Distance for Functional Data Clustering Based on
Smoothing Parameter Commutation

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Abstract

We propose a novel method to determine the dissimilarity between subjects for functional data clustering. Spline smoothing or interpolation is common to deal with data of such type. Instead of estimating the best-representing curve for each subject as fixed during clustering, we measure the dissimilarity between subjects based on varying curve estimates with commutation of smoothing parameters pair-by-pair (of subjects). The intuitions are that smoothing parameters of smoothing splines reflect inverse signal-to-noise ratios and that applying an identical smoothing parameter the smoothed curves for two similar subjects are expected to be close. The effectiveness of our proposal is shown through simulations comparing to other dissimilarity measures. It also has several pragmatic advantages. First, missing
values or irregular time points can be handled directly, thanks to the nature of smoothing splines. Second, conventional clustering method based on dissimilarity can be employed straightforward, and the dissimilarity also serves as a useful tool for outlier detection. Third, the implementation is almost handy since subroutines for smoothing splines and numerical integration are widely available. Fourth, the computational complexity does not increase and is parallel with that in calculating Euclidean distance between curves estimated by smoothing splines.

Keywords: Clustering, irregular longitudinal data, functional data, smoothing splines, dissimilarity, outlier.

1 Introduction

Clustering sets out to find groups for subjects based on several different characteristics (variables) with no subgroup labels other than the observed information. Ideal clustering memberships achieve the target such that subjects within a cluster are considered to be similar for the given characteristics (variables). The degree of similarity and dissimilarity can be defined in plenty of ways, and there are various methods for grouping subjects, including hierarchical clustering, k-means, and DBSCAN to name a few. See e.g. Berkhin (2006), Bouveyron and Brunet-Saumard (2014), Murtagh and Contreras (2012) for brief literature review of conventional clustering analysis in a multivariate data context.

In many situations, however, only one variable per subject was measured, but it was measured time after time. Functional data clustering is a somewhat distinctive notion to deal with grouping based on such data. The functional data clustering differs from conventional clustering in two aspects: data format and time coordinates. First, the data may be collected at unequally spaced time points, and many ‘missing’ values occur if an analyst aligns records into the conventional ‘variable-by-variable’ format. Second, even all subjects were observed at the same time points, the conventional clustering fails to take into account the coordinating order of variables, on which adjacent data collected for the same subject are expected to have similar values. Several methods for functional data have been suggested in the literature, and we review three major categories in the following: distance-based methods, decomposition-based methods, and model-based methods.
Distance-based methods, using pointwise distance between pairs of subjects, are the most straightforward approach (e.g., Tarpey and Kinateder [2003], Genolini and Falissard [2010]). They often deal with the two issues mentioned above by certain curve smoothing or imputation techniques, and subsequently distances between subjects are computed to which the conventional distance-based methods can be applied. Little attention, however, has been paid to the uncertainty of smoothing or imputation. To the best of our knowledge, the only two exceptions are (1) the prediction based approach of Alonso et al. [2006] that modified by Vilar et al. [2010], and (2) the hypotheses-testing-like approach of Maharaj [1996]. The former is computationally intensive and the latter is designed for invertible ARMA process, which restrict their application.

Decomposition-based methods, overcome the smoothing and sequential order issues through transforming the observed data into a finite series of common features, and the procedures deal with uncertainty of smoothing implicitly. For example, Abraham et al. [2003] used spline basis functions, James et al. [2000] used functional principal component analysis, and Warren Liao [2005] reviewed more sophisticated ‘feature-extraction’ algorithms. These approaches define common features for all groups and then assign weights to features by which groups are identified. Each group has different weights on those features and each group can be interpreted according to its lower-dimensional projection on features. Features extracted from a certain transformation of data are also popular, such as spectral densities (Fan and Zhang [2004]), periodogram (Caiado et al. [2006], De Lucas [2010]), and permutation distribution (Brandmaier [2012]). Nonetheless, in reality not all groups share the same number of features, and how to determine an appropriate number of dimensions is not easy.

In light of the difficulties encountered by the first two methods, many researchers suggest the third alternative, various model-based frameworks. They estimate individual underlying curves and cluster subjects simultaneously, and then statistical inference can be made based on the working models for clusters, such as measuring the uncertainty for cluster assignment and ‘within-cluster’ variation. Unfortunately, these approaches encounter other challenges. Purely parametric functional forms used in traj (Jones and Nagin [2007]) may not be realistic and its assumption of subjects sharing the same ‘un-
derlying’ curve within a group can be too restrictive. Applying semi- or non-parametric
methods has to do some dimension reduction within each group (e.g., FCM by James
and Sugar [2003] funHDDC by Bouveyron and Jacques [2011] Funclust by Jacques and
Preda [2013] and K-centre by Chiou and Li [2007]), but this encounters a similar problem
as decomposition-based methods. A pure likelihood-based framework (without dimension
reduction) called longclust is proposed by McNicholas and Murphy (2010). This method
is limited to short time series and breaks down easily due to the curse of dimensionality.
Even worse, the notion of distribution for random functions is not well-defined as curves
could have infinite dimensions (see e.g., Delaigle and Hall [2010]).

The aforementioned review describes the strengths and weaknesses of the existing
functional data clustering methods. Moreover, it is worth mentioning that the curve
variability is an important issue. Clustering curves can be a difficult ‘chicken-and-egg’
problem between (1) how to determine the within-cluster variations before identifying sub-
groups, and (2) how to separate subgroups when within-cluster variations are unknown.
This dilemma is related directly to the smoothing uncertainty problem in distance-based
approaches. Decomposition-based and model-based approaches estimate such variability
with necessity, but the estimation id often distorted when outliers occurs. A two-step
strategy exploiting relative merits of different methods seems reasonable: initially sepa-
rate potential outliers based on ‘outlier-invariant’ pairwise distance, and then form main
clusters with another appropriate clustering method. For such a strategy, a distance
measure concerning the variability of curve estimation or feature selection is crucial.

In this article, we develop an easily implementable and practically advantageous
method for distance measure between subjects. Instead of estimating the best-representing
curve for each subject as fixed during clustering, we propose to measure the dissimilarity
between subjects based on pair-by-pair varying curve estimates for a subject. By applying
the technique of smoothing splines, the curve smoothing is completely determined by the
chosen smoothing parameter. The intuitions behind our proposal are that smoothing pa-
rameters of smoothing splines reflect inverse signal-to-noise ratios and that the smoothing
results for two similar subjects are expected to be close if an identical smoothing param-
eter is applied. Specifically, if the unobserved true curves of subjects $i$ and $j$ are similar,
the estimates for them should resemble with each other, no matter whether we use a smoothing parameter primarily for the $i$-th or the $j$-th subject. Our distance is then calculated through commuting between the smoothing parameters for a pair.

The rest of the article is organized as follows. Section 2 describes the proposed dissimilarity and some of its properties. Its effectiveness is shown through simulations comparing to other dissimilarity measures in Section 3. An example of its application to methadone dosages observations is given in Section 4, where we also identified outliers with a rather simple method. Finally, Section 5 provides some concluding remarks and discussion concerning future directions.

2 The Proposed Distance

We utilize the smoothing spline as our smoothing method, and so we briefly introduce the smoothing spline before our proposal. Assume that the curve of $i$-th subject is observed at distinct finite time points $\{t_{i,1}, \ldots, t_{i,K_i}\}$ in an interval $[T_L, T_U]$ with measurement errors according to the model

$$y_{i,k} = f_i(t_{i,k}) + \epsilon_{i,k}, \quad k = 1, \ldots, K_i, \quad i = 1, \ldots, n,$$

(1)

where $\epsilon_{i,k} \sim N(0, \sigma^2)$. A reasonable estimation of $f_i$ is to minimize

$$\frac{1}{K_i}\sum_k (y_{i,k} - f_i(t_{i,k}))^2$$

but control the wiggleness of $f_i$ such as

$$\int_{T_L}^{T_U} (f''_i(t))^2 dt \leq \rho$$

for a positive $\rho$. This estimator is equivalent to a smoothing spline $\hat{f}_i(\cdot; \lambda)$ which minimizes

$$\frac{1}{K_i}(y_i - f_i)'(y_i - f_i) + \lambda \int_{T_L}^{T_U} (f''_i(t))^2 dt$$

(2)

given a smoothing parameter $\lambda$, where $y_i = (y_{i,1}, \ldots, y_{i,K_i})'$ and $f_i = (f_i(t_{i,1}), \ldots, f_i(t_{i,K_i}))'$ (see e.g., Wahba and Wendelberger, 1980; Green and Silverman, 1993). There are various methods to determine an appropriate $\lambda$ in (2), and once $\lambda$ chosen $\hat{f}_i(t; \lambda)$ for $t \in [T_L, T_U]$ is completely established. We exploit a mixed-effects model representation (e.g., Wang, 1998) of the problem in (2) as

$$y_i = X_i\beta_i + u_i + \epsilon_i,$$

(3)
where $\beta_i$ is the fixed effect, $X_i$ has two columns being 1's and $(t_{i,1}, \ldots, t_{i,K_i})'$, $\epsilon_i = (\epsilon_{i,1}, \ldots, \epsilon_{i,K_i})' \sim N(0, \sigma^2 I)$, and $u_i \sim N(0, \sigma_u^2 R)$ with $\sigma_u^2 = \sigma^2/(K_i\lambda)$ and the $(k,k^*)$ element of $R$ being

$$(TU - TL)^{-2} \int_{TL}^{TU} (t_{i,k} - \tau)^+(t_{i,k^*} - \tau)_+ d\tau$$

with $a_+ = \max(0, a)$. As a function of variance for $u_i$ in (3), $\lambda$ can be determined based on the restricted maximum likelihood method and $K_i\lambda$ has a useful interpretation of inverse signal-to-noise ratio as $\sigma_u^2/\sigma^2$. Additionally, it has been shown that the smoothing results are more robust even when the correlation structure of $\text{var}(\epsilon_i)$ is mis-specified (e.g. Wang 1998 and Krivobokova and Kauermann 2007).

Our proposal starts with finding $\hat{\lambda}_i$ in (3) for each subject based on $y_i$. The estimated curve is denoted by $\hat{f}_i(\cdot; \hat{\lambda}_i)$, which amounts to obtaining $\hat{f}_i(\cdot; \lambda)$ given $\lambda = \hat{\lambda}_i$ in (2) for observations $y_i$. Fixed on the smoothing parameter $\hat{\lambda}_i$, we can obtain $\hat{f}_j(\cdot; \hat{\lambda}_i)$ based on observations $y_j$. The roles of the two subjects can be exchanged, and similarly we have $\hat{f}_j(\cdot; \hat{\lambda}_j)$ and $\hat{f}_i(\cdot; \hat{\lambda}_j)$. Then the distance between subjects $i$ and $j$ is calculated as

$$d_{i,j} = \frac{1}{2} \left\{ \int_{TL}^{TU} \left( \hat{f}_i(t; \hat{\lambda}_i) - \hat{f}_j(t; \hat{\lambda}_j) \right)^2 dt \right\}^{1/2} + \left[ \int_{TL}^{TU} \left( \hat{f}_i(t; \hat{\lambda}_j) - \hat{f}_j(t; \hat{\lambda}_j) \right)^2 dt \right]^{1/2}.$$  

(4)

Due to the roles of $\hat{\lambda}_i$ and $\hat{\lambda}_j$ in (4), we call it a smoothing parameter commutation based distance, and explain its underlying rationale below. First if the ‘true’ $f_i$ and $f_j$ are similar, it is expected that $\hat{f}_i$ and $\hat{f}_j$ from $y_i$ and $y_j$ should be close, given an identical smoothing parameter. Second it takes the variation of smoothing into consideration with diverse $\lambda$’s for different pair of $(i,j)$’s. It focuses on how similar a pair of curves can be, instead of the distance between (fixed) estimated curves. Third $d_{i,j} \geq 0$, $d_{i,j} = 0$ if $i = j$, and $d_{i,j} = d_{j,i}$, so conventional distance based clustering methods can be applied straightforward. Fourth it reduces to rooted integral squared difference of $f_i$ and $f_j$ when no missing values and measurement errors present.

Our proposal also has several pragmatic advantages. First, missing values or irregular time points can be handled directly, thanks to the nature of smoothing splines. Second, the dissimilarity also serves as a useful tool for outlier detection (see Section 4). Third, the implementation is almost handy since subroutines for smoothing splines and numerical
integration are widely available. Although the computing burden for (4) seems heavy at first glance, it can be done more efficiently among \( n \) subjects. Given \( \lambda \) a fast \( O(K_i) \) algorithm to compute \( \hat{f}_i(t; \lambda) \) does exist (e.g., Hutchinson and De Hoog [1985]). Thus, one needs to solve \( \hat{\lambda}_i \) in (3) only \( n \) times for the \( n \) subjects, and then adopts the fast algorithm for \( \{\hat{f}_j(t; \hat{\lambda}_i) : i, j = 1, \ldots, n\} \). Therefore the computational complexity is proportional to that in treating \( f = \hat{f}_i(t; \lambda_i) \) as fixed and calculating distance as squared root of \( \int_T \left( \hat{f}_i(t; \lambda_i) - \hat{f}_j(t; \hat{\lambda}_j) \right)^2 \, dt \) (see Ramsay and Silverman [2005] and the latter procedure is referred to as \( d_{SS} \) in what follows).

3 Simulation

We conduct a simulation to investigate whether our proposed measure is more representative than other dissimilarity measures when observations were contaminated with (independent or dependent) noises. If an analyst is interested in the relative shape pattern of curves, regardless of shift, shrinkage, expansion, or magnitude, then several alignment, normalization, and warping tools can be applied in preprocessing (e.g., Berndt and Clifford [1994], Gaffney and Smyth [2004], and Liu and Yang [2009]). For fear of losing focus, we do not consider distance measures engaging with the preprocessing.

We consider the following four random curve models over \( t \in [0, 1] \)

\[
\begin{align*}
\hat{f}^{(1)}(t; \eta) &= \eta, \\
\hat{f}^{(2)}(t; \eta) &= \sin(2\pi t) - t + 2\eta \cos(4\pi t), \\
\hat{f}^{(3)}(t; \eta) &= 3t + 2\eta t, \\
\hat{f}^{(4)}(t; \eta) &= 5\eta \left\{ (t - 0.5)^2 - 2t(1 - t) \right\},
\end{align*}
\]

where \( \eta \sim N(1, 0.3^2) \). The four functional forms stand for constant, periodic, linear, and nonlinear (unobserved) true curves, respectively. The observed data are generated according to (1) merely at 200 time points, \( t_k \in \{0, 1/199, \ldots, 198/199, 1\} \), with noises
coming from four mechanisms

WN: \( \epsilon_k = \xi_k \),

AR : \( \epsilon_k = 0.8\epsilon_{k-1} + \xi_k \),

SARMA: \( \epsilon_k = 0.8\epsilon_{k-10} + 0.8\xi_{k-10} + \xi_k \),

BILR: \( \epsilon_k = 0.8\epsilon_{k-1} + 0.2\xi_{k-1} - 0.2\epsilon_{k-1}\xi_{k-1} + \xi_k \), (5)

where \( \xi_k \overset{i.i.d.}{\sim} N(0, 1) \) and \( \xi_k \) is independent of \( \epsilon_{k'} \) for \( k' \neq k \). That is, we set \( K_i \equiv 200, \ t_{ik} \equiv (k - 1)/199. \) The four noise mechanisms are examples of usual assumption for noises: purely independent process, stationary process, cyclostationary process, and nonstationary process. For each combination of \( f \in \{ f(1), f(2), f(3), f(4) \} \) and mechanism of \( \epsilon_k \), 10 series are generated according to 10 independent \( \eta \) as well as 10 sets of \( \epsilon_k \)'s, and totally there are 160 series mimicking the longitudinal observations from 160 subjects.

Then several distance measures are calculated based on the simulated data. Following the notation in [Montero and Vilar (2014)], we compare 10 measures, including our proposal (referred to as \( d_{OUR} \)) and point-wise Euclidean distance \( d_{EUCL} = \sqrt{\sum_k (y_{ik} - y_{jk})^2} \), and the eight others are listed in Table 1. Two comparison criteria are defined as follows:

\[
Q = \min_{a,b} \sum_i \sum_{j \neq i} \left( a + b\hat{d}_{i,j} - d_{i,j} \right)^2 \frac{d_{i,j}}{d_{i,j}},
\]

\[
R = \sum_i \sum_{j \neq i} (\hat{r}_{i,j} - r_{i,j})^2,
\]

where \( \hat{d}_{i,j} \) is one of the considered distance measures between the \( i \)-th and \( j \)-th subjects, \( d_{i,j} = \sqrt{\sum_k (f_i(t_{ik}) - f_j(t_{jk}))^2} \) is the true distance without noise, and \( \hat{r}_{i,j} \) and \( r_{i,j} \) are the corresponding rank of \( \hat{d}_{i,j} \) and \( d_{i,j} \) among all pairs of \((i, j)\)'s, respectively. The quantity \( Q \) reflects the loss, normalized by the true distance scales, for (linear) approximation to all the pairs of true distances, while \( R \) measures the deviation from monotonicity between \( \hat{d}_{i,j} \) and \( d_{i,j} \). A good measure should have a small value of \( Q \) or \( R \). The averaged \( Q \) and \( R \) values for the 10 measures over 200 simulation replicates are given in Table 2 and Table 3 respectively.

The two comparison criteria are highly coherent in that they almost always sort the
Table 1: Distance measures to be compared.

| Notation | Description                                                  | Literature |
|----------|--------------------------------------------------------------|------------|
| $d_{MAH}$ | parametric testing of equality of processes                  | Maharaj [1996] |
| $d_{GLK}$ | nonparametric equality testing of log-spectra                 | Fan and Zhang [2004] |
| $d_{SS}$  | based on spline smoothing curves                              | Ramsay and Silverman [2005] |
| $d_{CORT}$ | correlation-based modification of $d_{EUCL}$                  | Chouakria and Nagabhushan [2007] |
| $d_{IP}$  | based on integrated periodogram                               | De Lucas [2010] |
| $d_{PRED,h}$ | based on predicted values at future                          | Vilar et al. [2010] |
| $d_{CID}$ | complexity-based modification of $d_{EUCL}$                  | Batista et al. [2011] |
| $d_{PDC}$ | permutation distributions of order patterns                   | Brandmaier [2012] |

Table 2: Averaged Q values over 200 simulated replicates among 10 distance measures for each combination of $f$ and $\epsilon_k$ (with 10 random curves), and all the 160 curves. W, A, S, and B in the first column stand for WN, AR, SARMA, and BILR in [5], respectively. Bold digits are the best 3 within each row.

| $f$ $+$ $W$ | $f$ $+$ $A$ | $f$ $+$ $S$ | $f$ $+$ $B$ | $f$ $+$ $W$ | $f$ $+$ $A$ | $f$ $+$ $S$ | $f$ $+$ $B$ | $f$ $+$ $W$ | $f$ $+$ $A$ | $f$ $+$ $S$ | $f$ $+$ $B$ |
|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| $d_{EUCL}$  | $d_{OUR}$   | $d_{MAH}$   | $d_{GLK}$   | $d_{SS}$    | $d_{CORT}$  | $d_{IP}$    | $d_{PRED,h}$ | $d_{CID}$   | $d_{PDC}$   | $d_{EUCL}$  | $d_{OUR}$   |
| 1.59        | 0.36        | 8.45        | 8.55        | 0.37        | 3.82        | 9.32        | 1.85        | 2.19        | 8.63        | 1.59        | 0.36        |
| 5.61        | 5.66        | 8.07        | 8.02        | 5.66        | 6.4         | 9.54        | 4.61        | 5.82        | 7.96        | 5.61        | 5.66        |
| 8.07        | 6.15        | 8.67        | 8.55        | 6.16        | 8.68        | 10.53       | 7.32        | 8.19        | 8.78        | 8.07        | 6.15        |
| 7.65        | 7.66        | 8.48        | 8.48        | 7.65        | 7.89        | 11.88       | 5.62        | 7.87        | 8.48        | 7.65        | 7.66        |
| 2.21        | 0.87        | 3.79        | 3.56        | 0.83        | 3.54        | 1.35        | 3.96        | 2.76        | 4.06        | 2.21        | 0.87        |
| 3.94        | 3.94        | 3.91        | 3.97        | 3.94        | 3.94        | 5.69        | 4.01        | 3.95        | 3.97        | 3.94        | 3.94        |
| 3.96        | 3.81        | 3.83        | 3.83        | 3.63        | 3.94        | 5.71        | 4.04        | 3.93        | 3.95        | 3.96        | 3.81        |
| 3.99        | 3.99        | 4.05        | 4.06        | 3.99        | 3.99        | 12.32       | 4.04        | 4.04        | 4.09        | 3.99        | 3.99        |
| 1.49        | 1.05        | 1.40        | 1.40        | 0.99        | 1.52        | 1.38        | 1.58        | 1.50        | 1.53        | 1.49        | 1.05        |
| 1.49        | 1.49        | 1.47        | 1.49        | 1.49        | 1.50        | 2.38        | 1.51        | 1.49        | 1.49        | 1.49        | 1.49        |
| 1.53        | 1.49        | 1.49        | 1.49        | 1.49        | 1.52        | 4.07        | 1.54        | 1.52        | 1.51        | 1.53        | 1.49        |
| 1.56        | 1.56        | 1.55        | 1.56        | 1.56        | 1.57        | 12.44       | 1.58        | 1.56        | 1.56        | 1.56        | 1.56        |
| 2.31        | 0.79        | 3.17        | 3.19        | 0.81        | 2.94        | 3.53        | 2.69        | 2.54        | 3.18        | 2.31        | 0.79        |
| 3.20        | 3.20        | 3.21        | 3.27        | 3.20        | 3.23        | 4.01        | 3.04        | 3.23        | 3.22        | 3.20        | 3.20        |
| 3.29        | 3.19        | 3.23        | 3.22        | 3.18        | 3.29        | 4.74        | 3.32        | 3.28        | 3.25        | 3.29        | 3.19        |
| 3.35        | 3.35        | 3.38        | 3.38        | 3.35        | 3.36        | 9.01        | 3.31        | 3.38        | 3.37        | 3.35        | 3.35        |
| ALL         | 24.83       | 23.92       | 29.29       | 29.30       | 24.45       | 26.13       | 32.38       | 25.63       | 28.86       | 29.28       |

same best and worst measures. As expected, $d_{EUCL}$ is often among the best measures since there are no missing data and $d_{EUCL}$ is unbiased in many situations. But it does not good enough if the signal or noise is periodic ($f^{(2)}$, SARMA, respectively). Our method and $d_{SS}$ always fall in the best 3 measures, either for 10 curves within an individual group or for 160 curves as a whole. Note that $d_{SS}$ and $d_{EUCL}$ have almost identical result within a group, due to both utilize the mixed-effects model representation of smoothing splines. The difference lies in that $d_{SS}$ regarding $\hat{f}_i(t; \hat{\lambda}_i)$ as a fixed estimate of $f_i$. Our method outperforms for between-group distance, which indicates the advantage of accounting for smoothing variation via smoothing parameter commutation. In certain cases $d_{PRED,h}$ and $d_{MAH}$ are good measures, which also take estimation uncertainty into consideration.
| Method   | $d_{EUCL}$ | $d_{OUR}$ | $d_{MAH}$ | $d_{GLK}$ | $d_{SS}$ | $d_{CORT}$ | $d_{IP}$ | $d_{PRED,A}$ | $d_{CID}$ | $d_{PDC}$ |
|----------|------------|-----------|-----------|-----------|---------|------------|---------|-------------|---------|---------|
| $f^{(1)}+W$ | 0.73       | 0.24      | 12.26     | 12.15     | 0.24    | 2.22       | 12.01   | 1.11        | 1.16    | 12.39   |
| $f^{(1)}+A$ | 4.89       | 4.89      | 12.11     | 12.02     | 4.89    | 5.85       | 12.29   | 3.98        | 5.15    | 12.29   |
| $f^{(1)}+S$ | 7.79       | 5.21      | 11.82     | 11.94     | 5.24    | 10.20      | 12.29   | 7.23        | 8.87    | 12.18   |
| $f^{(1)}+B$ | 7.73       | 7.73      | 12.27     | 12.15     | 7.73    | 8.30       | 12.25   | 4.70        | 8.20    | 12.43   |
| $f^{(2)}+W$ | 3.01       | 1.04      | 8.88      | 6.69      | 1.01    | 6.27       | 1.29    | 11.69       | 4.21    | 12.27   |
| $f^{(2)}+A$ | 9.20       | 9.20      | 10.24     | 10.59     | 9.19    | 9.80       | 8.15    | 12.66       | 9.45    | 12.05   |
| $f^{(2)}+S$ | 10.99      | 8.19      | 10.14     | 10.18     | 7.88    | 11.71      | 7.85    | 13.45       | 11.33   | 12.35   |
| $f^{(2)}+B$ | 10.59      | 10.6      | 11.62     | 11.63     | 10.6    | 10.89      | 10.77   | 12.66       | 10.75   | 12.10   |
| $f^{(3)}+W$ | 9.18       | 4.49      | 8.16      | 8.10      | 4.27    | 10.79      | 6.78    | 14.54       | 10.09   | 12.35   |
| $f^{(3)}+A$ | 11.5       | 11.53     | 11.89     | 11.87     | 11.53   | 11.69      | 12.06   | 13.88       | 11.53   | 12.22   |
| $f^{(3)}+S$ | 11.90      | 11.53     | 11.72     | 12.17     | 11.34   | 11.95      | 12.10   | 14.09       | 11.87   | 11.96   |
| $f^{(3)}+B$ | 11.99      | 12.02     | 12.12     | 12.05     | 12.02   | 11.94      | 12.26   | 13.51       | 12.06   | 12.31   |
| $f^{(4)}+W$ | 4.63       | 1.31      | 11.56     | 12.23     | 1.32    | 7.87       | 12.29   | 7.49        | 5.79    | 12.21   |
| $f^{(4)}+A$ | 9.89       | 9.89      | 11.59     | 12.28     | 9.88    | 10.45      | 12.47   | 10.00       | 10.02   | 12.18   |
| $f^{(4)}+S$ | 11.71      | 10.23     | 11.34     | 12.11     | 10.23   | 11.87      | 12.19   | 13.08       | 11.72   | 12.20   |
| $f^{(4)}+B$ | 11.24      | 11.26     | 12.24     | 12.20     | 11.26   | 11.52      | 12.24   | 10.83       | 11.41   | 11.68   |
| ALL       | 1155.6     | 874.7     | 4160.5    | 4063.7    | 901.0   | 3768.6     | 2693.1  | 4191.6      |        |        |

Table 3: Averaged R values over 200 simulated replicates among 10 distance measures for each combination of $f$ and $\epsilon_k$ (with 10 random curves), and all the 160 curves. W, A, S, and B in the first column stand for WN, AR, SARMA, and BILR in (5), respectively. Bold digits are the best 3 within each row.

4 Real Data Application

We shall apply (4) to a methadone maintenance therapy data in Lin et al. (2015). Daily methadone dosages in mg for 314 participants between 01 January 2007 and 31 December 2008 were collected. The (partially) observed dose levels for each patient from day 1 to day 180 were used for clustering. Lin et al. (2015) categorized the dosages into 7 levels, one of which is missing value, and proposed a new dissimilarity measure for clustering ordinal data. The ordering of time coordinates, however, were discarded in their approach. In this example, we use the primary prescription dosage, and do not recode missing values separately. Smoothing splines take care the irregular follow-up time points of patients automatically, which may not be an easy task for other measures listed in Table 1.

The clustering procedure consists of three steps: (1) calculating the distance matrix, (2) detecting and removing outliers, and (3) forming clusters with the remaining data. We started from obtaining the pairwise distance matrix based on (4). Then two outliers were simply detected by calculating the average distance of each patient’s nearest 3 neighbors. Two had the distance in magnitude of 500 and 1 010, while all the others had distance falling [39,300]. Cluster identification result can be affected significantly by a few far away
noisy points, which should be removed in order to make more reliable clustering. Our
method to detect outliers is similar to [Ramaswamy et al. (2000)] based on dissimilarity.
Excluding the two outliers, the remaining 312 dosage curves of patients were clustered into
5 subgroups via “partitioning around medoids” (PAM), as shown in Figure 1. The mean
curves for each subgroup are also shown in Figure 2 (a).

It is obvious Group 1 and 2 are more stable, remaining a dose level roughly within
[10,40] and [40,80], respectively. Group 3 has an upward trend while Group 4 has a
downward trend, and from Figure 2 the two mean curves cross around day 85. Group 5
goes up quickly and stay a dose level around 80. Although Group 6 has a similar trend
to Group 5, it fluctuates heavily over a larger range and looks more unstable. Overall,
these figures indicate that a patient with early higher dosage taken (roughly above 60 mg
at day 45) tends not to reduce the level afterward and a monitoring between the second
and third month can be critical.

Results based on a model-based functional data clustering are also given for compar-
ison. We used the ‘funcit’ function in the ‘funcy’ package ([Yassouridis, 2016]) on The
Comprehensive R Archive Network (CRAN; [R Core Team, 2016]). The model option of
the function is set to be ‘iterSubspace’, i.e., an implementation of the algorithm in [Chiou
and Li, 2007]. The theoretical mean profiles of clusters based on participants including
and excluding outliers are shown in Figure 2 (c) and Figure 2 (d), respectively. Profiles
of the two outlier participants are also shown in Figure 2 (b).

Although PAM does not provide theoretical mean profiles so that it cannot be directly
compared to the model-based method, note the resemblance between Figures 2 (a) and 2
(d). Excluding the two outliers did improve the model-based method in that the average
distance to mean profile reduced 7.6% from 166.7 to 154.9, which gave more compact
clusters. Inspecting Figure 2 (b), we can realize the interlacing of the 2nd, 3rd, and 4th
subgroups in Figure 2 (c). Clearly, it is hard to group the two curves of outliers into the
found groups. Forcing to include them needs to exaggerate the within-group variation,
no matter which groups they are assigned to. Then the boundaries of groups are getting
blurred, so are the representativeness of mean profiles.

Unfortunately, identifying outlier during the model-based clustering procedure can
be tautological, since the unknown ‘ordinary’ within-group variation depends on telling apart which are ‘abnormal’ participants. In contrast, dissimilarity in a distance-based method (including our proposal) is not affected by whether outliers occurs, and can serve as an outlier detector. The simulations above reveal the stable superiority of the proposed dissimilarity, and it is usable in a beneficial preclean step for model-based clusterings.

5 Conclusion and Discussion

We have shown that distance based on smoothed data is better than distance based on specific time series assumptions, if the underlying curves are changed gradually. With smoothing parameter commutation, the proposed distance measure gains some improvement of the widely used approach in [Ramsay and Silverman (2005)] without introducing further computational complexity. We also demonstrated a simple method for outlier detection that helps model-based functional data clustering form more compact subgrous.

The ‘funcy’ package on CRAN integrated several model-based clustering methods for functional data, but most of them require regular measurements and do not fit the methadone dosage example with many missing values. The only two methods of the package allowing irregular measurements are ‘fitfclust’ and ‘iterSubspace’, and we apply the latter merely because the former was eating up more than 20GB memories and spending 6 hours at each iteration for the example, which is not yet a practical choice for general applications.

There are many other nonparametric regression methods other than smoothing splines, e.g., local polynomial regressions, wavelet analysis. Different techniques stand out in different situations. It is of interest to study whether there exist analogous parameter commutation operations and similar advantages when applying other nonparametric regressions. This direction is left as a future work.

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Figure 1: Subgroups from PAM clustering of the 312 patients in methadone maintenance therapy.
Figure 2: (a): Mean curves of subgroups in Figure 1; (b) Dosage profiles of the two excluded outliers; (c) Mean profiles of a model-based clustering method including the two outliers; (d) Mean profiles of the same clustering method with (c) but excluding the two outliers.
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