Outlier Detection for Functional Data with R Package fdaoutlier

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Abstract

Outlier detection is one of the standard exploratory analysis tasks in functional data analysis. We present the R package fdaoutlier which contains implementations of some of the latest techniques for detecting functional outliers. The package makes it easy to detect different types of outliers (magnitude, shape, and amplitude) in functional data, and some of the implemented methods can be applied to both univariate and multivariate functional data. We illustrate the main functionality of the R package with common functional datasets in the literature.

Keywords: functional data analysis, outlier detection, fdaoutlier, R.

1. Introduction

Outlier detection is a common task when carrying out exploratory data analysis. Identifying possible outliers is essential during the exploratory analysis process, because outliers can significantly bias any statistical analysis. The process of dealing with identified outliers may also provide new insights into the data generating process’s nature. In functional data analysis (FDA), observations are treated as functions observed on a domain. These functional observations can exhibit various outlyingness properties as pointed out by Hubert et al. (2015). For instance, an observation can be shifted from the mass of the data. Such outliers are referred to as magnitude outliers in the FDA literature. On the other hand, an observation can be a shape outlier because it differs in shape from the mass of the data (even if it lies completely
inside the mass of the data). For periodic functional observations, an observation may be outlying because it has an amplitude different from the mass of the data. Finally, any of the aforementioned outlyingness properties can be exhibited by a functional observation in a subset of the domain or all through the domain. Consequently, identifying outliers in FDA is challenging as there are many possible ways a functional observation can exhibit outlyingness.

Much work has been done regarding identifying outliers in the FDA context, with their corresponding software implementations made available in R (R Core Team 2020). A number of these methods have been obvious applications of a notion of functional depths, which induces a centre outward ordering on a sample of curves. For instance, the functional boxplot (Sun and Genton 2011) uses the (modified) band depth to define a 50% central region for the sample of curves with outliers identified as curves lying outside 1.5 times the central region in any part of the domain. In R, the functional boxplot is available in the fda package (Ramsay et al. 2020) with options to use the fast exact (modified) band depth defined by bands of two functions, proposed in Sun et al. (2012).

The fda.usc package (Febrero-Bande and Oviedo de la Fuente 2012) in R implements three functional outlier detection methods. The first method, proposed in Febrero et al. (2007), uses a likelihood ratio statistics to detect outlying curves (with cutoff determined by a bootstrap procedure). The two other methods identify outliers by comparing the depth values of the functions to a cutoff also obtained by a bootstrap procedure, based on either trimming of suspicious curves or placing more weights on the deeper curves (Febrero et al. 2008). These three methods are also implemented in the rainbow package (Shang 2011), as well as the functional bagplot and the functional highest density region plot (Hyndman and Shang 2010). The rainbow package also contains the integrated square forecast errors method for detecting functional outliers proposed in Hyndman and Shahid Ullah (2007) (see also Hyndman and Shang 2010).

Nagy et al. (2017) proposed the $j^{th}$ order integrated and infimal depths for identifying shape outliers, with implementations available in the ddaalpha package (Pokotylo et al. 2019). Rousseeuw et al. (2018) in their work proposed a directional outlyingness (DO) measure, its functional extension (fDO), and the variability of directional outlyingness (vDO). Then, they used the functional outlier map, a scatter plot of the fDO versus vDO, to identify outliers with cutoffs determined by the standardized logarithm of the combined functional outlyingness (LCFO) measure. The functional outlier map can also be used with the adjusted outlyingness (AO) measure proposed in Brys et al. (2005) (see also Hubert and Van der Veeken 2008, and Hubert et al. 2015), rather than the DO measure. These methods are available in the mrdDepth package (Segaert et al. 2020). Finally, the roahd package (Ieva et al. 2019) contains an implementation of the outliergram method proposed in Arribas-Gil and Romo (2014), as well as its multivariate generalisation proposed in Ieva and Paganoni (2020).

More recently proposed outlier detection methods include: the directional outlyingness for multivariate functional data proposed in Dai and Genton (2019) and further elaborated into the magnitude-shape plot (MS-Plot) in Dai and Genton (2018); the total variate depth (TVD) and modified shape similarity index (MSS) proposed in Huang and Sun (2019); and the CRO-FADALARA method, based on archetypoids proposed in Vinue and Epifanio (2020b), and available in the adamethods package (Vinue and Epifanio 2020a). Dai et al. (2020) also proposed detecting and classifying outliers using some sequence of transformations, e.g., shifting a curve to its centre and normalising it using the $L_2$ norm.
The objective of this paper is to describe the fdaoutlier package which aims to extend the available facility for outlier detection (in the FDA context) for R, with implementations of some of the latest outlier detection methods. The fdaoutlier package’s main contributions are:

- Implementations of the directional outlyingness and MS-Plot outlier detection methods proposed in Dai and Genton (2019) and Dai and Genton (2018).

- An implementation of the TVD and MSS proposed in Huang and Sun (2019). The fdaoutlier implementation of TVD/MSS is written in C++ using R’s .Call interface which leads to significant computational efficiency as TVD and MSS are computationally intensive.

- An implementation of the sequential transformation method described in Dai et al. (2020).

- An implementation of the massive unsupervised outlier detection (MUOD) method proposed in Azcorra et al. (2018).

- Various depth and ordering methods, including extremal depth, one and two-sided extreme rank length depth, directional quantile, among others, useful for ordering functional observations (e.g., in functional boxplots).

In the next section, we describe the theoretical background of the implemented outlier detection methods and demonstrate their implementations in fdaoutlier using simulated data. In Section 3, we apply fdaoutlier on two common datasets in the FDA outlier detection literature, replicating some of the analyses done in the literature. We then conclude in Section 4 with some remarks and a future outlook of fdaoutlier.

2. Outlier detection methods

We provide a brief primer of the implemented methods in the fdaoutlier package, and then describe their implementations. For illustrating the methods, we use the convenience functions simulation_model1() - simulation_model9() implemented in fdaoutlier to generate data with different types of outliers. These functions are useful for the rapid development and testing of new outlier detection methods and were curated from the functional outlier detection literature. Figure 1 shows plots of sample data generated by these nine models produced by calling simulation_model*(plot = TRUE).

2.1. Directional outlyingness and MS-Plot

The directional outlyingness for multivariate functional data proposed in Dai and Genton (2019) provides a way to measure not only the point-wise outlyingness of a functional observation but also the direction of outlyingness of that observation with respect to (w.r.t.) the rest of the data. Formally, let \( \mathbf{Y} : I \rightarrow \mathbb{R}^p \) be a stochastic process in the space of real continuous functions \( C(I, \mathbb{R}^p) \) defined on a compact interval \( I \). Let the probability distribution of \( \mathbf{Y} \) be \( F_{\mathbf{Y}} \). At each evaluation point, \( t \in I \), \( \mathbf{Y}(t) \) is a \( p \)-variate vector with probability
Figure 1: Simulation models: Plot of sample of data generated by each simulated model in \texttt{fdaoutlier}. Curves in orange are outliers.

The directional outlyingness for multivariate data is defined as:

$$ O(Y, F_Y) = o(Y, F_Y) \cdot v, $$

where $o(Y, F_Y)$ is the outlyingness of $Y$ w.r.t. to $F_Y$ and $v$ is the spatial depth defined at point $t$ by

$$ v(t) = \frac{|Y(t) - Z(t)|}{||Y(t) - Z(t)||}, $$

with $Z(t)$ being the unique median of $Y(t)$ w.r.t. $F_{Y(t)}$ (deepest point of $F_{Y(t)}$). $v(t)$ is a unit vector pointing from $Z(t)$ to $Y(t)$. Dai and Genton (2019) recommends using a distance-based outlyingness measure, like the Stahel-Donoho outlyingness defined by:

$$ SDO(Y(t), F_{Y(t)}) = \sup_{||u||=1} \frac{||u^\top Y(t) - \text{median}(u^\top Y(t))||}{\text{mad}(u^\top Y(t))}. $$

Thus, the Stahel-Donoho type directional outlyingness is given by:

$$ O(Y, F_Y) = SDO(Y, F_Y) \cdot v. $$

Then the functional directional outlyingness (FO) is defined, to capture the \textit{overall} outlyingness for functional data, as:

$$ FO(Y, F_Y) = \int I ||O(Y(t), F_{Y(t)})||^2 w(t) dt, $$
where $w(t)$ is a weight function defined on $I$. The mean directional outlyingness (MO) and variation of directional outlyingness (VO) were defined as:

$$MO(Y, F_Y) = \int_I O(Y(t), F_Y(t))w(t)dt,$$

(6)

and

$$VO(Y, F_Y) = \int_I ||O(Y(t), F_Y(t)) - MO(Y, F_Y)||^2w(t)dt.$$

(7)

These quantities measure the magnitude outlyingness and shape outlyingness of a functional observation, respectively. Dai and Genton (2019) further showed the relationship:

$$FO(Y, F_Y) = ||MO(Y, F_Y)||^2 + VO(Y, F_Y),$$

(8)

which decomposes the total functional outlyingness into the magnitude outlyingness and the shape outlyingness.

In practice, the functional observations are observed at a finite number of points, say $k$, on $I$, i.e., at points $t_1, t_2, \ldots, t_k \in I$. The finite dimensional version of $MO(Y, F_Y)$ is defined as:

$$MO_k(Y, F_Y) = \frac{1}{k} \sum_{i=1}^{k} O(Y(t_i), F_Y(t_i))w(t_i),$$

(9)

and the finite dimensional version of VO can be defined in a similar manner.

After obtaining the MO and VO for each curve, MS-Plot is then a scatterplot of the points $(MO^T, VO)^T$. To detect outliers, a multivariate data whose columns are the MOs and VOs is formed, and a robust Mahalanobis distance is computed for each of the $(MO^T, VO)^T$ pair in this data. The robust covariance matrix is estimated using the minimum covariate determinant (MCD) estimator (Rousseeuw and Driessen 1999). The distribution of these robust distances is approximated using the $F$ distribution (Hardin and Rocke 2005). Any observation with a robust distance greater than the cutoff obtained from the tails of the $F$ distribution is flagged as an outlier.

The directional outlyingness and MS-Plot methods procedures are implemented mainly through the `dir_out()` and `msplot()` functions in `fdaoutlier`. These functions accept a matrix or data frame of dimension $n \times p$ for a univariate functional data, or an array of dimension $n \times p \times d$ for multivariate functional data (where $n$ is the number of functions/curves, $p$ is the number of evaluation points in the domain, and $d$ is the dimension of the functional data with, $d \geq 2$ for multivariate functional data). The `dir_out()` function computes the directional outlyingness matrix $O(Y, F_Y)$, the mean directional outlyingness $MO(Y, F_Y)$ and the variation of directional $VO(Y, F_Y)$, while the `msplot()` function finds outliers using the mean and variation of outlyingness with the $F$ approximation.

We illustrate identifying outliers with `msplot()` using `simulation_model5()` to generate data of 100 curves, out of which 10 are shape outliers with a different covariance structure. The generated curves are observed on 50 domain points over the interval $[0, 1]$. A call to `simulation_model5()` returns a list containing the matrix of generated data and a vector containing the indices of the true outliers.

```R
R> simdata <- simulation_model5(n = 100, p = 50, + outlier_rate = 0.1, seed = 2)
```
```r
R> dt <- simdata$data
R> dim(dt)
[1] 100 50
R> simdata$true_outliers
[1] 6 10 20 21 34 38 48 49 66 93

Next we pass the generated data to the `msplot()` function to detect the outliers in `dt`. By default, `msplot()` also produces a plot of the VO against the MO (or ||MO|| in the case of a multivariate functional data) and returns a list containing `outliers` which is a vector of the indices of detected outliers. The plotting function can be turned off by setting the parameter `plot = FALSE`.

```r
R> ms <- msplot(dts = dt, return_mvdir = T, plot = FALSE)
R> ms$outliers
[1] 6 10 20 21 34 38 48 49 51 66 93 100
```

Setting the additional parameter `return_mvdir = TRUE` ensures that vectors of the mean and variation of outlyingness (MO and VO) of each curve are returned by `msplot()` (a matrix is returned for MO in the case of a multivariate functional data).

```r
R> head(ms$mean_outlyingness)
[1] 0.04718408 -0.76134612 1.30502807 0.20414153 0.81537363
[6] 2.27956644
```

The MS-Plot produced by the `msplot()` function when the parameter `plot = TRUE` is shown in Figure 2. Additional parameters `plot_title`, `title_cex`, `show_legend`, `ylabel` and `xlabel` can be passed to `msplot()` to further customise the MS-Plot generated.

```r
R> simdir <- dir_out(dts = dt, return_dir_matrix = T)
R> head(simdir$mean_outlyingness)
[1] 0.04718408 -0.76134612 1.30502807 0.20414153 0.81537363
[6] 2.27956644
```

If the aim is to compute either the MO and VO or the directional outlyingness matrix (or array for multivariate functional data), without the need for identifying outliers, then the `dir_out()` function, which is called by `msplot()` can be used directly. This returns a list containing the mean and variance of outlyingness, and the directional outlyingness matrix (if the parameter `return_dir_matrix = TRUE`).

```r
R> head(simdir$mean_outlyingness)
```
2.2. Total variation depth and modified shape similarity index

Suppose \( Y : I \to \mathbb{R} \) is a stochastic process defined on the interval \( I \) in \( \mathbb{R} \). Let the distribution of \( Y \) be \( F_Y \). For a function \( y \), let \( R_y(t) \) be the indicator function:

\[
R_y(t) = \mathbb{1}\{Y(t) \leq y(t)\},
\]

for \( t \in I \). The functional total variation depth (Huang and Sun 2019) of the function \( y \) w.r.t. \( F_Y \) is then defined as:

\[
TVD(y, F_Y) = \int_I D_y(t)w(t)dt,
\]
where \(w(t)\) is a weight function and \(D_y(t)\) is the pointwise total variation depth given by:

\[
D_y(t) = \text{var}\{R_y(t)\} = \mathbb{P}\{Y(t) \leq y(t)\} \mathbb{P}\{Y(t) > y(t)\}.
\]  

(12)

The constant weight function \(w(t) = \frac{1}{|I|}\) is suggested in (Huang and Sun 2019) but other weight functions (that place more emphasis on different regions of the interval) can be used in the formulation of the functional total variation depth. The pointwise total variation depth \(D_y(t)\) can be decomposed into a shape and magnitude component by breaking up the variance \(\text{var}\{R_y(t)\}\) using the law of total variance:

\[
D_y(t) = \text{var}\{R_y(t)\} = \text{var}\{\mathbb{E}\{R_y(t)|R_y(s)\}\} + \mathbb{E}\{\text{var}\{R_y(t)|R_y(s)\}\},
\]  

(13)

for \(s, t \in I\) and \(s = t - \Delta\). The shape similarity index of the functional observation \(y\) in a given time span \(\Delta\) is then the weighted ratio of the shape component \(\text{var}\{\mathbb{E}\{R_y(t)|R_y(s)\}\}\) to the total variation depth over the interval \(I\):

\[
SS(y, \Delta) = \int_I S_y(t, \Delta) v(t, \Delta) dt,
\]  

(14)

where

\[
S_y(t, \Delta) = \begin{cases} 
\text{var}\{\mathbb{E}\{R_y(t)|R_y(s)\}\}/D_y(t) & D_y(t) \neq 0 \\
1 & D_y(t) = 0,
\end{cases}
\]

and the weight function \(v(t, \Delta)\) is the normalised changes in \(y(t)\) over the interval \(I\):

\[
v(t, \Delta) = \frac{|y(t) - y(t - \Delta)|}{\int_I |y(t) - y(t - \Delta)|}.
\]

The shape similarity index is a measure of shape outlyingness with small indices associated with shape outliers. However, when \(D_y(t)\) is very small, the shape similarity index may not be small enough, so Huang and Sun (2019) further defined the modified shape similarity index (MSS) by shifting \((y(t - \Delta), y(t))\) to the centre. The modified shape similarity index is defined as:

\[
MSS(y, \Delta) = \int_I S_{\tilde{y}}(t, \Delta) v(t, \Delta) dt,
\]  

(15)

where \(\tilde{y}\) is given by:

\[
\tilde{y}(s, \Delta) = \begin{cases} 
\text{median}\{Y(s)\} & s = t \\
f(s) - f(s + \Delta) + \text{median}|Y(s + \Delta)| & s = t - \Delta,
\end{cases}
\]

and

\[
S_{\tilde{y}}(t, \Delta) = \text{var}\{\mathbb{E}[R_{\tilde{y}}(t)|R_{\tilde{y}}(s)\}] / D_{\tilde{y}}(t)\}.
\]

Details of the empirical versions of the total variation depth, the shape similarity index and its modified version are presented in the Appendix of Huang and Sun (2019). The total variation depth and the modified similarity index are implemented in the \texttt{total\_variation\_depth()}
function of \texttt{fdaoutlier} using C++ through R\textsc{’}s \texttt{.Call} interface for faster and efficient computation. This function accepts only a matrix, and calling it suffices to compute both the total variation depth and the modified shape similarity index. \texttt{total_variation_depth()} returns a list containing both the total variation depth and the modified shape similarity index:

\begin{verbatim}
R> tvdepth <- total_variation_depth(dt)
R> head(tvdepth$mss)
[1] 0.6388217 0.6208659 0.6975233 0.6853633 0.6618313 0.2167154
\end{verbatim}

\begin{verbatim}
R> head(tvdepth$tvd)
[1] 0.224578 0.156484 0.114386 0.197932 0.178926 0.072398
\end{verbatim}

In order to identify outliers, shape outliers are first identified and removed using a classical boxplot on the modified shape similarity indices. A functional boxplot is then used on the remaining curves (to identify magnitude outliers) using the total variation depth to identify their 50\% central region (relative to the original number of curves). The \texttt{tvdmss()} function implements these steps to detect the magnitude and shape outliers. It returns a function containing the indices of the magnitude outliers, shape outliers, and the combined (shape and magnitude) outliers. This is illustrated using the generated data \texttt{dt} from the previous section.

\begin{verbatim}
R> tvoutlier <- tvdmss(dts = dt)
R> tvoutlier$shape_outliers
[1] 6 10 20 21 34 38 48 49 66 93

R> tvoutlier$magnitude_outliers
NULL

R> tvoutlier$outliers
[1] 6 10 20 21 34 38 48 49 66 93
\end{verbatim}

In this case the total variation depth identifies all the shape outliers correctly and does not detect any magnitude outliers when compared to the index of the true outliers of the generated data:

\begin{verbatim}
R> simdata$true_outliers
[1] 6 10 20 21 34 38 48 49 66 93
\end{verbatim}
Additional arguments can be passed to the parameters \texttt{emp\_factor\_mas}, \texttt{emp\_factor\_tvd}, and \texttt{central\_region\_tvd} of \texttt{tvdmss()} to control the classical boxplot of the modified shape similarity index and the functional boxplot of the total variation depth.

### 2.3. Outlier detection using sequential transformations

\textit{Dai et al.} (2020) proposed using some sequence of transformations on the functional data to identify and classify functional outliers. By transforming the functional data, it is possible to turn shape outliers into magnitude outliers, consequently making it easier to identify shape outliers. More formally, let \( \{Y_i\}_{i=1}^n \) be a set of functional observations in the space of continuous functions \( C(I) \) defined on an interval \( I \in \mathbb{R} \). Suppose that \( Y_i \sim F_Y \), and let \( \Gamma \) be a transformation that is also defined on \( C(I) \). Furthermore, let \( F_{\Gamma(Y)} \) be the distribution of the transformed data \( \{\Gamma(Y_i)\}_{i=1}^n \). \textit{Dai et al.} (2020) proposed the following algorithm for functional outlier detection and taxonomy.

**Algorithm 1:** Functional outlier detection using sequential transformations.

1. Identify from \( \{Y_i\}_{i=1}^n \) the magnitude outliers using the functional boxplot, and denote the set of identified outliers by \( S_0 \). These are the \( \Gamma_0 \)-outliers (magnitude outliers).
2. Apply transformation \( \Gamma_1 \) on \( \{Y_i\}_{i=1}^n \) to get \( \{\Gamma_1(Y_i)\}_{i=1}^n \).
3. Repeat step 1 on \( \{\Gamma_1(Y_i)\}_{i=1}^n \) to obtain the set of detected outliers \( S_1 \); \( S_1 \setminus S_0 \) are the \( \Gamma_1 \)-shape outliers.
4. Apply transformation \( \Gamma_2 \) on \( \{\Gamma_1(Y_i)\}_{i=1}^n \) to get \( \{\Gamma_2 \circ \Gamma_1(Y_i)\}_{i=1}^n \).
5. Repeat step 1 on \( \{\Gamma_2 \circ \Gamma_1(Y_i)\}_{i=1}^n \) to obtain the set of detected outliers \( S_2 \); \( S_2 \setminus S_1 \cup S_0 \) are the \( \Gamma_2 \circ \Gamma_1 \)-shape outliers.
6. Repeat steps 4 and 5 if more transformations are considered.

\textit{Dai et al.} (2020) proposed the following useful (sequence of) transformations to identify and classify outliers:

- **Shifting and normalization of Curves:** \( T_2 \circ T_1 \circ T_0(Y_i) \)

This sequence involves first identifying the magnitude outliers using functional boxplot. This is the \( T_0 \) transformation and the identified outliers are the \( T_0 \) outliers (magnitude outliers). The second transformation \( T_1 \) involves shifting the raw curves \( Y_i \) to their centres:

\[
T_1(Y)(t) = Y(t) - \lambda(I)^{-1} \int_I Y(t) dt, \quad (16)
\]

where \( \lambda(I) \) is the Lebesgue measure of the interval \( I \). The \( T_1 \) outliers are then identified using functional boxplot (step 3 of Algorithm 1). The third transformation \( T_2 \) involves normalizing the centered curves, i.e., \( \{T_1(Y_i)\}_{i=1}^n \), with their \( L_2 \) norms:

\[
T_2(Y)(t) = \frac{T_1(Y)(t)}{[\int_I (T_1(Y)(t))^2 dt]^{1/2}}. \quad (17)
\]

- **Derivatives of curves:** \( D_2 \circ D_1 \circ D_0(Y_i) \)

The \( D_0 \) transformation first involves identifying the magnitude outliers using a functional boxplot without transforming the data (same as \( T_0 \)). These are the \( D_0 \) outliers. The second transformation \( D_1 \) involves finding the derivative of the curves, and the third transformation
\( D_2 \) computes the derivative of \( D_1(Y_i) \) again. After each transformation, outliers are identified using functional boxplot as indicated in Algorithm 1. \( D_1 \) and \( D_2 \) transforms are implemented in \texttt{fdaoutlier} by differencing the observed points of the functions on the domain.

**Directional outlyingness:** \( \mathcal{O}(Y(t)) \)

For multivariate functional data \( \{ Y_i \}_{i=1}^n \) taking values in \( \mathbb{R}^d \), the directional outlyingness transformation \( \mathcal{O} \) is especially useful. This transformation changes the multivariate functional observation \( Y_i \) to univariate functional data \( Y_i \) by finding the pointwise directional outlyingness described in Section 2.1 (Dai and Genton 2019). The univariate functional data (of the outlyingness values) can then be investigated for outliers, e.g., using functional boxplot with a one-sided ordering like the (one-sided) extreme rank length depth (see Myllymäki et al. 2017, and Dai et al. 2020).

Other transformations and sequences suggested in Dai et al. (2020) include elimination of phase variations using a warping function:

\[
R(Y)(t) = Y(r(t)),
\]  

where \( r(t) \) is a warping function on \( I \). Eliminating phase variations using \( R(Y) \) may make it easier to detect shape outliers. Other possible sequences of transformations are: \( D_1 \circ T_1 \circ T_0(Y) \) and \( D_2 \circ D_1 \circ T_2 \circ T_1 \circ T_0(Y) \).

In the intermediate steps of identifying outliers using functional boxplots, possible depths and outlyingness measures that can be used to order the functions are: modified band depth of López-Pintado and Romo (2009) (MBD), \( j \)th order integrated depth of Nagy et al. (2017) (\( FD_j \)), the \( L^\infty \) depth (Long and Huang 2016), and extreme rank length depth (ERLD) of (Myllymäki et al. 2017). Other methods include the robust Mahalanobis distance (RMD) of the \( (\text{MO}^\top, \text{VO})^\top \) pair, obtained from the directional outlyingness in Section 2.1, and directional quantile (DQ) (Myllymäki et al. 2017). DQ, RMD, and \( L^\infty \) are distance-based, while MBD, \( FD_j \), and ERLD are based on ranks. Dai et al. (2020) suggested using the distance-based methods, especially when the number of evaluation points on the interval \( I \) is small, as rank-based methods might suffer from a large number of ties. The distance-based methods also achieved the best results for detecting shape outliers in the simulation tests consisting of various shape outliers conducted in Dai et al. (2020). However, some transformations may require the use of specific ordering methods, e.g., the one-sided ERLD is best used with the \( \mathcal{O} \) transformation since it generates univariate functional data made up of point-wise directional outlyingness, and we want to consider only large values of these curves as extremes (rather than use a typical functional depth like MBD which considers both small and large values of curves as extremes). The \texttt{fdaoutlier} package implements all the transformations mentioned in Dai et al. (2020) except for the \( R(Y)(t) \) transformation which involves the use of a warping function. The ordering measures: band depth (BD) and MBD, \( L^\infty \), DQ, RMD, TVD, and ERLD (both one and two-sided) are available in \texttt{fdaoutlier} for ordering the functions in the intermediate functional boxplots.

The \texttt{seq_transform()} function in \texttt{fdaoutlier} finds outliers using sequential transformations. Like the other functions in \texttt{fdaoutlier}, \texttt{seq_transform()} accepts a matrix or data frame (of size \( n \) observations by \( p \) evaluation points) for a univariate functional data and an array (of size \( n \) observation by \( p \) evaluation points by \( d \) dimension). The sequence of transformations to apply on the data is specified to the \texttt{sequence} parameter which accepts a character vector containing a combination of the following strings: "T0", "D0", "T1", "T2", "D1", "D2", and
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"O". The strings "T0", "T1" and "T2" represent the transformations $T_0$, $T_1$ and $T_2$ respectively, while the strings "D0", "D1", and "D2" represent $D_0$, $D_1$ and $D_2$ respectively. The string "O" indicates the outlyingness transformation $O(Y(t))$. Thus, to specify the sequence of transformations: $D_1 \circ T_1 \circ T_0(Y)$, one should pass the argument c("T0", "T1", "D1") to the parameter sequence in the call to seq_tranform(), i.e., set sequence = c("T0", "T1", "D1"). We provide some examples below on the use of the seq_transform() function for detecting outliers using some suggested sequences in Dai et al. (2020).

First we generate some data with outliers from simulation_model4():

```r
R> simdata4 <- simulation_model4(n = 100, p = 50, outlier_rate = 0.05, + deterministic = T, seed = 50)
R> dt4 <- simdata4$data
```

Next, we call the seq_transform() using the sequence $T_2 \circ T_1 \circ T_0(Y(t))$ and specifying modified band depth as the ordering function of choice for the intermediate functional boxplots.

```r
R> seq1 <- seq_transform(dts = dt4, + sequence = c("T0", "T1", "T2"), + depth_method = "mbd")
R> seq1$outliers

$T0
integer(0)

$T1
[1] 43 53

$T2
[1] 43 53 96
```

seq_transform() returns a list of named lists, with each named lists containing the indices of the outliers found at each step of the sequence of transformations. The names of the lists are the different transformations conducted at each step. In this example, the sequence $T_2 \circ T_1 \circ T_0(Y(t))$ (with modified band depth) identifies only three of the five true outliers contained in the simulated data:

```r
R> unique(unlist(seq1$outliers))

[1] 43 53 96
```

```r
R> simdata4$true_outliers

[1] 20 43 53 70 96
```

Next we try the sequence $D_1 \circ T_1 \circ T_0(Y(t))$ but now with the total variation depth in the intermediate functional boxplot:
The sequence $D_1 \circ T_1 \circ T_0(Y)(t)$ with total variation depth identifies only two of the five true outliers as seen below:

```r
R> unique(unlist(seq2$outliers))
[1] 43 53
```

Another suggested sequence is the sequence $D_2 \circ D_1 \circ D_0(Y)(t)$. We use this sequence but now with the $L^\infty$ depth as the ordering function:

```r
R> seq3 <- seq_transform(dts = dt4,
+   sequence = c("D0", "D1", "D2"),
+   depth_method = "linfinity")
R> seq3$outliers

$D0
integer(0)

$D1
integer(0)

$D2
integer(0)
```

This time, the sequence $D_2 \circ D_1 \circ D_0(Y)(t)$ does not identify any of the outliers. This is not surprising as the sequence $D_2 \circ D_1 \circ D_0(Y)(t)$ is advisable for identifying pure magnitude (captured by $D_0$) and pure shape outliers (captured by $D_1$ and $D_2$) and this result is in line with the results of the simulation tests conducted in Dai et al. (2020) where the sequence...
\( D_2 \circ D_1 \circ T_0(Y)(t) \) performed the worst on this simulation model (See Table 4 of Dai et al. (2020)). Note that the sequence \( D_2 \circ D_1 \circ T_0(Y)(t) \) can also be specified with the `sequence` argument \( c("D0", "D1", "D1") \) or \( c("D0", "D2", "D2") \) or \( c("T0", "D1", "D2") \) since both "D1" and "D2" do the same thing, i.e., perform a lag-1 differencing and "D0" and "T0" also do the same thing (identify magnitude outliers in the raw untransformed data). When there are repeated transformations in the argument passed to `sequence` (e.g., when `sequence = c("D0", "D1", "D1")` is passed), a warning is shown and the labels of the output outliers list are changed, so that outliers for the two \( D_1 \) transformations are accessed with `output$outliers$D1_1` and `output$outliers$D1_2` respectively:

```r
R> seq4 <- seq_transform(dt = dt4,
+  sequence = c("D0", "D1", "D1"),
+  depth_method = "linfinity")
R> seq4$outliers

$D0
integer(0)

$D1_1
integer(0)

$D1_2
integer(0)
```

Sometimes, it may be necessary to inspect or save the intermediate transformed data for further analysis. Each intermediate transformed data can be saved by setting the parameter `save_data = TRUE` in the call to `seq_transform()`. These data can then be assessed with the form `object_name$transformed_data$transform`:

```r
R> seq5 <- seq_transform(dt = dt4,
+  sequence = c("D0", "D1", "D1"),
+  depth_method = "mbd", save_data = T)
R> str(seq5$transformed_data$D1_1)
num [1:100, 1:49] 0.409 0.659 0.657 0.307 0.397 ...  
- attr(*, "dimnames")=List of 2
  ..$: NULL
  ..$ : chr [1:49] "2" "3" "4" "5" ...
```

As mentioned earlier, the \( O(Y)(t) \) transformation should be used with a one-sided ERLD ordering (in the functional boxplot) so that only large values of the resulting outlyingness data are considered as extremes:

```r
R> seq6 <- seq_transform(dt = dt4,
+  sequence = "O",
+  depth_method = "erld",
+  erld_type = "one_sided_right")
R> seq6$outliers
```
The additional parameter `erld_type` specifies whether large values should be considered as extremes (`erld_type = "one_sided_right"`), or small values should be considered as extremes (`erld_type = "one_sided_left"`) or both small and large values should be considered as extremes (`erld_type = "two_sided"`). The two sided ordering is used by default if `erld_type` is not specified.

### 2.4. Massive unsupervised outlier detection

The massive unsupervised outlier detection (MUOD) detects and classifies outliers into shape, magnitude, and amplitude outliers. It was proposed in Azcorra et al. (2018) as a support method to identify influential users in social networks. MUOD works by computing for each curve three indices which measure outlyingness in terms of shape, magnitude, and amplitude. The shape index of $Y_i$ w.r.t. $F_Y$ denoted by $I_S(Y_i, F_Y)$ is defined as

$$I_S(Y_i, F_Y) = \left| \frac{1}{n} \sum_{j=1}^{n} \hat{\rho}(Y_i, Y_j) - 1 \right|,$$

where $\hat{\rho}(Y_i, Y_j)$ is the Pearson correlation coefficient between the observed points of curves $Y_i$ and $Y_j$, given by

$$\hat{\rho}(Y_i, Y_j) = \frac{\text{cov}(Y_i, Y_j)}{s_{Y_i}s_{Y_j}}, \quad s_{Y_i}, s_{Y_j} \neq 0.$$  (20)

The magnitude and amplitude indices of $Y_i$ w.r.t. $F_Y$ are defined are:

$$I_M(Y_i, F_Y) = \left| \frac{1}{n} \sum_{j=1}^{n} \hat{\alpha}_j \right|,$$

and

$$I_A(Y_i, F_Y) = \left| \frac{1}{n} \sum_{j=1}^{n} \hat{\beta}_j - 1 \right|,$$

respectively, where

$$\hat{\beta}_j = \frac{\text{cov}(Y_i, Y_j)}{s_{Y_j}^2}, \quad s_{Y_j}^2 \neq 0,$$

$$\hat{\alpha}_j = \bar{x}_i - \hat{\beta}_j \bar{x}_j,$$

and

$$\bar{x}_i = \frac{\sum_{t \in I} Y_i(t)}{p}.$$  

Generally, magnitude outliers will have larger magnitude indices, and the same applies to shape and amplitude outliers. To identify a cutoff for the indices, Azcorra et al. (2018)
proposed to use a “tangent” method, which searches for the line tangent to the maximum index and uses as cutoff the point where this tangent line intercepts the x-axis. This method is especially problematic and prone to false positives, as pointed out by Vinue and Epifanio (2020b). A alternative is to use a classical boxplot on the indices to identify extremely large indices.

MUOD is implemented in fdaoutlier and can be accessed through the muod() function. The tangent method or the classical boxplot can be specified for determining the indices cutoffs. The function returns a list containing the outliers and the MUOD indices. The outliers list contains vectors with names shape, amplitude and magnitude all containing the indices of the detected shape, amplitude, and amplitude outliers, respectively.

```r
R> simdata1 <- simulation_model1(n = 100, p = 50, +     outlier_rate = 0.1, seed = 2)
R> moutlier <- muod(dts = simdata1$data, cut_method = "tangent")
R> moutlier$outliers

$shape
[1] 100 58 35 79 21 40 50 14

$amplitude
[1] 51 100 58 14 94

$magnitude
 [1] 20 21 66 48 38 34 10 49 6 93 67

R> moutlier2 <- muod(dts = simdata1$data, cut_method = "boxplot")
R> moutlier2$outliers

$shape
[1] 100 58 35 79 21 40

$amplitude
[1] 51 100 58

$magnitude
 [1] 20 21 66 48 38 34 10 49 6 93

Furthermore, the muod magnitude (\(I_M\)), amplitude (\(I_A\)) and shape (\(I_S\)) indices can be accessed for further analysis:

```r
R> str(moutlier$indices)

'data.frame': 100 obs. of 3 variables:
$ shape   : num 0.1007 0.092 0.0845 0.1153 0.0721 ... 
$ magnitude: num 0.404 0.437 1.188 1.21 0.371 ... 
$ amplitude: num 0.08081 0.26492 0.00309 0.51515 0.11212 ...
3. Usage examples

In this section, we demonstrate the use of the `fdaoutlier` package on some common real datasets in the functional data analysis literature. In particular, we replicate some of the application examples from Dai and Genton (2018) and Dai et al. (2020). First, we analyse the Spanish ('aemet') weather dataset, followed by the population growth dataset. These datasets have been analysed extensively in the literature, and they provide meaningful applications for outlier detection in functional data analysis.

The Spanish weather data contains the daily average temperature, log precipitation, and wind speed of 73 Spanish weather stations measured between 1980-2009. This data was analysed in Dai and Genton (2018), Dai and Genton (2019), and Dai et al. (2020) where the directional outlyingness, MS-Plot, and sequential transformation methods were proposed. The data is originally available in the `fda.usc` package (with the name `aemet`) but a stripped-down version is also made available in `fdaoutlier` (with the name `spanish_weather`). In this analysis, we focus on the average temperature and log precipitation, and the aim is to find outlying curves (weather stations with outlying weather data). Following Dai and Genton (2019), we smooth the data with 11 B-spline basis functions by obtaining a smoothing matrix (without roughness penalty) using the `fda.usc` package.

```r
R> library("fda.usc")
R> data("spanish_weather")
R> b_spline <- create.bspline.basis(c(0, 365), nbasis = 11)
R> smoothing_matrix <- S.basis(tt = 0.5:364.5, basis = b_spline)
R> temp <- spanish_weather$temperature %*% smoothing_matrix
R> logprecip <- spanish_weather$log_precipitation %*% smoothing_matrix
```

A plot of the original and smoothed versions of the temperature and log precipitation data is shown in Figure 3. Next, we apply MS-Plot on the individual smoothed temperature and log precipitation data using the `msplot()` function to detect the marginal outliers.

```r
R> temp_ms <- msplot(dts = temp, plot = F)
R> logprecip_ms <- msplot(dts = logprecip, plot = F)
```

Using the indices of the outliers returned, we can identify the weather stations detected as marginal outliers using the station information data (`station_info`).

```r
R> head(spanish_weather$station_info$name[temp_ms$outliers])
[1] "A CORUÑA"
[2] "A CORUÑA/ALVEDRO"
[3] "SANTIAGO DE COMPOSTELA/LABACOLLA"
[4] "ASTURIAS/AVILÉS"
[5] "OVIEDO"
[6] "TARIFA"

R> head(spanish_weather$station_info$name[logprecip_ms$outliers])
```
Figure 3: Plot of temperature and log precipitation and their smoothed (with 11 B-spline basis) versions.

Using the vectors of the mean and variation of directional outlyingness returned by `msplot()`, we can make a plot of the outliers detected and the plots of VO against MO as shown in Figure 4.

We can also apply `msplot()` on the multivariate functional constructed by combining both the smoothed temperature and log precipitation using an `array` in order to detect and identify the joint temperature and log precipitation outliers:

```R
R> joint_dt <- array(data = c(as.vector(temp), as.vector(logprecip)), +                     dim = c(nrow(temp), ncol(temp), 2))
R> joint_ms <- msplot(joint_dt, plot = F)
R> joint_ms$outliers
```

[1] 1 2 3 9 20 21 31 33 34 35 36 39 44 52 55 56 57 58 59 60 66 70
Figure 4: Plot of temperature and log precipitation and their MS-Plots. Lines and points in color are outliers.

R> head(spanish_weather$station_info$name[joint_ms$outliers])

[1] "A CORUÑA"
[2] "A CORUÑA/ALVEDRO"
[3] "SANTIAGO DE COMPOSTELA/LABACOLLA"
[4] "ASTURIAS/AVILÉS"
[5] "TARIFA"
[6] "SANTANDER/PARAYAS"

Figure 5 shows the plot of the variation of outlyingness VO against the norm of the mean of outlyingness $||MO||$ produced by fdaoutlier (by setting plot = TRUE in the call to msplot()). Another option to detect joint outliers is to use the directional outlyingness transformation O(Y)(t) (together with a one-sided ERLD in the functional boxplot) in Dai et al. (2020). This can be achieved using the seq_transform() function in fdaoutlier.

R> joint_seq <- seq_transform(dts = joint_dt, sequence = "O",
+    depth_method = "erld", erld_type = "one_sided_right")
R> joint_seq$outliers

$0
[1] 33 34 35 36 39 44 45 55 56 58 60 66
As a second example, we consider the world population data analysis carried out in Dai et al. (2020). The data consists of the population of 105 countries as of July 1 in the years 1950-2010. These 105 countries are countries with a population between 1 million and fifteen million on July 1, 1980. The preprocessed data is available in fdaoutlier under the name world_population. A plot of the data is shown in Figure 6. Using the seq_tranform() function, we try to reproduce the results of the analysis carried out in Dai et al. (2020) which identified different types of outliers in the data using the the transformation $T_2 \circ T_1 \circ T_0$ (and the $L^\infty$ depth in the functional boxplots).

```r
R> seq_pop <- seq_transform(dts = world_population,
+ sequence = c("T0", "T1", "T2"),
+ depth_method = "linfinity")
```

The magnitude outliers are then the $T_0$ outliers which can be obtained with:

```r
R> seq_pop$outliers$T0
[1]  5  9 18 25 40 41 44 49 55
```

```r
R> (t0_outliers <- rownames(world_population)[seq_pop$outliers$T0])
```
Figure 6: World population in thousands of 105 countries from 1950-2010.

[1] "Mozambique" "Uganda"    "Sudan"    "Ghana"
[5] "Afghanistan" "Nepal"     "Malaysia" "Iraq"
[9] "Saudi Arabia"

and the $T_1$ outliers:

\begin{verbatim}
R> seq_pop$outliers$T1
[1] 3 5 9 12 13 18 24 25 36 40 41 44 49 55 57 59
\end{verbatim}

\begin{verbatim}
R> (t1_outliers <- rownames(world_population)[seq_pop$outliers$T1])
[1] "Madagascar"   "Mozambique"
[3] "Uganda"       "Angola"
[5] "Cameroon"     "Sudan"
[7] "Cote d'Ivoire" "Ghana"
[9] "Kazakhstan"   "Afghanistan"
[11] "Nepal"        "Malaysia"
[13] "Iraq"         "Saudi Arabia"
[15] "Syrian Arab Republic" "Yemen"
\end{verbatim}
In Dai et al. (2020), they considered the $T_1$ outliers which are not $T_0$ outliers as amplitude outliers for classification purposes. These can be obtained with:

```r
R> amp_ind <- seq_pop$outliers$T1[!(seq_pop$outliers$T1 + %in% seq_pop$outliers$T0)]
R> rownames(world_population)[amp_ind]
```

[1] "Madagascar" "Angola"
[3] "Cameroon" "Cote d'Ivoire"
[5] "Kazakhstan" "Syrian Arab Republic"
[7] "Yemen"

Finally, the shape outliers are the $T_2$ outliers that are neither $T_0$ outliers nor $T_1$ outliers.

```r
R> shape_ind <- seq_pop$outliers$T2[!(seq_pop$outliers$T2 + %in% seq_pop$outliers$T0)]
R> shape_ind <- shape_ind[!(shape_ind %in% seq_pop$outliers$T1)]
R> rownames(world_population)[shape_ind]
```

[1] "Rwanda" "Armenia"
[3] "Georgia" "Belarus"
[5] "Bulgaria" "Czech Republic"
[7] "Hungary" "Republic of Moldova"
[9] "Estonia" "Latvia"
[11] "Lithuania" "Bosnia and Herzegovina"
[13] "Croatia"

The $T_0$ and $T_1$ outliers are mostly countries in Africa and the Middle East while the shape outliers ($T_2$ outliers) are mostly Eastern and Central European countries. The outliers detected are visualised in Figure 7, and these results are consistent with Dai et al. (2020, Table 5). We can also use `tvdmss()` and `muod()` on the world population data:

```r
R> wptvdout <- tvdmss(dts = world_population)
R> wpmout <- muod(dts = world_population, cut_method = "boxplot")
```

TVD did not detect any magnitude outlier but MSS does find a couple of “shape” outliers all of which are in Africa and the Middle East, and these countries are those classified as $T_0$ and $T_1$ outliers by sequential transformations above:

```r
R> wptvdout$magnitude_outliers
NULL
```

```r
R> rownames(world_population)[wptvdout$shape_outliers]
```

[1] "Mozambique" "Uganda"
[3] "Sudan" "Cote d'Ivoire"
Figure 7: Outliers detected in world population data using sequential transformation. Curves in red are magnitude outliers, in blue are shape outliers, in green are amplitude outliers and in grey are normal observations.

[5] "Ghana" "Kazakhstan"
[7] "Afghanistan" "Nepal"
[9] "Malaysia" "Iraq"
[11] "Saudi Arabia" "Syrian Arab Republic"
[13] "United Arab Emirates" "Yemen"

The countries flagged as magnitude outliers by muod() are very similar to those flagged by sequential transformations as $T_0$ outliers:

R> rownames(world_population)[wpmout$outliers$magnitude]

[1] "Sudan" "Saudi Arabia" "Uganda" "Iraq"
[5] "Cote d'Ivoire" "Malaysia"

The amplitude outliers detected by muod() that are also not magnitude outliers are:

R> wpamp_ind <- wpmout$outliers$amplitude[!(wpmout$outliers$amplitude + %in% wpmout$outliers$magnitude)]
R> rownames(world_population)[wpamp_ind]
Finally, the shape outliers flagged by \texttt{muod()} that are neither amplitude nor magnitude outliers are mostly the Eastern and Central European countries flagged as $T_2$ outliers by sequential tranformations:

\begin{verbatim}
R> wpshape_ind <- wpmout$outliers$shape[!(wpmout$outliers$shape + %in% wpmout$outliers$magnitude)]
R> wpshape_ind <- wpshape_ind[!(wpshape_ind %in% wpmout$outliers$amplitude)]
R> rownames(world_population)[wpshape_ind]
\end{verbatim}

In conclusion, the outliers detected and the classification of such outliers may vary across different outlier detection methods as shown by this world population data example. While the results of the outlier detection and classification for MUOD and sequential transformations are quite similar, those of TVD and MSS are quite different and in particular, countries identified as shape outliers by TVD and MSS are those flagged as magnitude and amplitude outliers by MUOD and sequential tranformations.

\section*{4. Summary and future outlook}

This article introduces the \texttt{fdaoutlier} package, which extends the available tools for outlier detection in functional data analysis in \texttt{R}. \texttt{fdaoutlier}'s focus so far has been the implementation of the latest state-of-the-art outlier detection methods in the FDA literature that are not yet implemented in \texttt{R} and that are especially useful for detecting shape outliers. These include the directional outlyingness and MS-Plot, the total variation depth and modified shape similarity, and sequential transformations. These implementations will be especially useful to FDA researchers for testing and comparissons in the development of new outlier detection and exploratory methods. Likewise, \texttt{fdaoutlier} will be useful for practitioners in the exploratory analysis of their functional data.

We will continue adding more outlier detection methods for functional data to the \texttt{fdaoutlier} package, especially (future) outlier detection methods not yet implemented in \texttt{R}, and also those with implementations in \texttt{R} but that can be improved upon. We will also continue adding useful tools for development and testing of new outlier detection methods for functional data, e.g., additional simulation models and functions for comparing outlier detection methods, and these will be directed by the trends in the FDA literature. Our long-term goal for the
The development of \texttt{fdaoutlier} is for it to be a helpful package for practitioners and researchers alike for conducting robust analysis and outlier detection for functional data.

\section*{Computational details}

The results in this paper were obtained using R 3.6.3 with the \texttt{fdaoutlier} 0.2.0 package and \texttt{fda.usc} 2.0.2. R itself and all packages used are available from the Comprehensive R Archive Network (CRAN) at \url{https://CRAN.R-project.org/}.

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