Stratigraphic Data

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Introduction

Introduction

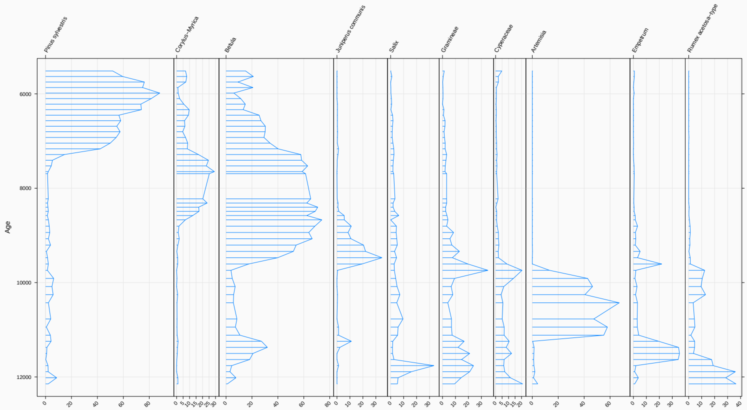
Summarising stratigraphic data

Summarising change in stratigraphic data

- 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

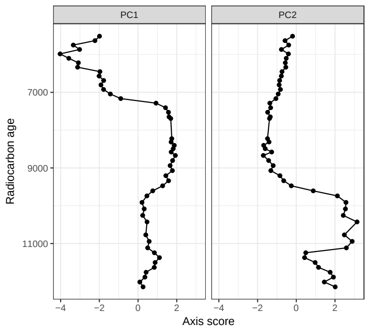


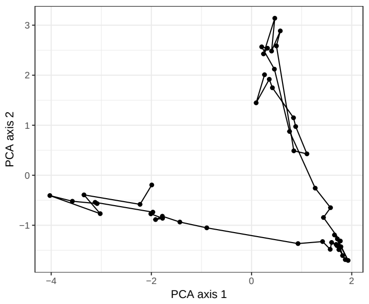
Abernethy Forest pollen data (Birks & Mathewes, 1978)

Principal Curves

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

Trend is broken over two or more axes:



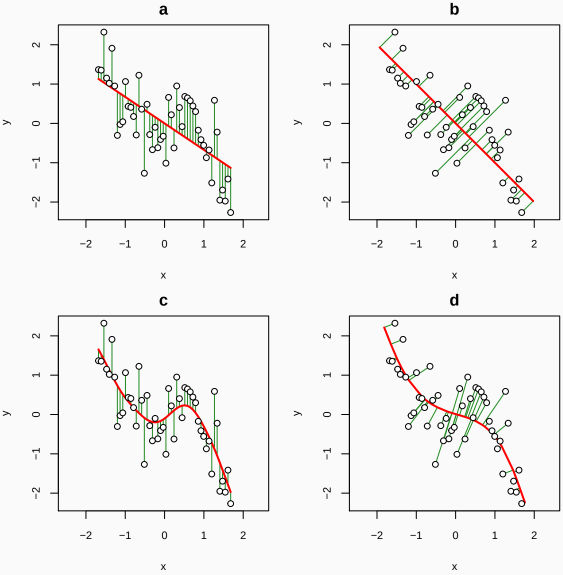


Can we generalise the PCA solution to be a smooth, non-linear surface?

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



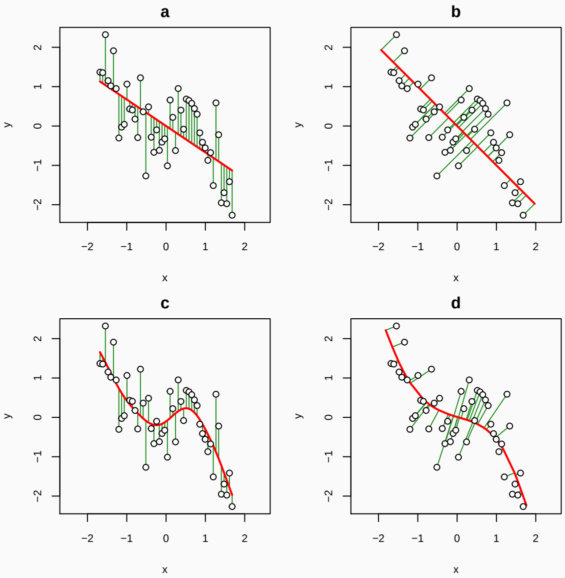
We can generalise the OLS model to a regression of y on x using a smooth function of x, $f(x)$, as the predictor

$f(x)$ 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, with smoothness determined by minimising a penalised sums of squares criterion under CV (or GCV): **Errors are still assessed in y only**

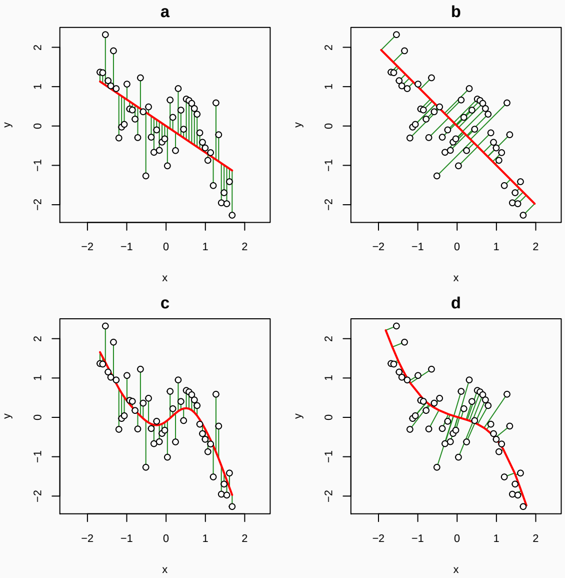
Principal Curves — Comparison of estimation techniques



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

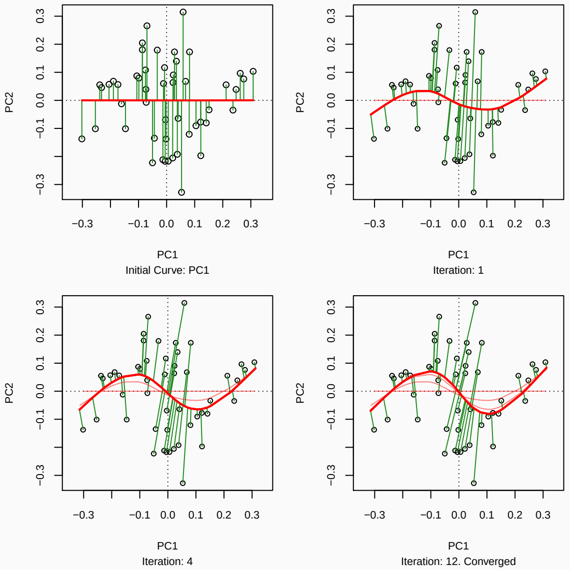
Principal Curves — Comparison of estimation techniques



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

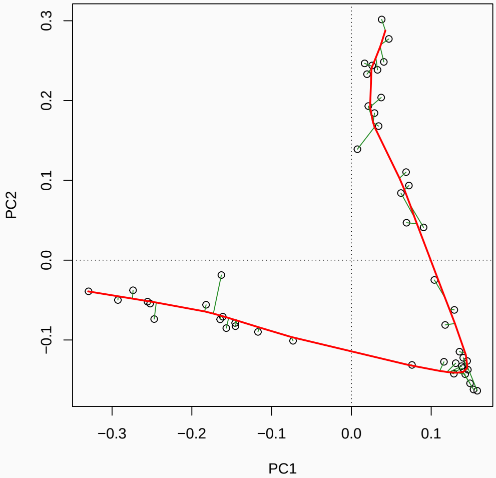
```
> aber.pc <- prcurve(abernethy2, trace = FALSE, vary = TRUE, penalty = 1.4)
> aber.pc
```

```

    Principal Curve Fitting

Call: prcurve(X = abernethy2, vary = TRUE, trace = FALSE, penalty
= 1.4)

Algorithm converged after 6 iterations

           SumSq Proportion
Total     103234      1.000
Explained  98864      0.958
Residual    4370      0.042

Fitted curve uses 218.3391 degrees of freedom.
```

```
> varExpl(aber.pc)
```

```
      PrC
0.9576693
```

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

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
- Could also use
    - derivatives of splines from principal curve
    - derivatives of GAM(s) fitted to variables of interest

Rate of change analysis

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

Rate of change analyis

TODO - needs an example

Chronological clustering (zonation)

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

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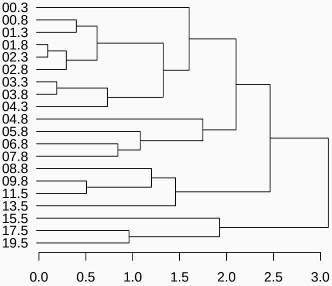
Chronological clustering

TODO insert HJBB's figure 1 from chpt 11 DPER5

CONISS


00.3
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1.0
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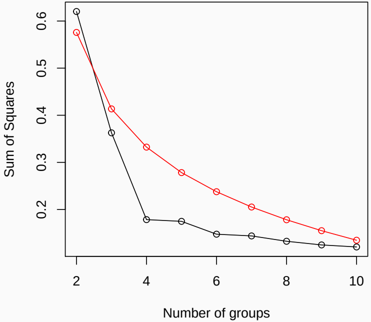
2.0
2.5
3.0


Sum of Squares
0.2
0.3
0.4
0.5
0.6
2
4
6
8
10
Number of groups

Binary splitting via MRT