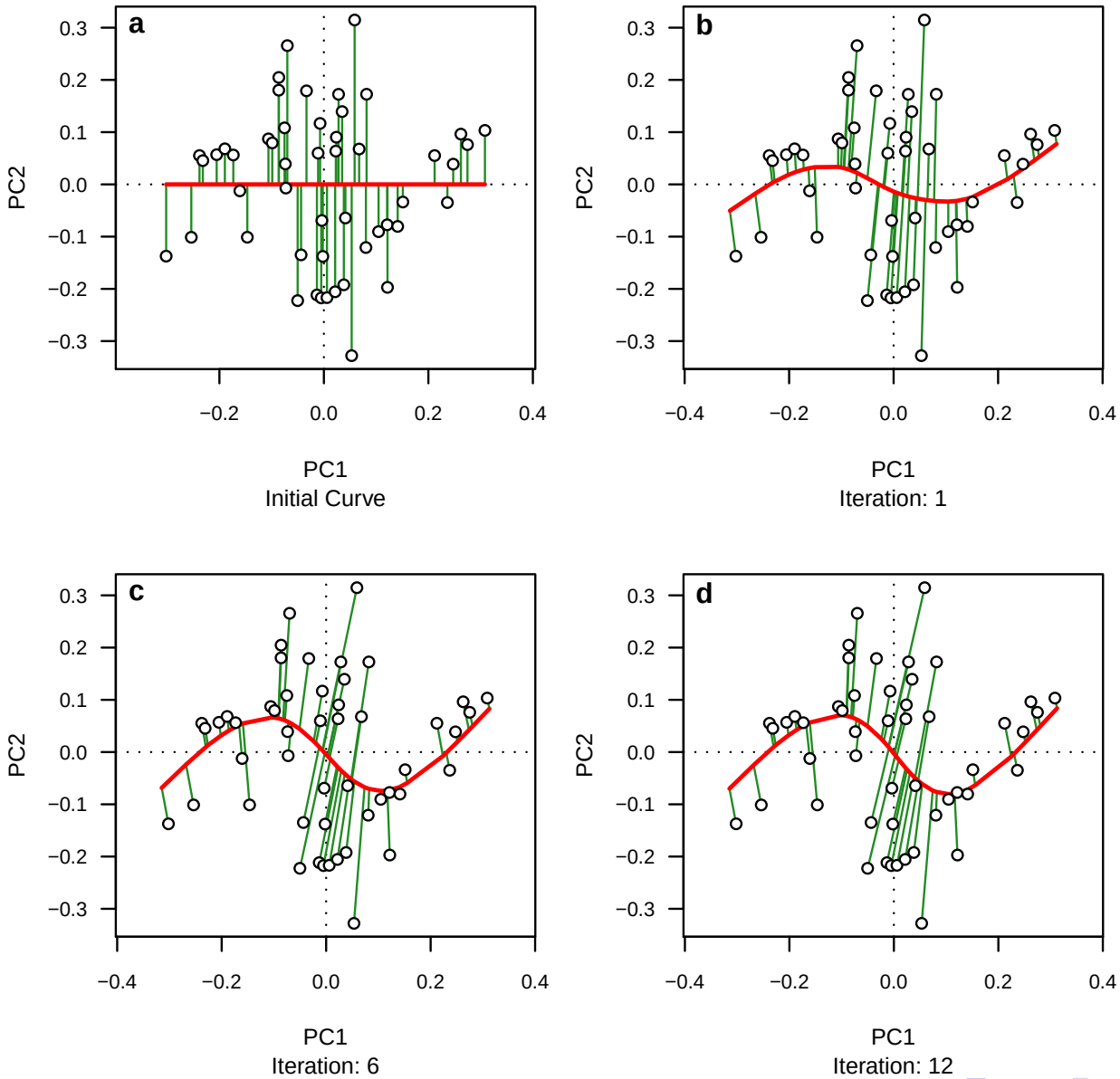
Principal Curves — Comparison of estimation techniques



Principal Curves — Fitting algorithm

- Start with any smooth curve — the first or second PCA or CA axis
- Begin the Projection Step
  - All objects are projected onto a point on the smooth curve that they are closest too
  - The distances of the points along the curve that each object projects onto are determined
- Begin the Local Averaging Step
  - Bend the current smooth curve towards the data so that the sum of squared orthogonal distances is reduced
  - Taking each species (variable) in turn as the response, fit a smoother to predict the response using distance along the current curve as the predictor variable
  - Repeat for all species (variables) and collect the fitted values of the individual smoothers into a matrix that described the new location of the curve in high dimensions
- If the new curve is sufficiently similar to the current curve, declare convergence
- If algorithm has not converged, iterate the projection and local averaging steps until convergence

Principal Curves — Fitting algorithm

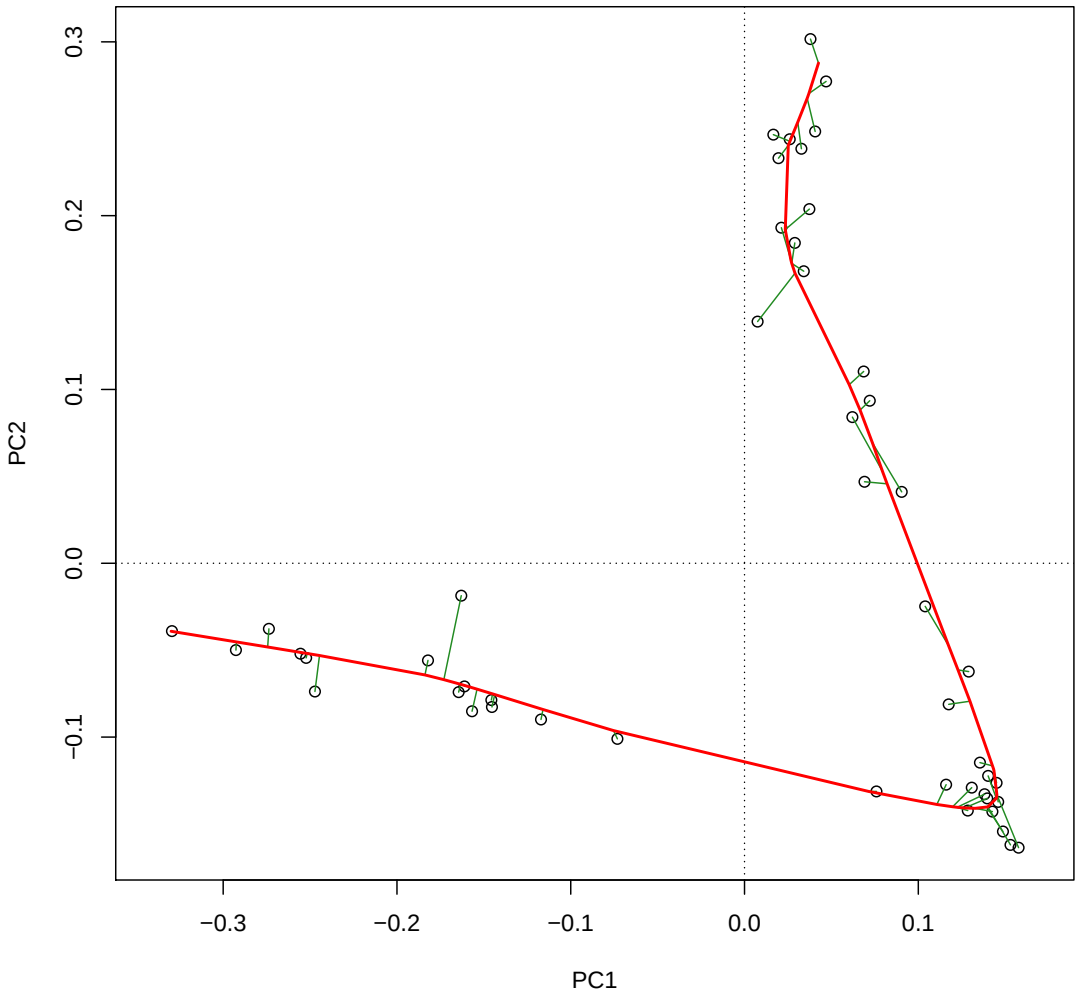


Principal Curves — How Smooth?

- The smoother fitted to produce the principal curve is a plug-in element of the algorithm
- Can use any smoother; here used cubic regression splines
- Important to not over fit the data by allowing too-complex a curve
- Several options
  - Fit PCs with a large span (few df), note error, then reduce span (increase df), note error, etc. Use screeplot to determine optimal span
  - Fit smoothers to each species using starting curve, allowing (G)CV to choose optimal smoothness for each species. Fit the PC using the median of the smoothness values over all species
  - Allow the optimal degree of smoothness to be determined for each species individually during each local averaging step
- Advantage of latter is that those species that vary along the curve more strongly can use more degrees of freedom than those species that only vary lineally

Principal Curves — Abernethy Forest

Visualise the fitted curve in PCA space



Principal Curves — Comparison with PCA and CA

- The PC describes the long, sequential gradient in vegetation in a single variable
- The PC explains 96% of the variance in the absolute pollen data
- PCA axis 1 explains 47% and CA axis 1 31% of the variance in the data
- We need at least 2 PCA axes to fully capture the single gradient (80.2%)
- Distance along the curve between adjacent time points is a measure of compositional change
- Can be expressed as a rate of compositional change — highlights the periods of rapid compositional change in the Abernethy sequence

Rate of change analysis

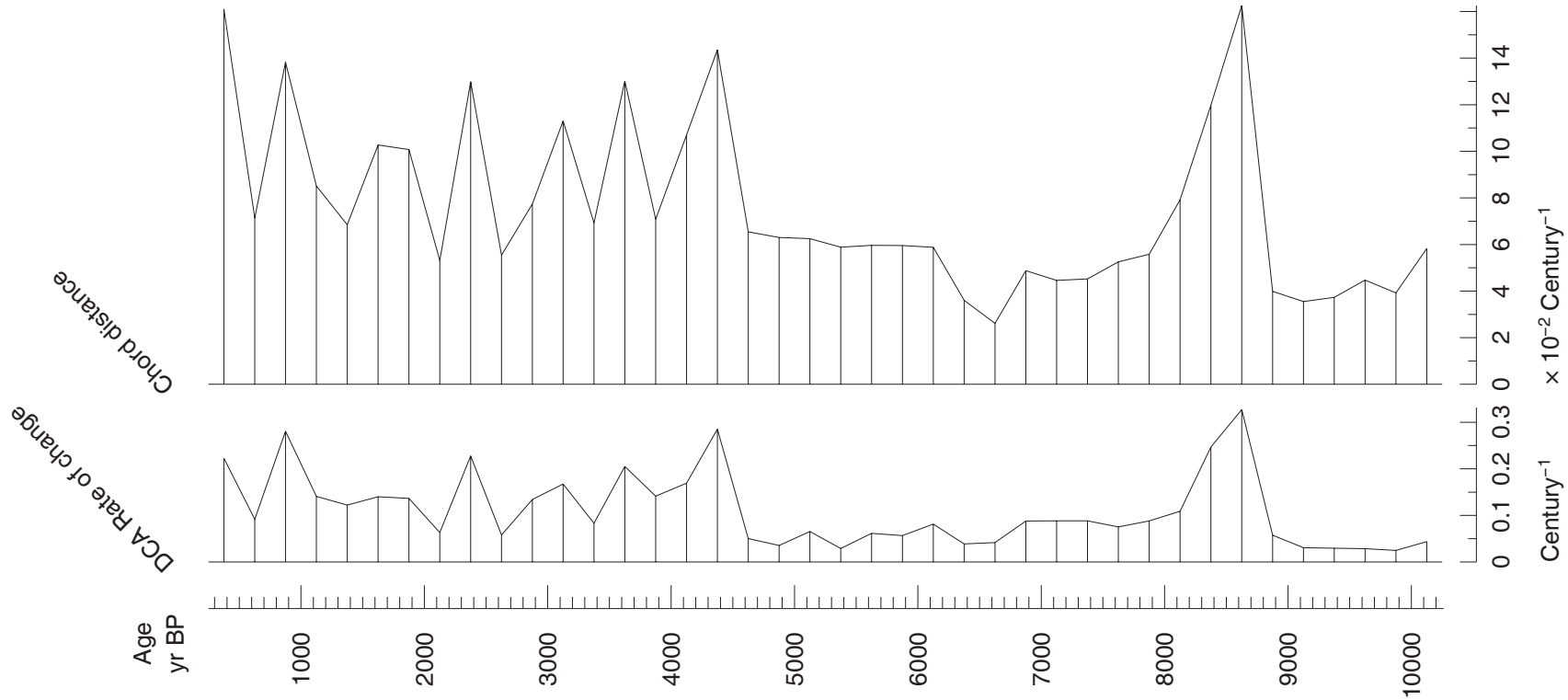
- Stratigraphic sequences record changes over time
- How quickly do these changes take place?
- Rate of change analysis aims to answer this
- Two general approaches
  - change in ordination units
  - change measured in dissimilarity

Rate of change analysis

- Jacobsen & Grimm (1988) method involves
  1. smooth the data
  2. interpolate to constant time intervals
  3. ordinate smoothed, interpolate data (e.g. using DCA)
  4. calculate change in ordination/axis score units as measure of RoC
- Dissimilarity-based approach can be performed two ways
  1. Smooth the data & interpolate, *then* compute dissimilarity between interpolated levels
  2. Compute dissimilarity between adjacent samples directly, then standardise dissimilarity by time interval between samples.

Rate of change analysis — RLGH diatoms

DCA-based (lower) & dissimilarity-based (upper) rate of change analysis. DCA distance based on 3 axes). All data smoothed (5 term cubic spline) & interpolated to 250 yr intervals.



Birks (2012)

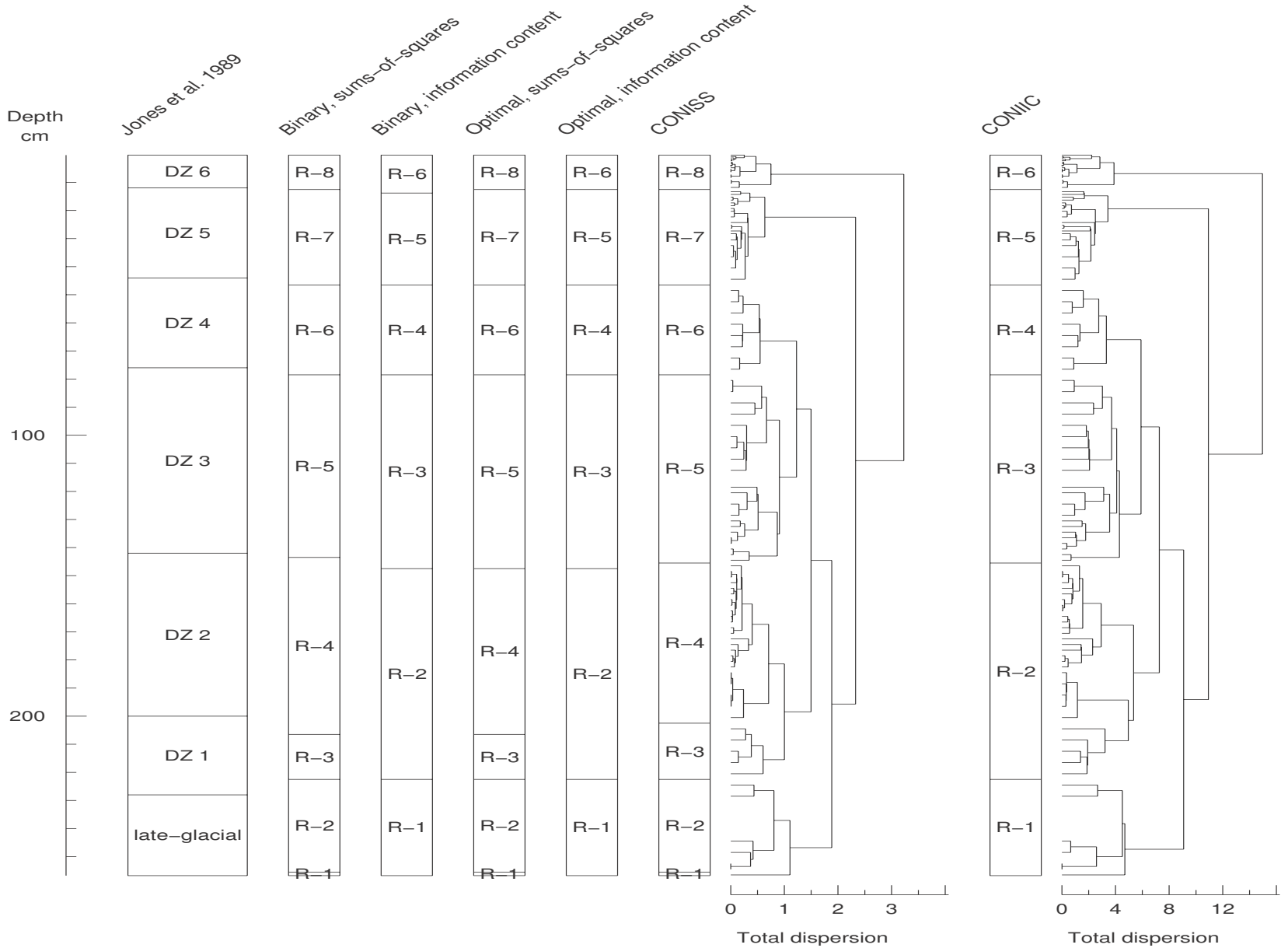
Chronological clustering

- Chronological (or constrained) clustering commonly used to partition a sediment sequence into 2 or more zones
- Useful for, *inter alia*
  - delineating periods of similar species composition
  - identifying discontinuities or periods of rapid change
  - to facilitate description of a stratigraphic sequence
- As with standard cluster analysis, plethora of methods available
  - Optimal partitioning
  - Binary (divisive) splitting
  - Agglomerative partitioning
- Can be used with any dissimilarity (in theory), but common ones are
  - Cluster sums of squares (within-group Euclidean distance)
  - Cluster-wise information statistic

Chronological clustering

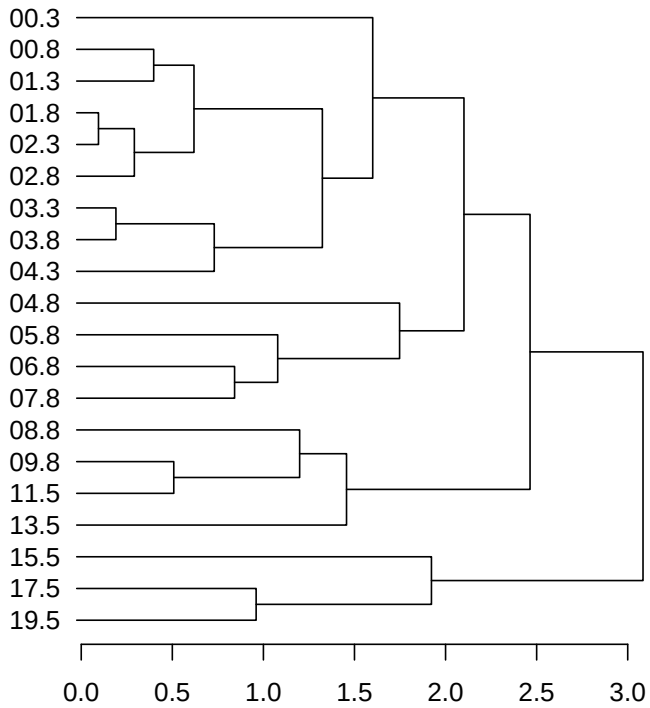
- Optimal partitioning
  - Identifies optimal locations for splits to form k zones
  - Non-hierarchical, 3 zone solution **not** found by splitting one of the zones from the two zone solution
  - Split placed to minimise within-cluster sum of squares or information content
- Binary (divisive) splitting
  - Similar to optimal method but *is* hierarchical
  - Split sequence into two zones, then split one of the 2 resulting zones, repeat
  - Zone that is split is the one that would reduce within-group SS or IC the most
- Agglomerative partitioning
  - Start with all samples in separate zones and fuse the most similar adjacent samples
  - Repeat, each time fusing most similar samples or zones

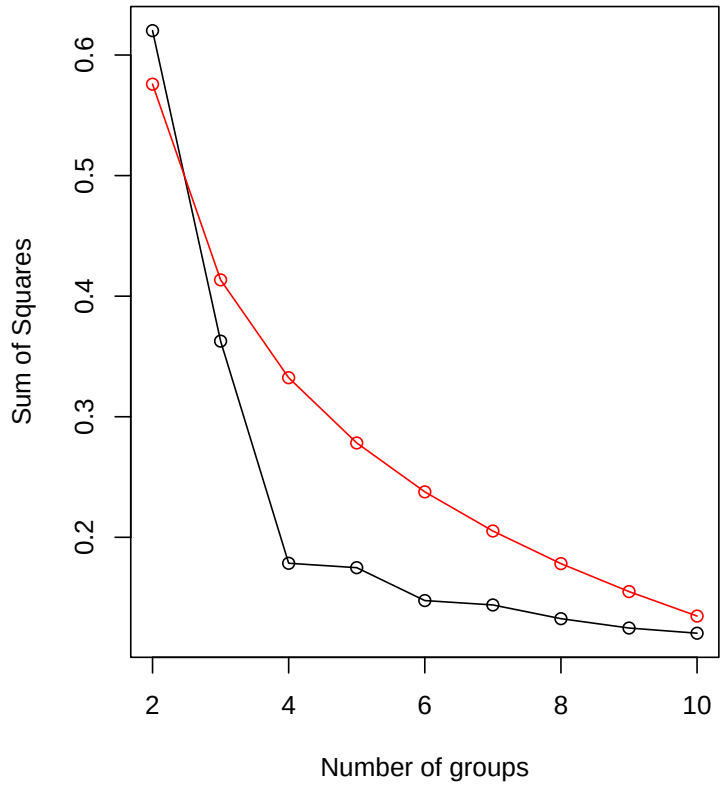
Chronological clustering



CONISS

```
> require(rioja)
> data(RLGH)
> diss <- dist(sqrt(RLGH$spec/100))
> clust <- chclust(diss)
> plot(clust, hang=-1, horiz=TRUE, x.rev = TRUE)
> bstick(clust, 10)
```





Binary splitting via MRT