Inference for Data Visualization

Christof Seiler

Stanford University, Spring 2016, Stats 205

Introduction

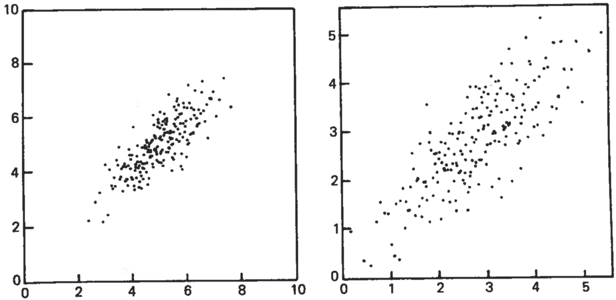
- Exploratory data analysis is usually not parametric
- For instance, in Principle Component Analysis (PCA), we do not assume any parametric model (the data doesn't need to be normally distributed)
- What is described by PCA is a decomposition of the data into Principle Components (PCs) along which the variance is maximized after projecting the data
- But, as we have seen in this course, it is in general not necessary to assume a parametric model for inference

Introduction

- We successfully used ranks that allowed to remove the normality assumptions in one and two-sample tests
- We successfully used the bootstrap to sample from the empirical distribution and construct confidence intervals
- We successfully used permutation tests for hypothesis testing
- In all these examples we have found ways to make inference
- Is this possible for data visualization?
- That's the topic for today

Magical Thinking

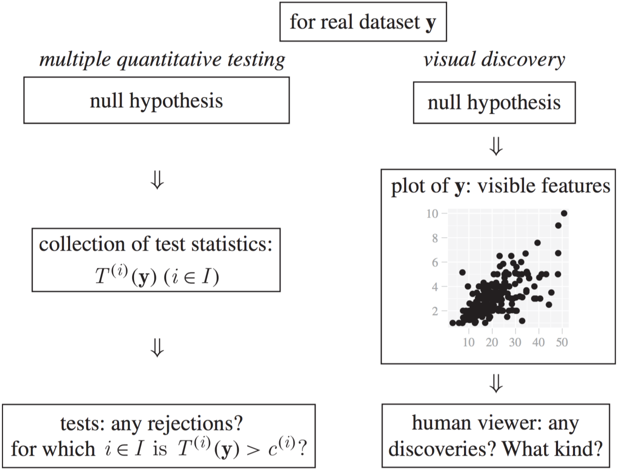
- Professional statisticians and other scientists with statistical training were ask “How associated the two variables were”



Source: Diaconis (1983)

- Most of the subjects judged left plot as more associated than right plot (the same data points)
- Rescaling can shift the perceived association by 10 to 15%

Inference for Plots: The Lineup



Source: Buja et al. (2009)

Inference for Plots: The Lineup

- Generate 19 null plots
- Arrange all 19 plots and insert the real data at random location
- Ask human viewer to single out the real plot
- Under the null hypothesis that all plots are the same, there is a one in 20 chance to single out the real one
- If the viewer chooses the plot of the real data, then the discovery can be assigned a p-value of $1/20 = 0.05$
- Larger number of null plots could yield a smaller p-value
- But there is a limit of how many plots a human can consider

Inference for Plots: The Lineup

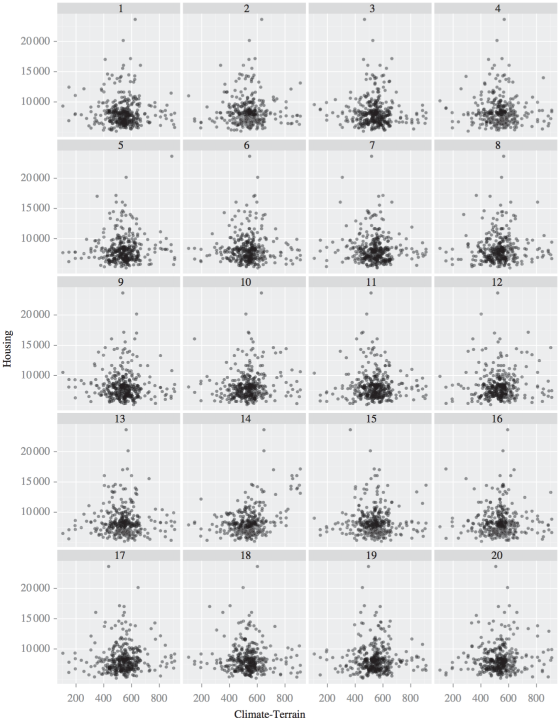
- This protocol can be repeated with multiple independently recruited viewers
- Consider K viewers and $k \leq K$ selected the plot of the real data
- Then the combined p-value is probability $P(X \geq k)$ following a binomial distribution with K trials and success probability $1/20$
- Can be as small as 0.05^K if all viewers picked the plot of the real data

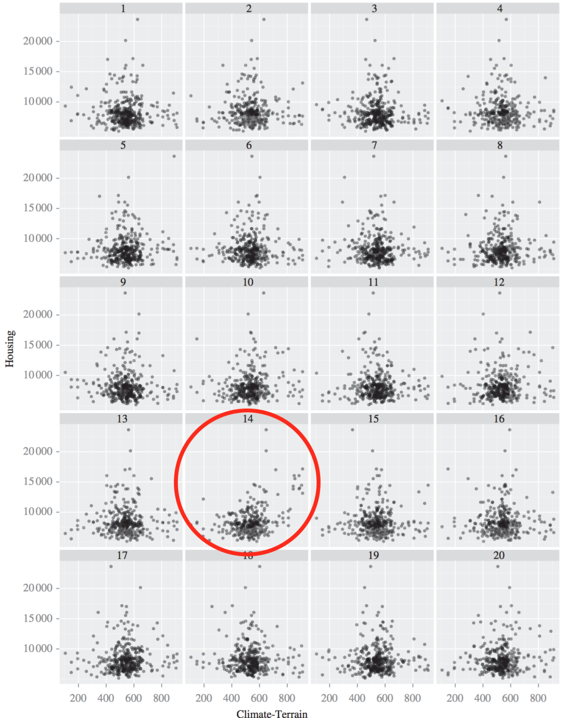
Inference for Plots: The Lineup (Example)

- Example comes from Boyer & Savageau (1984) where cities across the USA were rated in 1984
- Question: Is 'Climate-Terrain' associated to 'Housing'?
- Low values on 'Climate-Terrain' imply uncomfortable temperatures (either hot or cold)
- High values of 'Housing' indicate a higher cost of owning a single family residence

Inference for Plots: The Lineup (Example)

- The null hypothesis for this example is
  H_0: Housing is independent of Climate-Terrain
- The null plots are generated by permuting the values of the variable Housing
- Pick out the plot of the real data: Is any plot different from the others?
- Plots on next slide are taken from Buja et al. (2009)


Housing
Climate-Terrain
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
20000
15000
10000
200
400
600
800


1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
Housing
20000
15000
10000
200
400
600
800
Climate-Terrain

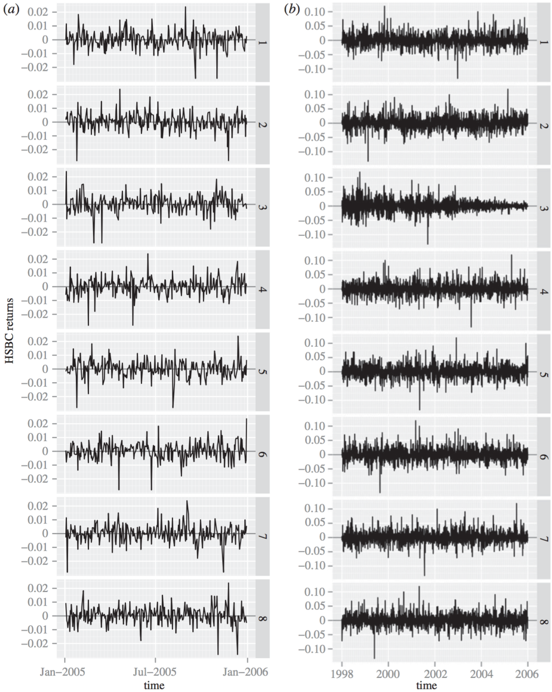
- In class experiment

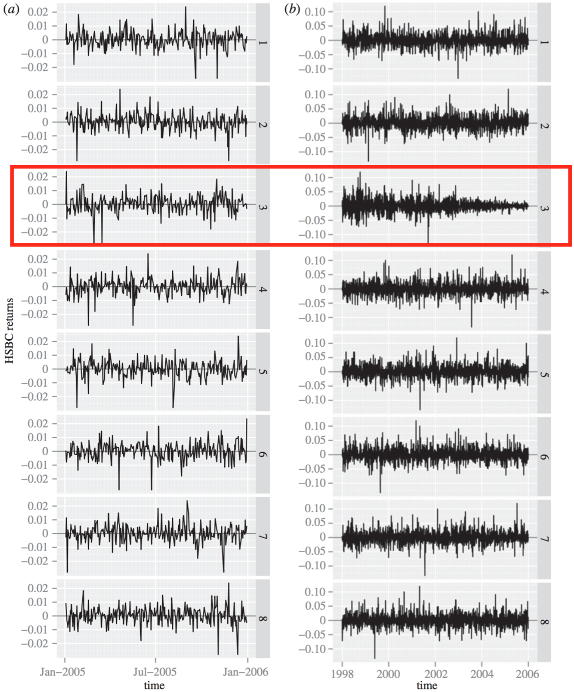
```r
# number of students
K = 8
# number of correct picks
k = 2
pvalue = sum(dbinom(k:K,K,1/20)); pvalue
```

```
## [1] 0.05724465
```

Inference for Plots: The Lineup (Example)

- HSBC (The Hongkong and Shanghai Banking Corporation) daily stock returns
  - two panels, the first showing the 2005 data only,
  - the second the more extensive 1998–2005 data
- In each panel, select which plot is the most different
- Plots on next slide are taken from Buja et al. (2009)


(a)
(b)
HSBC returns
0.02
0.01
0
−0.01
−0.02
0.10
0.05
0
−0.05
−0.10
1
2
3
4
5
6
7
8
Jan−2005
Jul−2005
Jan−2006
time
1998
2000
2002
2004
2006
time



(a)
(b)
HSBC returns
0.02
0.01
0
−0.01
−0.02
0.10
0.05
0
−0.05
−0.10
1
2
3
4
5
6
7
8
Jan−2005
Jul−2005
Jan−2006
time
1998
2000
2002
2004
2006
time

- In class experiment

```
# number of students
K = 8
# number of correct picks
k = 4
pvalue = sum(dbinom(k:K,K,1/8)); pvalue
```

```
## [1] 0.01124781
```

Inference for Plots: The Lineup (Example)

- For 2005, the viewer should have had difficulty selecting the real data
  - This is a year of low and stable volatility
- For 1998–2005, it should be easy
  - features two volatility bursts
  - one in 1998 due to the Russian bond default and the LTCM collapse
  - the other in 2001 due to the 9/11 event
  - after, volatility stabilizes at a low level

Principal Component Analysis

- Principal Component Analysis (PCA) is a data exploration tool
- PCA finds a low-dimensional subspace that minimizes the distances between projections points and subspace
- Consider observations $x_1, x_2, \ldots, x_n$
- Center and combine them in matrix X of dimension $p \times n$
- PCA solves this minimization problem with $\langle v_1, v_1 \rangle = 1$

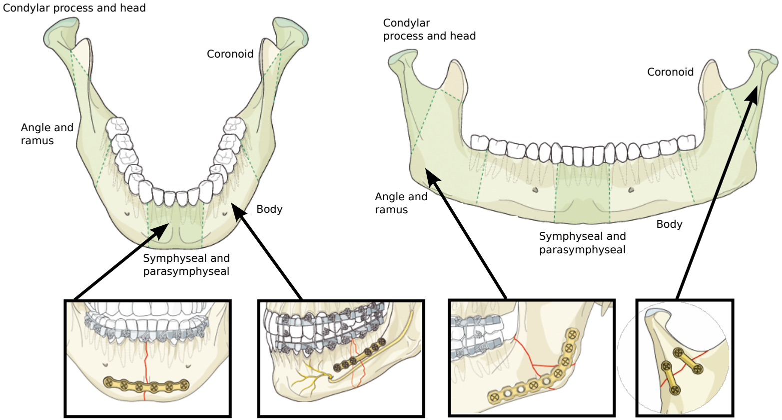
$$\hat{v}_1 = \underset{v_1}{\text{maximize}} \Big\{ \text{Var}(Xv_1) \Big\}$$

- And for v_2 with $\langle v_1, v_2 \rangle = 0$ and $\langle v_2, v_2 \rangle = 1$

$$\hat{v}_2 = \underset{v_2}{\text{maximize}} \Big\{ \text{Var}(Xv_2) \Big\}$$

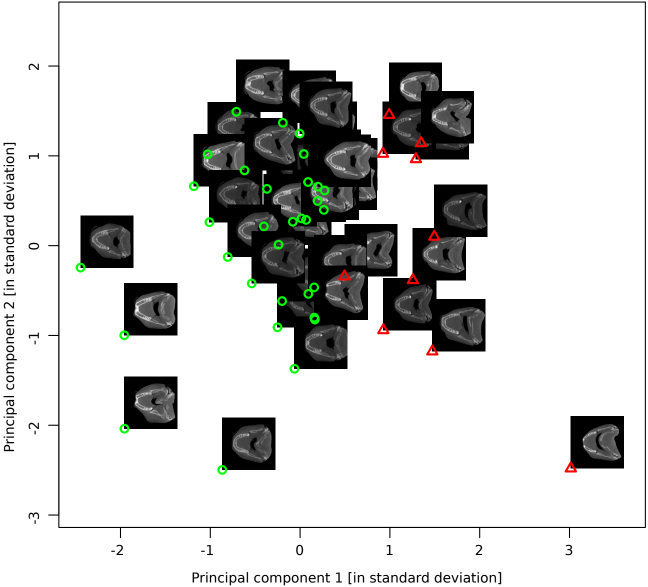
- Keep going the same way until $\hat{v}_1, \ldots, \hat{v}_q$ have been collected and put them in $\hat{V}_q$ of dimensions $p \times q$

Principal Component Analysis (Example)



Source: www.aofoundation.org

Principal Component Analysis (Example)



Source: S., Pennec, and Reyes 2012

Principal Component Analysis (Example)

Two animations of mandible "eigenanatomy":

- `http://christofseiler.github.io/phd/`

Bootstrap PCA

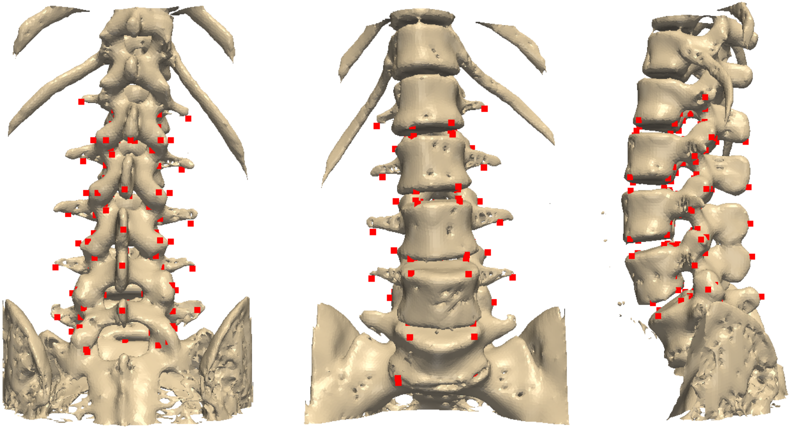
- Two ways to bootstrap PCA in case of random rows X
- Partial bootstrap and total bootstrap
- Partial bootstrap:
  - Project B replications onto initial subspace
  - Initial subspace is obtained by PCA on original X
  - Underestimates variation of parameters (Milan 1995)
- Total bootstrap:
  - Perform new PCA on each replication
  - Problem: Need to align PCA's
  - Nuisance variations: reflections and rotations

Bootstrap PCA

- For the total bootstrap, need to align PCA's
- This is usually done using Procrustes analysis
- Procrustes refers to a bandit from Greek mythology who made his victims fit his bed by stretching their limbs (or cutting them off)
- Procrustes analysis is used in statistical shape analysis to compare aligned shapes after removing "nuisance" parameters:
  - translation in space
  - rotation in space
  - sometimes scaling of the objects

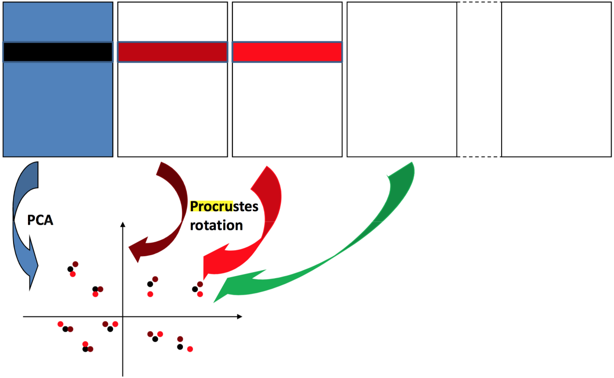
Bootstrap PCA

- Shape example: landmarks for the human spine



Bootstrap PCA

- Same idea can be applied to align projected observations
- In PCA, shapes are the projected observations onto the lower dimensional subspace spanned by say PC1 and PC2



Source: Josse, Wager, and Husson (2014)

Bootstrap PCA

- Collecting B bootstrap sampled PCA's by resampling rows of data matrix X
$$\hat{V}_q^{*1}, \ldots, \hat{V}_q^{*B}$$
- Align all the projected point set using Procrustes alignment
- Meaning, we find rotation ($R^T R = I$)
$$\hat{R}^b = \underset{R}{\text{minimize}} = \left\{ \|X^{*1}\hat{V}_q^{*1} - X^{*b}\hat{V}_q^{*b}R\|^2 \right\}$$
- and apply rotation to projected data points
$$X^{*b}\hat{V}_q^{*b}\hat{R}^{*b}$$
- Overlay points and draw contours around it

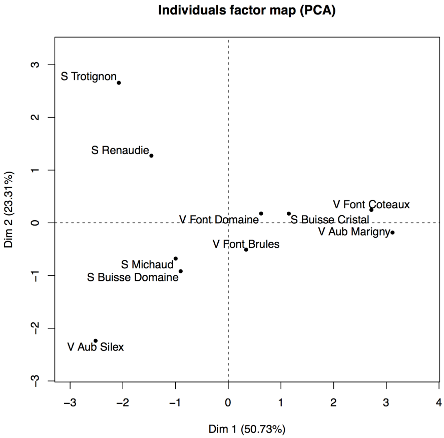
Parametric Bootstrap PCA

- In case of fixed rows and columns X, we can use parametric bootstrap
- It is good alternative when the model is too difficult or before the asymptotics regime
- Steps:

1. Perform PCA on X to estimate $\hat{V}_p$
2. Estimate error σ^2 from residual matrix $\epsilon_{n\times p} = X - \hat{V}_q \hat{V}_q^T X$ (assume elementwise iid normal noise)
3. Bootstrap $1, \ldots, B$:
    - Draw ϵ_{ij}^{*b} from $N(0, \hat{\sigma}^2)$
    - Generate new matrix $X^{*b} = \hat{V}_q \hat{V}_q^T X + \epsilon^{*b}$
    - Perform PCA on X^{*b}

Parametric Bootstrap PCA (Example)

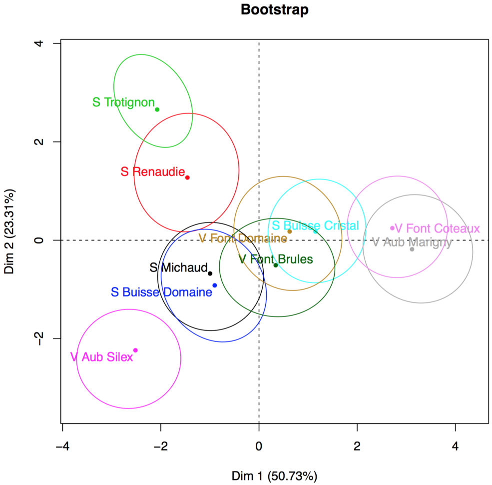
- Consumers describe 10 white wines with 15 sensory attributes
- Consumers score wines between 1 and 10 for each attribute
- Collect averages across consumers in 10×15 matrix X



Source: Josse et al.

Parametric Bootstrap PCA (Example)

- With boostraped confidence ellipses



Source: Josse et al.

References

- Diaconis (1983). Theories of Data Analysis: From Magical Thinking Through Classical Statistics
- Buja, Cook, Hofmann, Lawrence, Lee, Swayne, and Wickham (2009). Statistical Inference for Exploratory Data Analysis and Model Diagnostics
- Milan and Whittaker (1995). Application of the Parametric Bootstrap to Models that Incorporate a Singular Value Decomposition
- Josse, Wager, and Husson (2014). Confidence Areas for Fixed-Effects PCA
- Seiler, Pennec, and Reyes (2012). Capturing the Multiscale Anatomical Shape Variability with Polyaffine Transformation Trees