

## From Last Meeting

Finished ICA

Analysis of Mass Flux data:

- Insights from “clustering”
- Explored “rotation of PCA directions”

# Goodness of Approximation

I.e. how many basis elements to use?

E.g. Corpora Callosa data

Recall “shape representations” are based on  
 $d = 80$  dimensional “feature vectors”

Show CCFrawAlls3.mpg

How big does  $d$  need to be?

A personal working assumption:

“shape is complicated, so need  $d$  large”

## Major sticking point

For medical image shapes, usually have “few data points”,  
 $n < d$

Personal approach:

- that complicates matters
- but “shape” is “complex” and requires complex rep'n
- hence need to develop new statistical methods:

High Dimension Low Sample Size

## Classical Approach

- Statistical Multivariate Analysis is based on “standardizing”
- Multiply by  $\hat{\Sigma}^{-1/2}$  (for covariance matrix)
- Requires  $n > d$  (else matrix inverse doesn't exist)
- For  $n \leq d$ , do “dimension reduction”
- For example, keep only the “1<sup>st</sup> few Principal Components”

## Questions:

Is dimension reduction (e.g. PCA based) “good enough”?

Or is it important to develop HDLSS methods?

Aside: how well do ANOVA sums of squares “capture shape”?

Study in context of corpus colosum data

## Fourier Approximation Background:

Represent:

$$Shape = \sum_{j=1}^d c_j BE_j$$

where the  $c_j$  are the “Fourier Coefficients”

and where the  $BE_j$  are “basis element” shapes

## Fourier Approximation Background (Cont.):

Problem:  $BE_j$  have “parametric representation”,  
so hard to view individually

Solution: Interesting web site:

<http://www.cs.unc.edu/~seanho/migggg/fourdem.html>

show CorpColl\BdryFourDemo\fourdem.html

Some examples of generated shapes:

Show CorpColl\CCFbasis.ps

# Approximation 1: Raw Fourier Coefficients

View “goodness of approximation” of

$$k - \text{approx. Shape} = \sum_{j=1}^k c_j BE_j$$

for  $k = 0, 1, 2, \dots, d$

show CCFappFourAlls3C4.mpg

- $k = 0$  single point: the “zero function”
- $k = 1$  just a line
- $k = 2, 3$  still a line (due to “shape normalization”)



## Approximation 1: Raw Fourier Coefficients (cont.)

- $k = 4$  ellipse
- $k > 4$  more complicated shapes
- larger  $k$  get convergence towards full shape
- $k = 80 = d$  blue completely covers white

## Approximation 1: Raw Fourier Coefficients (cont.)

ANOVA style Sums of Squares:

$$\text{Signal Power}(k - \text{Approx.}) = \sum_{j=1}^k c_j^2$$

Measures “goodness of fit”, on scale of “energy”

Energy decomposition:  $c_j^2$  is “power in signal in direction  $BE_j$ ”

Show upper left of CCFappFourAlls3.ps

# Approximation 1: Raw Fourier Coefficients (cont.)

Useful scales:

- log scales

Show bottom row of CCFappFourAlls3.ps

- relative scale:  $c_j^2 / \sum_{j'=1}^d c_{j'}^2$

Show center of CCFappFourAlls3.ps

- cumulative relative scale:

$$\frac{\sum_{k=1}^k c_k^2}{\sum_{j'=1}^d c_{j'}^2}$$

Show right of CCFappFourAlls3.ps

## Approximation 1: Raw Fourier Coefficients (cont.)

What does “cumulative relative signal power” really measure?

Again show CCFappFourAlls3C4.mpg

- $k = 2$  line alone is 93%
- $k = 6$  nearly elliptical is 95%???
- $k = 12$  99%, but still “misses lots of shape”
- $k = 25$  99.9%, still don't have all of this “shape”?

Have looked at some others: similar lessons

## Approximation 2: Centered Fourier Coefficients

Main idea: subtract out the mean first

- standard in ANOVA (often huge part of Sums of Squares)
- results in much different interpretation (of relative SS)

When is “90% of SS explained”?

- **Case 29:** 31 terms: all of shape

show CCFappCFourAlls3C3.mpg

- **Case 2:** 11 terms: missed a lot of shape

show CCFappCFourAlls3C1.mpg

## Approximation 2: Centered Fourier Coefficients (Cont.)

Paradox of cumulatives (“data compression” plots):

- **Case 2** has “great compression” (high curve), yet needs ~50 terms (99.8% explained) for “good shape rep’n”
- **Case 29** has “poor compression” (low curve), yet needs only ~32 terms (92.53% explained) for “good shape rep’n”

Personal conclusion:

“shape” manifestations of Sum of Square Analysis is “slippery”

## Approximation 3: Principal Component Analysis

### Recall Ideas:

- Find “directions of greatest variability”
- Will “maximize signal compression”
- Works in an “average sense”, **not** individually
- Use  $1^{\text{st}}$   $k$  for “dimensionality reduction”

## Approximation 3: Principal Component Analysis (cont.)

### Overlay of cumulatives:

Show CCFappPCAAlls3.ps

- cumulative eigenvalues (“average”) shown in yellow
- much better signal compression than centered Fourier

flip back to CCFappCFourAlls3.ps

- colored cases are extremes of signal compression:
- **Case 2** is “great”, **Case 13** and **Case 29** are “poor”
- **Case 35** is “closest to average”



## Approximation 3: Principal Component Analysis (cont.)

How well does “90%” capture “shape”?

- **Case 2**: poor (happens at  $k = 1$ )

Show CCFappPCAAlls3C1.mpg

- **Case 13** and **Case 29** good (happens at  $k = 16$  and  $k = 17$ )

Show CCFappPCAAlls3C2.mpg and CCFappPCAAlls3C3.mpg

- **Case 35** not quite (happens at  $k = 6$ )

Show CCFappPCAAlls3C4.mpg

- $k$  is more useful than “% variability”?

## Approximation 3: Principal Component Analysis (cont.)

How many terms are needed to capture shape?

- **Case 2:**  $k = 17?$

Show CCFappPCAAlls3C1.mpg

- **Case 13**  $k = 15?$

Show CCFappPCAAlls3C2.mpg

- **Case 29**  $k = 16?$

Show CCFappPCAAlls3C3.mpg

- **Case 35**  $k = 15?$

Show CCFappPCAAlls3C4.mpg

## Personal conclusions

- “Sums of Squares” are very crude surrogate for “shape”
- Not enough to “just work with 1<sup>st</sup>  $k$  PCs”
- Not enough to “just work with PCs with top 95% of signal”
- Careful about “average fit” (as in PCA), vs. “individuals”
- 15 – 20 PCs “captures shape for Corpus Callosum data”
- Expect more needed for higher dim’nal objects

Show GreggTracton.html

Still worth developing **HDLSS**