

Bagplots, boxplots and outlier detection for functional data

Han Lin Shang & Rob J Hyndman

Business & Economic Forecasting Unit



MONASH University

Outline

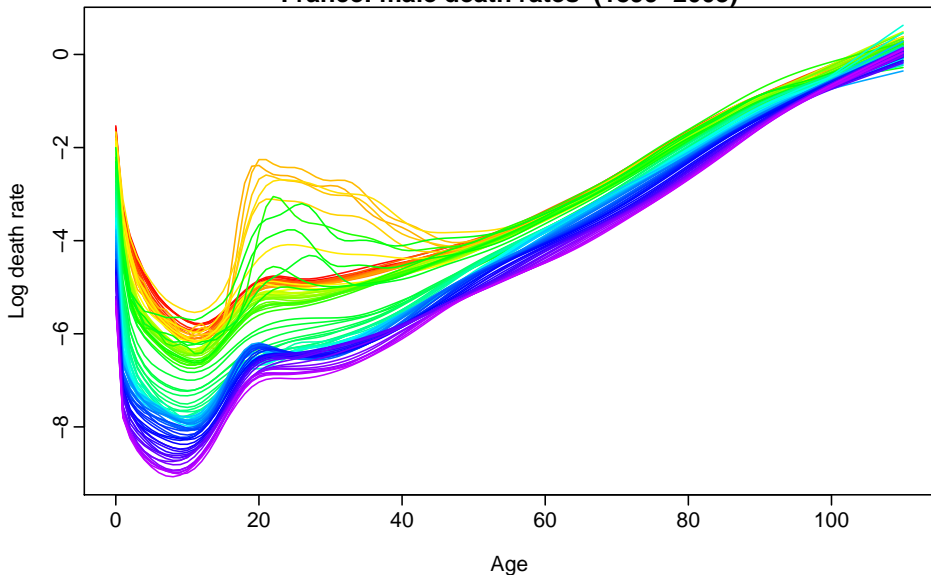
- 1 Introduction
- 2 Functional bagplot and HDR boxplot
- 3 Outlier detection
- 4 Conclusions

Outline

- 1 **Introduction**
- 2 Functional bagplot and HDR boxplot
- 3 Outlier detection
- 4 Conclusions

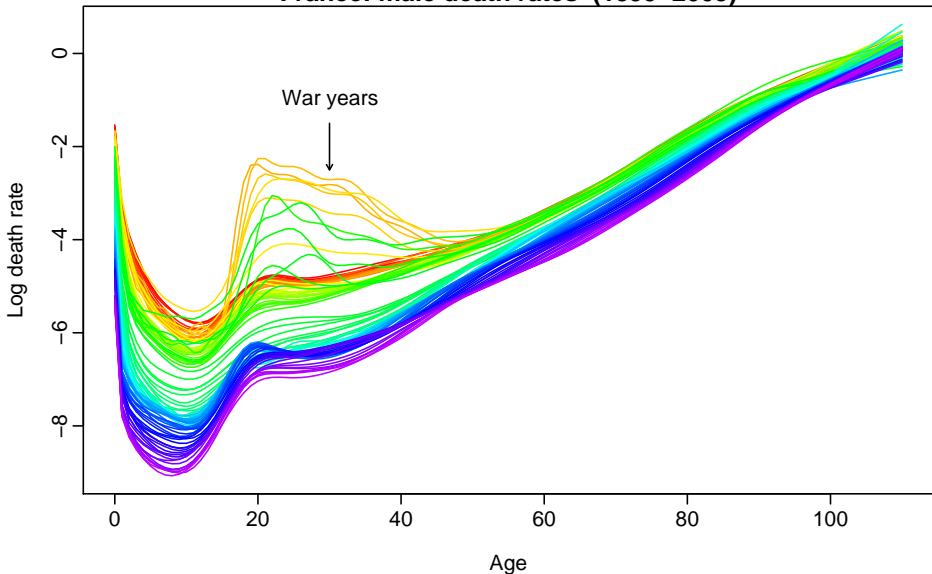
French male mortality rates

France: male death rates (1899–2003)



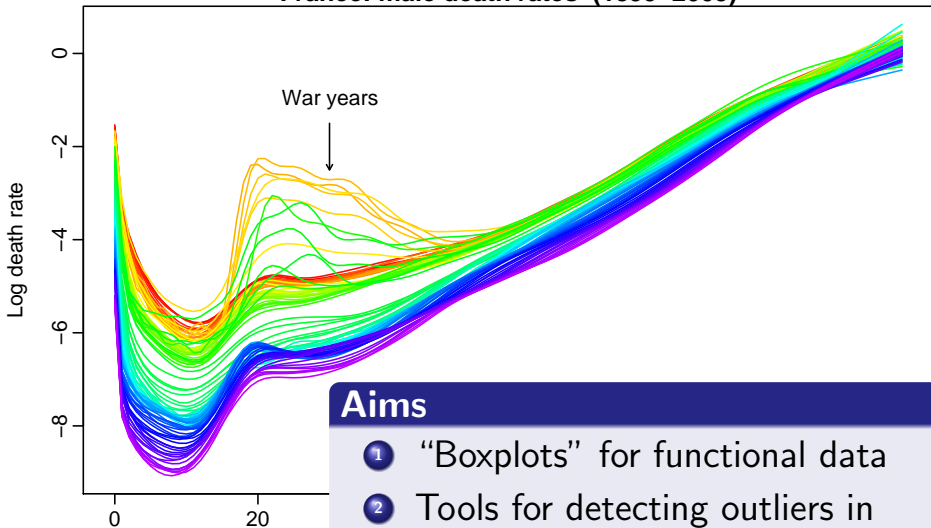
French male mortality rates

France: male death rates (1899–2003)



French male mortality rates

France: male death rates (1899–2003)



Aims

- 1 "Boxplots" for functional data
- 2 Tools for detecting outliers in functional data

Robust principal components

Let $\{y_i(x)\}$, $i = 1, \dots, n$, be a set of curves.

Robust principal components

Let $\{y_i(x)\}$, $i = 1, \dots, n$, be a set of curves.

- 1 **Apply a robust principal component algorithm**

$$y_i(x_i) = \mu(x) + \sum_{k=1}^{n-1} z_{i,k} \phi_k(x)$$

Robust principal components

Let $\{y_i(x)\}$, $i = 1, \dots, n$, be a set of curves.

- 1 **Apply a robust principal component algorithm**

$$y_i(x_i) = \mu(x) + \sum_{k=1}^{n-1} z_{i,k} \phi_k(x)$$

- $\mu(x)$ is mean curve

Robust principal components

Let $\{y_i(x)\}$, $i = 1, \dots, n$, be a set of curves.

① Apply a robust principal component algorithm

$$y_i(x_i) = \mu(x) + \sum_{k=1}^{n-1} z_{i,k} \phi_k(x)$$

- $\mu(x)$ is mean curve
- $\{\phi_k(x)\}$ are principal components

Robust principal components

Let $\{y_i(x)\}$, $i = 1, \dots, n$, be a set of curves.

1 Apply a robust principal component algorithm

$$y_i(x_i) = \mu(x) + \sum_{k=1}^{n-1} z_{i,k} \phi_k(x)$$

- $\mu(x)$ is mean curve
- $\{\phi_k(x)\}$ are principal components
- $\{z_{i,k}\}$ are PC scores

Robust principal components

Let $\{y_i(x)\}$, $i = 1, \dots, n$, be a set of curves.

1 Apply a robust principal component algorithm

$$y_i(x_i) = \mu(x) + \sum_{k=1}^{n-1} z_{i,k} \phi_k(x)$$

- $\mu(x)$ is mean curve
- $\{\phi_k(x)\}$ are principal components
- $\{z_{i,k}\}$ are PC scores

2 Plot $z_{i,2}$ vs $z_{i,1}$

Robust principal components

Let $\{y_i(x)\}$, $i = 1, \dots, n$, be a set of curves.

1 Apply a robust principal component algorithm

$$y_i(x_i) = \mu(x) + \sum_{k=1}^{n-1} z_{i,k} \phi_k(x)$$

- $\mu(x)$ is mean curve
- $\{\phi_k(x)\}$ are principal components
- $\{z_{i,k}\}$ are PC scores

2 Plot $z_{i,2}$ vs $z_{i,1}$

Robust principal components

Let $\{y_i(x)\}$, $i = 1, \dots, n$, be a set of curves.

1 Apply a robust principal component algorithm

$$y_i(x_i) = \mu(x) + \sum_{k=1}^{n-1} z_{i,k} \phi_k(x)$$

- $\mu(x)$ is mean curve
- $\{\phi_k(x)\}$ are principal components
- $\{z_{i,k}\}$ are PC scores

2 Plot $z_{i,2}$ vs $z_{i,1}$

➡ Each point in scatterplot represents one curve.

Robust principal components

Let $\{y_i(x)\}$, $i = 1, \dots, n$, be a set of curves.

1 Apply a robust principal component algorithm

$$y_i(x_i) = \mu(x) + \sum_{k=1}^{n-1} z_{i,k} \phi_k(x)$$

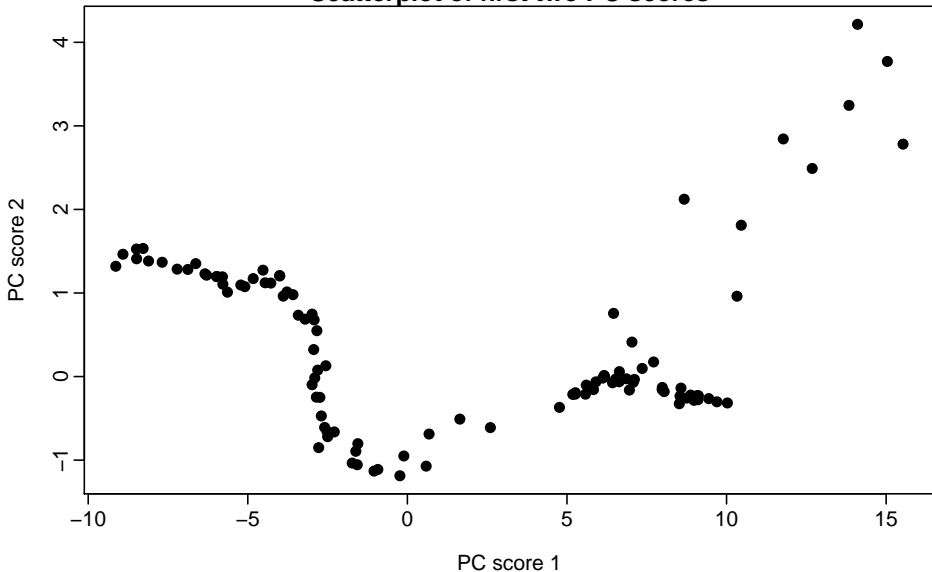
- $\mu(x)$ is mean curve
- $\{\phi_k(x)\}$ are principal components
- $\{z_{i,k}\}$ are PC scores

2 Plot $z_{i,2}$ vs $z_{i,1}$

- ➡ Each point in scatterplot represents one curve.
- ➡ Outliers show up in bivariate score space.

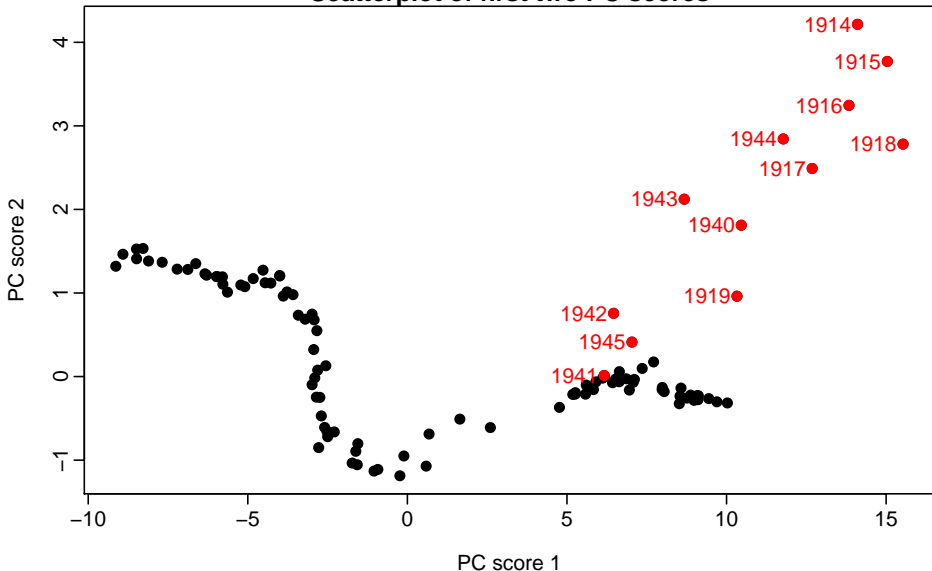
Robust principal components

Scatterplot of first two PC scores



Robust principal components

Scatterplot of first two PC scores



Outline

1 Introduction

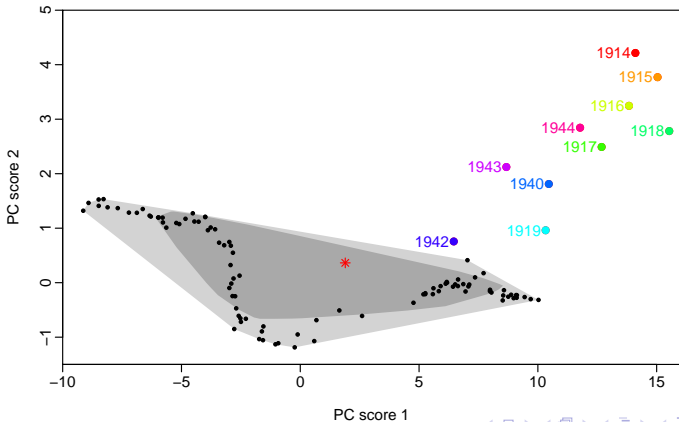
2 Functional bagplot and HDR boxplot

3 Outlier detection

4 Conclusions

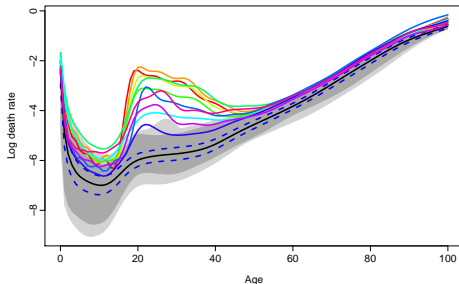
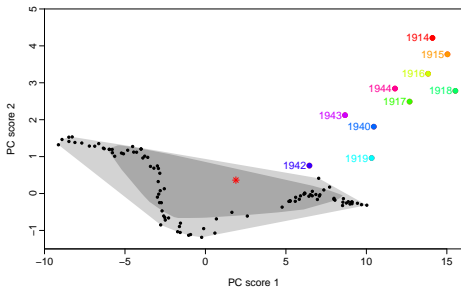
Functional bagplot

- Bivariate bagplot due to Rousseeuw et al. (1999).
- Rank points by halfspace location depth.
- Display median, 50% convex hull and outer convex hull (with 99% coverage if bivariate normal).

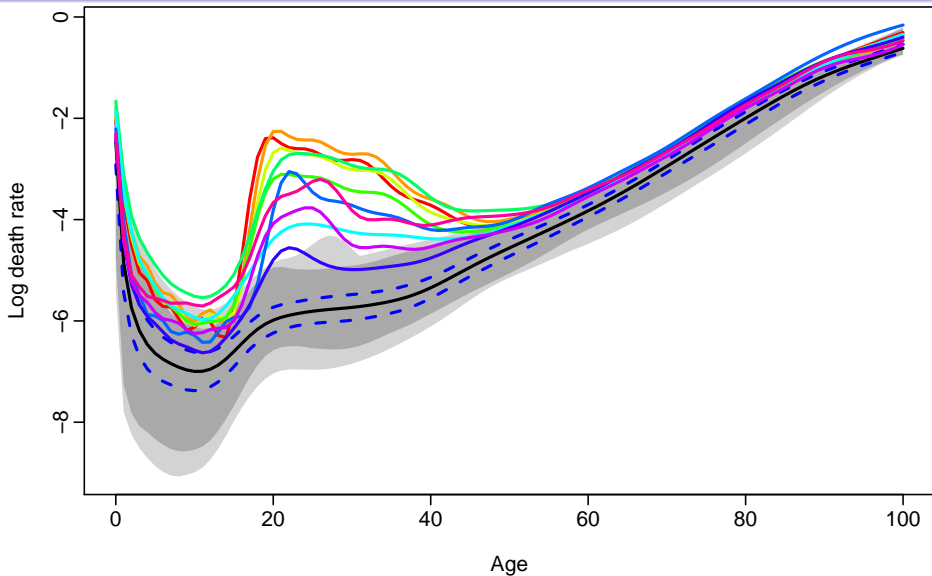


Functional bagplot

- Bivariate bagplot due to Rousseeuw et al. (1999).
- Rank points by halfspace location depth.
- Display median, 50% convex hull and outer convex hull (with 99% coverage if bivariate normal).
- Boundaries contain all curves inside bags.
- 95% CI for median curve also shown.

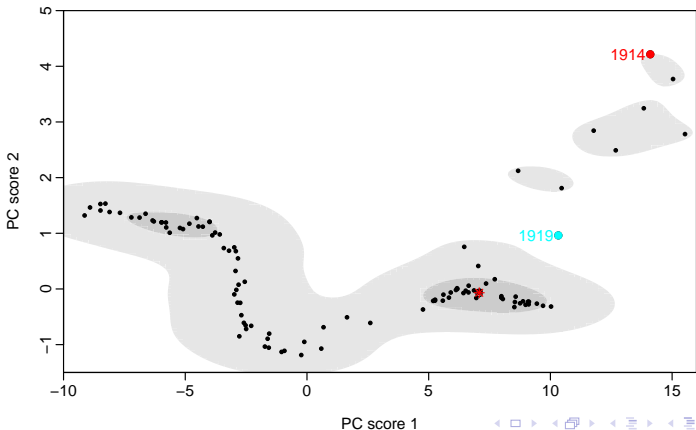


Functional bagplot



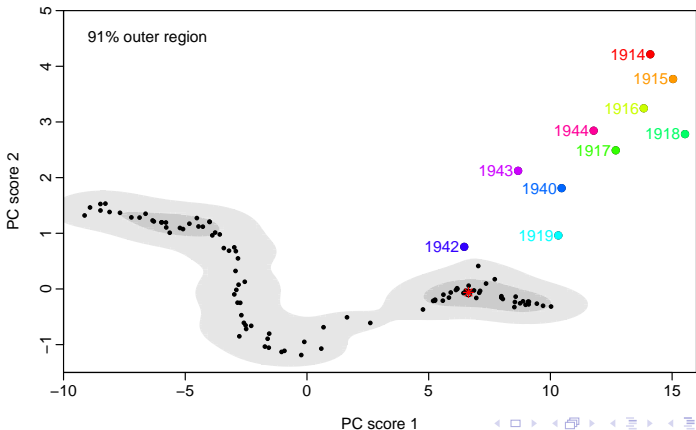
Functional HDR boxplot

- Bivariate HDR boxplot due to Hyndman (1996).
- Rank points by value of kernel density estimate.
- Display mode, 50% and (usually) 99% highest density regions (HDRs) and mode.



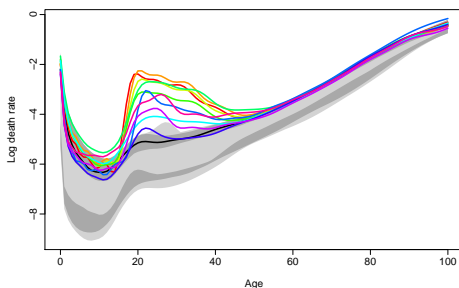
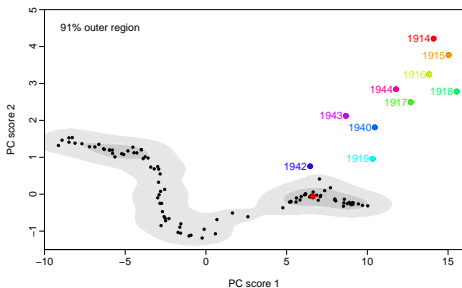
Functional HDR boxplot

- Bivariate HDR boxplot due to Hyndman (1996).
- Rank points by value of kernel density estimate.
- Display mode, 50% and (usually) 99% highest density regions (HDRs) and mode.

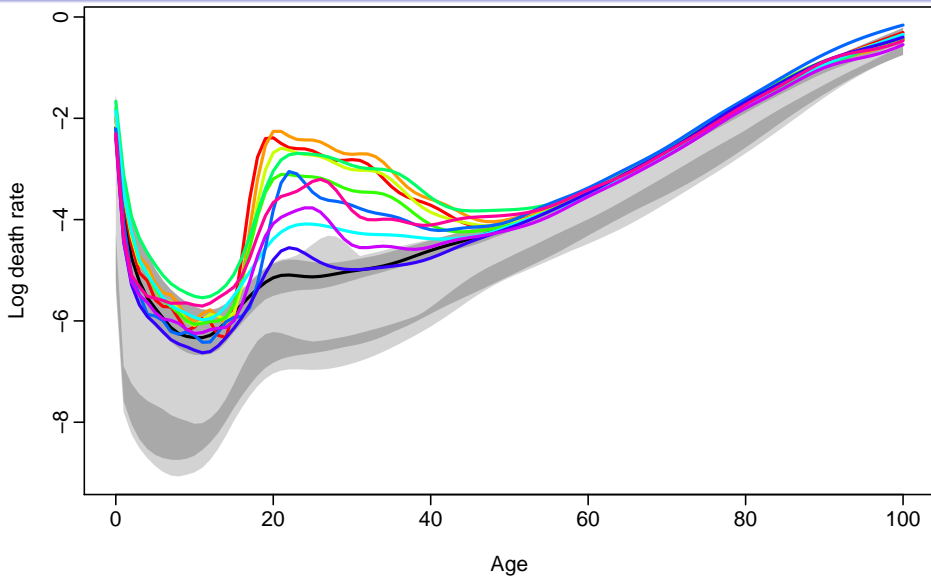


Functional HDR boxplot

- Bivariate HDR boxplot due to Hyndman (1996).
- Rank points by value of kernel density estimate.
- Display mode, 50% and (usually) 99% highest density regions (HDRs) and mode.
- Boundaries contain all curves inside HDRs.



Functional HDR boxplot



Outline

- 1 Introduction
- 2 Functional bagplot and HDR boxplot
- 3 Outlier detection**
- 4 Conclusions

Outlier detection: existing methods

Likelihood ratio method

- Febrero et al. (2007) find curve that maximizes LRT statistic.
- If $LRT > C$, then curve is considered outlier.
- C is computed via smoothed bootstrap.
- Process continues until no more outliers.

Outlier detection: existing methods

Likelihood ratio method

- Febrero et al. (2007) find curve that maximizes LRT statistic.
- If $LRT > C$, then curve is considered outlier.
- C is computed via smoothed bootstrap.
- Process continues until no more outliers.

Disadvantages

- Computationally intensive.
- Ignores shape outliers.
- If trimmed mean is used and there is no outlier, C will be downward biased.

Outlier detection: existing methods

Integrated squared error method

- Hyndman & Ullah (2007) proposed the use of

$$v_i = \int_x \left[\hat{y}_i(x) - \mu(x) - \sum_{k=1}^K z_{i,k} \phi_k(x) \right]^2 dx$$

where $z_{i,k}$ and (robust) PC scores and $\phi_k(x)$ are PCs.

Outlier detection: existing methods

Integrated squared error method

- Hyndman & Ullah (2007) proposed the use of

$$v_i = \int_x \left[\hat{y}_i(x) - \mu(x) - \sum_{k=1}^K z_{i,k} \phi_k(x) \right]^2 dx$$

where $z_{i,k}$ and (robust) PC scores and $\phi_k(x)$ are PCs.

- Curve is outlier if $v_i > s + \lambda\sqrt{s}$, where $s = \text{median}(v_1, \dots, v_t)$ and λ is tuning parameter.

Outlier detection: existing methods

Integrated squared error method

- Hyndman & Ullah (2007) proposed the use of

$$v_i = \int_x \left[\hat{y}_i(x) - \mu(x) - \sum_{k=1}^K z_{i,k} \phi_k(x) \right]^2 dx$$

where $z_{i,k}$ and (robust) PC scores and $\phi_k(x)$ are PCs.

- Curve is outlier if $v_i > s + \lambda\sqrt{s}$, where $s = \text{median}(v_1, \dots, v_t)$ and λ is tuning parameter.

Outlier detection: existing methods

Integrated squared error method

- Hyndman & Ullah (2007) proposed the use of

$$v_i = \int_x \left[\hat{y}_i(x) - \mu(x) - \sum_{k=1}^K z_{i,k} \phi_k(x) \right]^2 dx$$

where $z_{i,k}$ and (robust) PC scores and $\phi_k(x)$ are PCs.

- Curve is outlier if $v_i > s + \lambda\sqrt{s}$, where $s = \text{median}(v_1, \dots, v_t)$ and λ is tuning parameter.

Disadvantages

- Depends on K and λ .
- If K large, outliers modelled by higher components.

Outlier detection: comparison

French male mortality data set

Based on historical information, the outliers are expected to be 1914–1919 & 1940–1945.

Method

Outliers detected

Likelihood ratio

—

Integrated squared error

1914–1918, 1940, 1943–1944

Bagplot

1914–1919, 1940, 1942–1944

91% HDR boxplot

1914–1919, 1940, 1942–1944

Outlier detection: comparison

French male mortality data set

Based on historical information, the outliers are expected to be 1914–1919 & 1940–1945.

Method

Outliers detected

Likelihood ratio

—

Integrated squared error

1914–1918, 1940, 1943–1944

Bagplot

1914–1919, 1940, 1942–1944

91% HDR boxplot

1914–1919, 1940, 1942–1944

Method

Sensitivity Specificity Time (s)

Likelihood ratio

0%

100%

18.8

Integrated squared error

50%

94%

3.4

Bagplot

83%

98%

0.6

91% HDR boxplot

83%

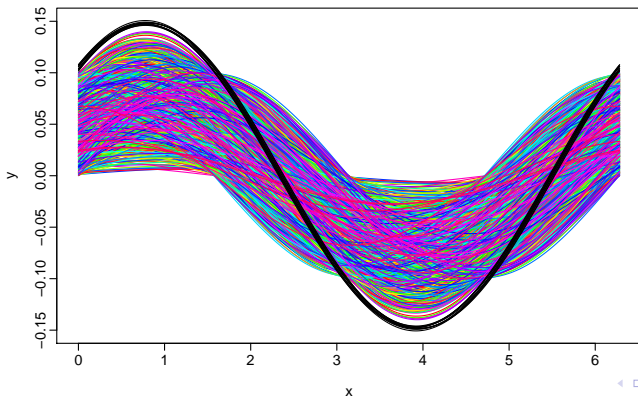
98%

0.3

Outlier detection: comparison

Simulation

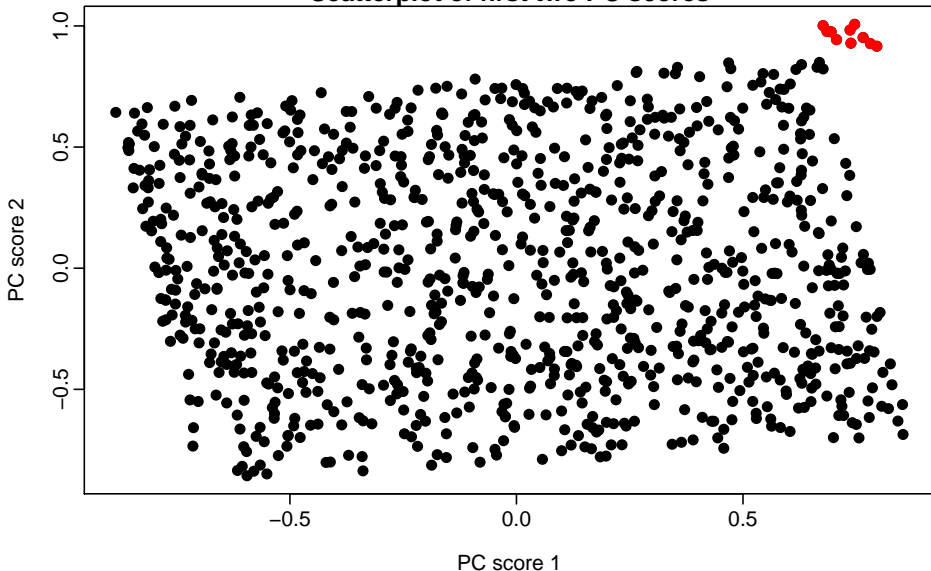
- $y_i(x) = a_i \sin(x) + b_i \cos(x), \quad 0 < x < 2\pi$
- $a_i, b_i \sim \text{Unif}(0, 0.1)$ with probability 99%
- $a_i, b_i \sim \text{Unif}(0.1, 0.108)$ with probability 1%



Outliers shown
in black

Outlier detection: comparison

Scatterplot of first two PC scores



Outlier detection: comparison

Simulation

Method	Outliers detected
Likelihood ratio	—
Integrated squared error	—
Bagplot	—
99% HDR boxplot	All

Outlier detection: comparison

Simulation

Method Outliers detected

Likelihood ratio	—
Integrated squared error	—
Bagplot	—
99% HDR boxplot	All

Method Sensitivity Specificity Time (s)

Likelihood ratio	0%	100%	28.5
Integrated squared error	0%	100%	18.8
Bagplot	0%	100%	7.3
99% HDR boxplot	100%	100%	6.9

Outline

- 1 Introduction
- 2 Functional bagplot and HDR boxplot
- 3 Outlier detection
- 4 Conclusions**

Conclusions

- Functional bagplot highly robust but sometimes misses outliers.

Conclusions

- Functional bagplot highly robust but sometimes misses outliers.
- Functional HDR boxplot more flexible but coverage probability needs tuning.

Conclusions

- Functional bagplot highly robust but sometimes misses outliers.
- Functional HDR boxplot more flexible but coverage probability needs tuning.
- Functional HDR boxplot can detect bimodality and inliers.

Conclusions

- Functional bagplot highly robust but sometimes misses outliers.
- Functional HDR boxplot more flexible but coverage probability needs tuning.
- Functional HDR boxplot can detect bimodality and inliers.
- Existing depth method performs poorly and ignores shape outliers.

Conclusions

- Functional bagplot highly robust but sometimes misses outliers.
- Functional HDR boxplot more flexible but coverage probability needs tuning.
- Functional HDR boxplot can detect bimodality and inliers.
- Existing depth method performs poorly and ignores shape outliers.
- Existing ISE method often misses outliers.

Conclusions

- Functional bagplot highly robust but sometimes misses outliers.
- Functional HDR boxplot more flexible but coverage probability needs tuning.
- Functional HDR boxplot can detect bimodality and inliers.
- Existing depth method performs poorly and ignores shape outliers.
- Existing ISE method often misses outliers.

Conclusions

- Functional bagplot highly robust but sometimes misses outliers.
 - Functional HDR boxplot more flexible but coverage probability needs tuning.
 - Functional HDR boxplot can detect bimodality and inliers.
 - Existing depth method performs poorly and ignores shape outliers.
 - Existing ISE method often misses outliers.
- ➡ Paper and R code: www.robhyndman.info
- ➡ Comments to: Han.Shang@buseco.monash.edu