Robust Functional Manifold Clustering

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Abstract

In machine learning it is common to interpret each data sample as a multivariate vector disregarding the correlations among covariates. However, the data may actually be functional i.e. each data point is a function of some variable such as time and the function is discretely sampled. The naive treatment of functional data as traditional multivariate data can lead to poor performance due to the correlations. In this paper we focus on subspace clustering for functional data or curves, and propose a new method robust to shift and rotation. The idea is to define a function or curve and all its versions generated by shift and rotation as an equivalent class, and then find the subspace structure among all equivalent classes as the surrogate for all curves. Experimental evaluation on synthetic and real data reveals that this method massively outperforms prior clustering methods in both speed and accuracy when clustering functional data.

Keywords: Functional Data, Curves, Manifold, Clustering

1 Introduction

In machine learning it is common to interpret each data point as a vector in Euclidean space [1]. Such a discretisation is chosen because it allows for

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easy manipulations and fast computation, even with large datasets. However these methods choose to ignore that the data may not naturally fit into this assumption. In fact much of the data collected for practical machine learning are actually functions or curves. In contrast to feature vectors, functional data encode gradient information, which is vital to analysis. For example financial data such as stock or commodity prices are functions of monetary values over time [2]. Recently functional data have become increasingly important in many scientific and engineering research areas such as ECG (electrocardiogram) or EEG (Electroencephalography) in healthcare [3], subject outlines in both macro and micro-biology [4], weather or climate data [5], astronomy [6] and motion trajectories from computer vision [5, 7].

Analyzing functional data has been an emerging topic in statistical research [8, 9, 10, 11] and has attracted great attention from machine learning community in recent years [12, 13]. One of the important challenges in analyzing functional data for machine learning is to efficiently cluster and to learn better representations for functional data. Theoretically functional data are of infinite dimension. Due to discretisation, there are only limited samples taken from a functional observation. Strong correlation between neighbouring samples and information loss during discretisation are major challenges for analysis. A desired model for functional data is expected to properly and parsimoniously characterise the nature and variability hidden in the data. The classic functional principal component analysis (fPCA) [14, 15] is one of such examples to discover dominant modes of variation in the data. However fPCA may fail to capture patterns if the functional data are not well aligned in its domain. For time series, a special type of functional data, dynamic time warping (DTW) has long been proposed to compare time series based on shape and distortions (e.g., shifting and stretching) along the temporal axis [16, 17].

Another important type of functional data is shape [10, 18]. Shape is an important characterizing feature for objects, and in computer vision shape has been widely used for the purpose of object detection, tracking, classification, and recognition. In fact, a natural and popular representation for shape analysis is to parametrise boundaries of planar objects as 2D curves. In object recognition, images of the same object should be similar regardless of resolution, lighting, or orientation. Hence an efficient shape representation or shape analysis scheme must be invariant to scale, translation and rotation.

Our intention in this study is to consider functional data clustering by accounting for the possible invariance in scaling/stretching, translation and
rotation of functional data. The focus of this paper is upon functional data including continuous functions parameterised by a single variable such as time and shapes in Euclidean spaces. The main characteristic we are interested in is that the functions are actually clustered in underlying subspaces. In other words, the original functions are sampled from several subspaces, which is embedded in a space with infinitely many dimensions. However, the observed functions are affected by geometric distortions and noise for some reason. The distortions creep in the multivariate representations of the functions and effectively breaks down the subspace identification methods built on classic multivariate data, even for those with robustness designed in the models to handle fairly large noises. Our experiments shown in Section 5 reveal this quite clearly. The reason is straightforward as the geometric distortions are themselves structural and do not fit into any probability distribution.

The solution to this problem relies on countering distortions, and the way we approach it is to manipulate the observed functions such that the transformed versions are invariant to distortions. Or in other words, we group the distorted versions of one function to be an equivalent class and treat the whole class as a datum in clustering. The equivalent class as a new representation accommodates all possible distortions and hence an infinite class. However, the cost is that the new representation of functions has some geometric structure, which has to be dealt with to achieve the final goal. This geometric structure in particular is a quotient manifold where each point is an equivalent class of functions that are transformed version of each other. The original subspace then becomes subspaces in this quotient manifold. However, it has no obvious coordinate representation, and hence no computation can be carried out directly. We get around this problem by projecting points into tangent space, a vector space regarded as a local approximation of the manifold, where we model the relations among the images of the points for clustering purpose. A very useful shape representation we consider is the square-root velocity function (SRVF) representation [10, 19]. In general, the resulting SRVF of a continuous shape is square integrable, belonging to the well-defined Hilbert space where appropriate measurement can be applied. Refer to Section 3 for more details. By acknowledging the true nature of the data we develop more robust clustering method that exploit features that would otherwise be ignored or lead to erroneous results with simple linear models.

The rest of the paper is organised as follows. In section 2 we discuss related work in this field. In Section 3, we review the preliminaries about the SRVF and more importantly the manifold of open curves and introduce
our robust functional manifold clustering model. Section 4 is dedicated to explaining an efficient algorithm for solving the optimisation in the realisation of our model based on the linearised alternative direction method with adaptive penalty (LADMAP) and the algorithm convergence and complexity are also analysed. In Section 5, the proposed model is assessed on both synthetic and real world databases against several state-of-the-art methods. Finally, conclusions are discussed in Section 6.

2 Related Work And Motivation

The simplest approaches for clustering functional data have relied heavily on Dynamic Time Warping (DTW). DTW is an alignment technique which aims to warp the time axis of the data until the difference between the two sequences is minimised [20]. DTW also provides a distance measurement between the two sequences, once aligned. Historically DTW has been mainly used for large scale data mining, where queries are performed to quickly find the nearest neighbours to sequences of data [6]. However the aligned distance produced by DTW has been used for clustering of functional data. In its simplest form DTW is used to produce a pairwise distance matrix for the entire dataset [21, 22]. Then the distance matrix is used by a hierarchical or spectral clustering method to produce the final clusters. Although these DTW based approaches are computationally cheap, their clustering accuracy leaves much to be desired. This is due to two flaws in DTW. Firstly, the distance measurement for DTW is based on Euclidean distance between each point in the sequence. This totally ignores any gradient based information in the sequence. Secondly, the warping accuracy is dependant on the correct choice of window size. Poor choices of warping window size can have a dramatic impact on warping and alignment accuracy [23]. Other methods such as DTW-HMM [24] have used DTW based clusters as an initialisation point for more advanced methods such as Hidden Markov Models.

A more sophisticated approach for functional data clustering is to use probabilistic methods [20]. Early methods used simple Gaussian probability models [5, 25, 26, 27]. However these models only hold for Euclidean vector data where the notions of cluster centres and cluster variance can be easily quantified [28]. In [29] Zhang et al proposed Bayesian clustering of curves, which is similar in nature to DTW pairwise distance clustering with advances that address most of the drawbacks. The distance matrix is based on analysis of the data points in the curve manifold. Then the clustering is performed on the distance matrix by using a probabilistic method that simultaneously
finds the cluster assignment and the number of clusters automatically.

We now draw the readers attention to subspace clustering methods, as they apply to many situations that traditional clustering methods cannot handle well [30, 31]. Different from finding spatially concentrated clusters measured by usual Euclidean metric, these methods aim to segment the data into clusters with each cluster corresponding to a unique subspace. More formally, given a data matrix of observed column-wise data samples \( \mathbf{A} = [\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_N] \in \mathbb{R}^{p \times N} \) and \( \mathbf{a}_i \in \mathbb{R}^p, \forall i = 1, \ldots, N \), the objective of subspace clustering is to assign each data sample to its underlying subspace. The basic assumption is the following.

**Subspace assumption:** The data is drawn from a union of \( c \) subspaces \( \{S_i\}_{i=1}^c \) with bases \( \{B_i\}_{i=1}^c \), and intrinsic dimensions \( \{d_i\}_{i=1}^c \).

Based on above assumption, simple linear algebra shows that for any given point in a subspace, the most parsimonious or consistent (measured by matrix rank) reconstruction of it is formed by the points from the same subspace as that of the given one. Many methods are constructed on this observation such as Sparse Subspace Clustering (SSC) [32] and low-rank representation (LRR) [33] while different methods seek different structures in the reconstruction matrices in their formulations. For any given datum \( \mathbf{a}_i \), the reconstruction is expressed as

\[
\mathbf{w}_i = \arg \min_{\mathbf{z}_i} \| \mathbf{a}_i - \mathbf{A}_{-i} \mathbf{w}_i \|, \quad (2.1)
\]

where \( \mathbf{A}_{-i} \) is the matrix of \( \mathbf{A} \) with the \( i \)th column removed, and \( \mathbf{w}_i \) is a vector with the reconstruction weights for \( \mathbf{a}_i \). Let \( \mathbf{W} = [\mathbf{w}_1, \ldots, \mathbf{w}_N] \) be the matrix consisting of all reconstruction weights. The restriction to \( \mathbf{W} \) as being sparse or low rank has the effect of selecting points from subspaces. Therefore, \( \mathbf{W} \) can be used as an affinity matrix to form a graph and a spectral clustering method like nCUT [34] to obtain the final subspace labels. Of course, there is always noise in the observed data, which has to be modelled for robustness.

Let us go back to functional data case where \( \mathbf{a}_i \) is actually a function of time \( t \) without loss of generosity, i.e. \( \mathbf{a}_i(t) \in \mathbb{R}^\infty \). The subspace assumption can still be valid for the bases being functions as well. This is obvious in spectroscopy where some material spectrum is a mix of several spectra of pure materials [35] which is one set of bases. Segmenting spectra according to their constituents is exactly subspace clustering. Similar applications like this are abundant in many areas such as computer vision where the data are essentially functions, and therefore subspace clustering is very useful in functional setting. As a consequence of validity of the subspace assumption, the reconstruction in (2.1) still holds. This justifies the direct application of
the subspace clustering to the multivariate representation of functional data *when they are clean*. However, the observed functionals can be affected by many things except for additive noise. The most serious one is distortions in shape. For example in thermal infra-red data of geological substances, a curve may contain a key identifying feature such as a dip near a particular frequency. This dip may shift or vary position even for the same substance due to impurities as shown in Fig. 4. Or in other cases the feature may be elongated, shrunk or subject to some non-uniform warping or scaling. Unfortunately, these distortions commonly exist in functional data. For example, the trajectories of writing a letter look very similar but never quite the same with different orientation, starting point and features, nonetheless they are the same letter. These distortions effectively break down (2.1) in obvious way, e.g. a shifted version of a function can not even reconstruct its original version using the formulation of (2.1), and therefore multivariate subspace clustering is no long appropriate.

DTW correction can alleviate the problem to some extent, with the limitation of only dealing with shift effectively. Moreover, when two functions are from different subspaces, the optimal alignment is not clear and the alignment outcome can be misleading as the shape features of functions can be misaligned during the process. Nonetheless the DTW idea is interesting. What if we take another route? Instead of carrying out the alignment explicitly, we pack all the common distortions into a map $\mathcal{F}$ from a function to its equivalent class, i.e. $\mathcal{F} : a(t) \mapsto [a(t)]$, meaning that if one function is the distorted version of the other, they end up in the same equivalent class by using $\mathcal{F}$. $[x]$ stands for equivalent class containing all objects that are equivalent to $x$ in some sense. Now the data in the subspace assumption becomes equivalent classes instead of individual functions. Although the equivalent class has no explicit vector form, its geometric structure may be used for computational purpose to recover the subspaces underpinning these equivalent classes. So we need two components at the same time, the map $\mathcal{F}$ accounting for distortions which has a suitable geometric structure. The next section is dedicated to explaining the details of the development of our method.

### 3 Robust Functional Manifold Clustering

Please note that differential geometry is involved in this method. [36] is an excellent reference for all the concepts used in this paper.

We start with a few observations. The first is the distinct features of
functions are usually in rate of changes such as valleys and peaks which can be better captured by first derivative. The second is that shift, stretch and compression of functions can be regarded as re-parametrisation of the time \( t \), i.e. the distorted version is actually \( a(\gamma(\tau)) \), where \( \gamma(\tau) \) is the re-parametrisation function replacing \( t \). The third is that the rotation is a simple linear operation whose matrix representation is a rotation matrix. These observations lead us to the square-root velocity function (SRVF) representation [10, 19] with rotation group detailed in the following sections.

### 3.1 The Curve Manifold

We formalise the function as a smooth parameterised \( n \)-dimension curve \( a : D \rightarrow \mathbb{R}^n \), where \( D = [0,1] \). Here the smoothness requirement means that the function has continuous first order derivative. We represent it using the square-root velocity function (SRVF) representation given by

\[
q(t) = \frac{\dot{a}(t)}{\sqrt{|\dot{a}(t)|}},
\]

where \( \dot{a}(t) \) is the derivative of \( a(t) \) and \( \|\dot{a}(t)\| \) the \( L^2 \) norm of \( \dot{a}(t) \). Apparently we exclude constant curve which has norm 0. The SRVF mapping transforms the original curve \( a(t) \) into a gradient based representation, which facilitates the comparing of the shape information.

In this paper, we focus on the set of open curves, i.e. \( a(0) \neq a(1) \). For handling general curves, we refer readers to [10]. The SRVF facilitates a measure and geometry bearing invariance to scaling, shifting and reparameterising in the curves domain. For example, all the translated curves (in \( \mathbb{R}^n \)) from a curve \( a(t) \) will have the same SRVF. Robinson [37] proved that if the curve \( a(t) \) is absolutely continuous, then its SRVF \( q(t) \) is square-integrable, i.e., \( q(t) \) is in a functional Hilbert space \( L^2(D, \mathbb{R}^n) \). Conversely for each \( q(t) \in L^2(D, \mathbb{R}^n) \), there exists a curve \( a(t) \) whose SRVF corresponds to \( q(t) \). Thus the set \( L^2(D, \mathbb{R}^n) \) is a well-defined representation space of all the curves. The most important advantage offered by the SRVF framework is that the natural and widely used \( L^2 \)-measure on \( L^2(D, \mathbb{R}^n) \) is invariant to reparameterisation. That is, for any two SRVFs \( q_1 \) and \( q_2 \) and an arbitrarily chosen reparametrisation function (non-decreasing) \( t = \gamma(\tau) \), we have

\[
\|q_1(t) - q_2(t)\|_{L^2} = \|q_1(\gamma(\tau)) - q_2(\gamma(\tau))\|_{L^2}.
\]

This property give us the invariance to some distortions we mentioned earlier. Furthermore, this reparameterisation together with \( L^2(D, \mathbb{R}^n) \) form
a quotient manifold. To see this, we introduce some more notations. Let \( \Gamma \) be the set of all diffeomorphisms from \( D = [0, 1] \) to \( D = [0, 1] \). This set collects all the reparametrisation mappings. \( \Gamma \) is a Lie group with composition as the group operation and the identity mapping as the identity element. Then all the orbits \([q] = \{ q \circ \gamma = q(\gamma(t)) \mid \forall \gamma \in \Gamma \}\) together define the quotient manifold \( L^2(D, \mathbb{R}^n)/\Gamma \), i.e. all reparametrised \( q(t) \) are treated as the same.

Without loss of generality, we assume that all curves are normalised to unitary length, i.e., \( \int_D \| \dot{a}(t) \| dt = 1 \). The SRVF\s associated with these curves are elements of a unit sphere in the Hilbert space \( L^2(D, \mathbb{R}^n) \) because \( \int_D \| q(t) \|^2 dt = 1 \). Therefore, under the curve normalisation assumption, instead of \( L^2(D, \mathbb{R}^n) \), we consider the following unit sphere manifold

\[
C^o = \left\{ q \in L^2(D, \mathbb{R}^n) : \int_D \| q(t) \|^2 dt = 1 \right\}.
\]

The manifold \( C^o \) has some nice properties, see [38]. For any two points \( q_0 \) and \( q_1 \) in \( C^o \), the geodesic, i.e. the shortest path connecting two points on the manifold, is given by \( \alpha : [0, 1] \to C^o \),

\[
\alpha(\tau) = \frac{1}{\sin(\theta)} (\sin(\theta(1 - \tau))q_0 + \sin(\theta\tau)q_1),
\]

(3.1)

where \( \theta = \cos^{-1}(\langle q_0, q_1 \rangle) \) is the length of the geodesic and \( \langle \cdot, \cdot \rangle \) is the inner product defined in \( L^2(D, \mathbb{R}^n) \). Taking the derivative of \( \alpha \) at \( \tau = 0 \), we obtain the tangent vector at \( q_0 \)

\[
v = \frac{\theta}{\sin(\theta)} [q_1 - \langle q_0, q_1 \rangle q_0].
\]

(3.2)

The above formula is regarded as the Logarithm mapping \( \log_{q_0}(q_1) \) on the manifold \( C^o \), i.e. the map that takes the points on the manifold to the tangent space rooted at some point.

As we are concerned with the shape invariance, i.e., we need to additionally remove the shape-preserving transformations: rotation and curve reparametrisation. For this purpose, we introduce rotation group \( SO(n) \) for all the rotations in \( \mathbb{R}^n \). Combining \( SO(n) \) with \( \Gamma \), we define the equivalence relation between pair of points \( q_i \) and \( q_j \), i.e. we claim \( q_i \) equivalent to \( q_j \), written as \( q_i \sim q_j \), if they are rotated and reparametrised version of each other. The quotient manifold \( S^o = C^o/(SO(n) \times \Gamma) \) then has the property we need. Each element \([q] \in S^o \) is an equivalence class defined by

\[
[q] = \left\{ Oq(\gamma(t))\sqrt{\dot{\gamma}(t)} \mid O \in SO(n) \text{ and } \gamma \in \Gamma \right\}.
\]
Now $[q_i]$ is the a family of curves that are transformed version of each other. More concretely, given a set of $N$ unit-length curves $\{a_1(t),...,a_N(t)\}$, their SRVF$s$ are $\{q_1(t),...,q_N(t)\}$ such that $[q_i] \in S^o$ and $q_i(t)$ is a representative of the equivalent class $[q_i]$. So if $a_i(t)$ is the distorted version of $a_j(t)$ and then $[q_i]=[q_j]$ and these two will be reflected as a single point in $S^o$.

### 3.2 The Proposed Clustering Method

It is clear that $S^o$ is a good representation for curves which is invariant to many distortions we focus on. From the line of its development, we see that the functional subspace assumption holds because the gradient and rotation are linear operators and reparameterisation works on function bases as well. However, the obstacle now is that $S^o$ is an abstract unitary sphere with no obvious vector form. Recovering the subspace structure is not straightforward. Nonetheless the tangent space of any smooth manifold at any point is a well defined vector space with the same dimensionality as the manifold $[39]$. Observe that the projection to tangent space on unitary sphere $S^o$ in $\mathbb{R}^{n+1}$ preserves subspace structure of the points on the sphere. If the foot of a tangent space is from one subspace, then this subspace will have one less dimension in the tangent space. This is illustrated in Fig. 1. This prompts us to use tangent space on $S^o$. Fortunately, the computation is readily available.

Given any two points $[q_0]$ and $[q_1]$ in $S^o$, a tangent representative $[38]$ of $[q_1]$ in the tangent space $T_{[q_0]}(S^o)$ can be calculated in the following way, as
suggested in [40, 41] based on (3.2),
\[
\tilde{v} = \log_{\tilde{q}_0}(\tilde{q}_1) = \frac{\tilde{\theta}}{\sin(\tilde{\theta})}[\tilde{q}_1 - (\tilde{q}_0, \tilde{q}_1)\tilde{q}_0].
\]  

(3.3)

where \( \tilde{q} \) is the representative of \([q]\) given by the well-defined algorithm in [40, 41] and \( \tilde{\theta} = \cos^{-1}(\langle \tilde{q}_0, \tilde{q}_1 \rangle) \). In fact, \( \tilde{v} \) is the lifting representation of tangent vector \( \log_{\tilde{q}_0}(\tilde{q}_1) \) in \( T_{\tilde{q}_0}(S^o) \) for \([q_1]\), or in other words, the projection of \([q_1]\) in \( T_{\tilde{q}_0}(S^o) \).

We are ready to recover the subspace structure now in tangent space. We start with

\[
\sum_{j=1}^{N} w_{ij} \log_{\tilde{q}_i}(\tilde{q}_j) = 0, \quad \forall i = 1, \ldots, N.
\]

(3.4)

Note that \( \log_{\tilde{q}_i}(\tilde{q}_i) = 0 \), i.e. \([q_i]\) is the origin of its tangent space. This introduces indeterminacy for \([q_i]\). Therefore, we have the constraint \( \sum_{j=1}^{N} w_{ij} = 1, i = 1, 2, \ldots, N \) to avoid trivial solution and other indeterminacy such as arbitrary scaling. Moreover, tangent space of every point is utilised as in (3.4) to form a multiple view of the subspaces. The advantage of doing this is not only avoiding a vanishing point, but also increasing the stability of subspace recovery process. The next step is to consolidate the multiple views. One critical observation is that although every tangent space is different depending on the support point, the null space is the same. If \([q_i]\)'s have subspace structure, the most efficient way to recover null space is to pick points from subspaces consistently which is reflected as the lowest rank in coefficient matrix \( W \), whose \( ij \)th element is \( w_{ij} \). This leads to the following objective

\[
\min_{W} \lambda \|W\|_* + \sum_{i=1}^{N} \frac{1}{2} \| \sum_{j=1}^{N} w_{ij} \log_{\tilde{q}_i}(\tilde{q}_j) \|_{[q]}^2,
\]

(3.5)

\[
\text{s.t. } \sum_{j=1}^{N} w_{ij} = 1, i = 1, 2, \ldots, N.
\]

where \( \| \cdot \|_{[q]} \) is the metric defined on the manifold, which is defined by the classic \( L^2 \) Hilbert metric on the tangent space, quantifying the deviation from 0, and \( \|W\|_* \) is the nuclear norm as a convex approximation to matrix rank. Note that the above objective function reflects the trade-off between low rank and null space recovery, i.e. (3.4), controlled by \( \lambda \).
Denote \( w_i \) the \( i \)-th row of matrix \( W \) and define
\[
B^i_{jk} = \langle \log_{[q_i]}([q_j]), \log_{[q_i]}([q_k]) \rangle.
\] (3.6)

Then with some algebraic manipulation we can re-write (3.5) into the following simplified form,
\[
\min_{W} \lambda \|W\|_* + \sum_{i=1}^{N} w_i B^i w_i^T,
\]
\[
\text{s.t.} \quad \sum_{j=1}^{N} w_{ij} = 1, i = 1, 2, \ldots, N.
\] (3.7)

where \( B^i = (B^i_{jk}) \).

Once solved, \( W \) can be used as affinity to build graph. As \( W \) has consistent pattern within each subspace, the graph should consist of several connected components corresponding to subspaces and graph cut can then be applied to segment them.

4 Optimisation

4.1 Algorithm

To solve the objective function in (3.7) we use the Linearised Alternative Direction Method with Adaptive Penalty (LADMAP) [42, 43]. First take the augmented Lagrangian of the objective (3.7)
\[
L = \lambda \|W\|_* + \frac{1}{2} \sum_{i=1}^{N} w_i B^i w_i^T + \langle y, W1 - 1 \rangle + \beta \frac{1}{2} \|W1 - 1\|_F^2
\] (4.1)

where \( y \) is the Lagrangian multiplier (vector) corresponding to the equality constraint \( W1 = 1 \), \( \| \cdot \|_F \) is the matrix Frobenius-norm, and \( \beta \) is the proximal parameter which will be updated in the iterative algorithm to be introduced.

Denote by \( F(W) \) the function defined by (4.1) except for the first term \( \lambda \|W\|_* \). We adopt a linearisation of \( F(W) \) at the current location \( W^{(k)} \) in the iteration process, that is, we approximate \( F(W) \) by the following
linearisation with a proximal term

\[ F(W) \approx F(W^{(k)}) + \langle \partial F(W^{(k)}), W - W^{(k)} \rangle \]

\[ + \frac{\eta_W \beta_k}{2} \| W - W^{(k)} \|_F^2, \]

where \( \eta_W \) is an approximate constant with a suggested value given by \( \eta_W = \max \{ \| B \|_2 \} + N + 1 \) (this value is presented in the convergence theorem in the next section), and \( \partial F(W^{(k)}) \) is the gradient matrix of \( F(W) \) at \( W^{(k)} \).

Denote by \( B \) the 3-order tensor whose \( i \)-th frontal slice is \( B^i \). Write \( W \odot B \) the matrix whose \( i \)-th row is given by \( w^i B^i \). Then it is easy to show

\[ \partial F(W^{(k)}) = W \odot B + y^T + \beta_k (W1 - 1)1^T. \] (4.2)

Then (4.1) can be approximated by linearisation and \( W \) will be updated by the following

\[ W^{(k+1)} = \arg \min_W \lambda \| W \|_*, \] (4.3)

\[ + \frac{\eta_W \beta_k}{2} \| W - \left( W^{(k)} - \frac{1}{\eta_W \beta_k} \partial F(W^{(k)}) \right) \|_F^2. \]

Problem (4.3) admits a closed form solution by using SVD thresholding operator [44], given by

\[ W^{(k+1)} = U_W S_{\frac{1}{\eta_W \beta_k}}(\Sigma_W) V_W^T, \] (4.4)

where \( U_W \Sigma_W V_W^T \) is the SVD of \( W^{(k)} - \frac{1}{\eta_W \beta_k} \partial F(W^{(k)}) \) and \( S_\tau(\cdot) \) is the Singular Value Thresholding (SVT) [44, 45] operator defined by

\[ S_\tau(\Sigma) = \text{diag}(\max \{ |\Sigma_{ii}| - \tau, 0 \}). \] (4.5)

The updating rule for \( y \) is

\[ y^{(k+1)} = y^{(k)} + \beta_k (W^{(k)}1 - 1) \] (4.6)

and the updating rule for \( \beta_k \)

\[ \beta_{k+1} = \min \{ \beta_{\max}, \rho \beta_k \}, \] (4.7)

where

\[ \rho = \begin{cases} \rho_0, & \text{if } \beta_k \| W^{k+1} - W^k \| \leq \varepsilon_1, \\ 1, & \text{otherwise}. \end{cases} \]

We summarise the above as Algorithm 1. Once the coefficient matrix \( W \) is found, a spectral clustering is applied to the affinity matrix \( \frac{|W| + |W^T|}{2} \) to obtain the segmentation of the data. In particular we use nCUT [34] for its good performance in both accuracy and efficiency in spectral clustering. We call our method robust functional manifold clustering, or rFMC for short.

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Algorithm 1 Optimisation for (3.7)

Require: \{X_i\}^N_{i=1}, \lambda

1: Initialise: \mathbf{W} = \mathbf{0}, \mathbf{y} = \mathbf{0}, \beta = 0.1, \beta_{\text{max}} = 10, \rho^0 = 1.1, \eta = \max\{\|\mathbf{B}^i\|_F\} + N + 1, \epsilon_1 = 1e^{-4}, \epsilon_2 = 1e^{-4}

2: Construct each \mathbf{B}^i as per (3.6)

3: while not converged do

4: Update \mathbf{W} using (4.4)

5: Check convergence criteria

\[ \beta^{(k)}\|\mathbf{W}^{(k+1)} - \mathbf{W}^{(k)}\|_F \leq \epsilon_1 \]
\[ \|\mathbf{W1 - 1}\|_F \leq \epsilon_2 \]

6: Update Lagrangian Multiplier

\[ \mathbf{y}^{(k+1)} = \mathbf{y}^k + \beta^{(k)}(\mathbf{W1 - 1})^T \]

7: Update \rho

\[ \rho = \begin{cases} \rho_0 & \text{if } \beta^{(k)}\|\mathbf{W}^{(k+1)} - \mathbf{W}^{(k)}\|_F \leq \epsilon_1 \\ 1 & \text{otherwise}, \end{cases} \]

8: Update \beta

\[ \beta^{(k+1)} = \min(\beta_{\text{max}}, \rho\beta^{(k)}) \]

9: end while

10: return \mathbf{W}
4.2 Complexity Analysis

For ease of analysis, we firstly define some symbols used in the following. Let $K$ and $r$ denote the total number of iterations and the lowest rank of the matrix $W$, respectively. The size of $W$ is $N \times N$. The major computation cost of our proposed method contains two parts, calculating all $B^i$'s and updating $W$. In terms of the formula (3.6) through (3.2) and (3.3), the computational complexity of Log algorithm is $O(T^2)$ where $T$ is the number of terms in a discretised curve; therefore, the complexity of $B^i_{jk}$ is at most $O(T^2)$ and $B^i$’s computational complexity is $O(N^2T^2)$. Thus the total for all the $B^i$ is $O(N^3T^2)$. In each iteration of the Algorithm, the singular value thresholding is adopted to update the low rank matrix $W$ whose complexity is $O(rN^2)$ [33]. Suppose the algorithm is terminated after $K$ iterations, the overall computational complexity is given by

$$O(N^3T^2) + O(KrN^2)$$

4.3 Convergence Analysis

Algorithm 1 is adopted from the algorithm proposed in [43]. However due to the terms of $B^i$’s in the objective function (4.1), the convergence theorem proved in [43] cannot be directly applied to this case as the linearisation is implemented on both the augmented Lagrangian terms and the term involving $B^i$’s. Fortunately we can employ the revised approach, presented in [46], to prove the convergence for the algorithm. Without repeating all the details, we present the convergence theorem for Algorithm 1 as follows.

**Theorem 1 (Convergence of Algorithm 1)**  If $\eta_W \geq \max\{\|B_i\|^2\} + N + 1$, $\sum_{k=1}^{+\infty} \beta_k^{-1} = +\infty$, $\beta_{k+1} - \beta_k > C_0 \frac{\sum_i \|B_i\|^2}{\eta_W - \max\{\|B_i\|^2\} - N}$, where $C_0$ is a given constant and $\| \cdot \|$ is the matrix spectral norm, then the sequence $\{W^k\}$ generated by Algorithm 1 converges to an optimal solution to problem (3.7).

In all the experiments we have conducted, the algorithm converges very fast with $K < 100$.

5 Experimental Analysis

In this section we evaluate the clustering performance of rFMC on synthetic, semi-synthetic and real world datasets. We compare our algorithm
to two baseline algorithms k-means and spectral clustering of a DTW distance matrix, and the state of the art Bayesian Clustering of Curves. We also compare against LRR and SSC, two highly cited multivariate subspace clustering methods. Note that we used nCUT to find final clustering solution for LRR and SSC as well.

In an effort to maximise transparency and repeatability, all code and data used for these experiments can be found online at https://staff.scem.uws.edu.au/~yiguo/code/rfmc.

To help evaluate consistency we fixed the parameters to the same values for every experiment. Parameters were selected by testing a wide range of values over all datasets so that the best average result for each method was obtained. For rFMC and LRR, $\lambda$ was set to 0.1, and for SSC, $\lambda$ was 0.05. Overall we found that the segmentation accuracy of LRR and SSC did not vary that much with changes in $\lambda$. For our DTW baseline algorithm we set the warping window to 10% of the data length, which has been shown to be suitable in most cases [23].

Segmentation accuracy was measured using the subspace clustering accuracy (SCA) metric [32], which is defined as

$$\text{SCA} = 1 - \frac{\text{num. of misclassified points}}{\text{total num. of points}},$$

where higher SCA means greater clustering accuracy. The SCA metric is taken over all possible pairwise assignments of clusters.

5.1 Toy Synthetic Data Clustering

First we attempt to verify that rFMC achieves its design purpose for robustness against distortions in subspace recovery. While other methods without
<table>
<thead>
<tr>
<th>Method</th>
<th>Mean</th>
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<th>Max</th>
<th>Min</th>
<th>Std</th>
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<tr>
<td><strong>kmeans</strong></td>
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<td>41.7%</td>
<td>60.0%</td>
<td>35.0%</td>
<td>7.4%</td>
<td>0.01</td>
</tr>
<tr>
<td>DTW</td>
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<td>59.9%</td>
<td>81.7%</td>
<td>36.7%</td>
<td>12.0%</td>
<td>0.11</td>
</tr>
<tr>
<td>LRR</td>
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<td>36.7%</td>
<td>14.7%</td>
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</tr>
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<td>15.6%</td>
<td>0.10</td>
</tr>
<tr>
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<td>65.0%</td>
<td>100.0%</td>
<td>25.0%</td>
<td>23.7%</td>
<td>48.71</td>
</tr>
<tr>
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<td>83.3%</td>
<td>98.3%</td>
<td>36.7%</td>
<td>17.7%</td>
<td>11.18</td>
</tr>
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<td>23.0%</td>
<td>6.4%</td>
<td>0.01</td>
</tr>
<tr>
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<td>39.4%</td>
<td>20.0%</td>
<td>4.1%</td>
<td>0.01</td>
</tr>
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<td>40.0%</td>
<td>48.8%</td>
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<td>8.0%</td>
<td>0.27</td>
</tr>
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<td>0.15</td>
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<td><strong>49.4%</strong></td>
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<td><strong>31.2%</strong></td>
<td><strong>7.2%</strong></td>
<td><strong>64.73</strong></td>
</tr>
</tbody>
</table>

Table 1: Synthetic data results with 3, 5 and 8 clusters
Figure 3: SCA means and medians of different methods on synthetic data.
Figure 4: Example plots of curves used in the Semi-synthetic TIR Data Experiment. Each cluster has a base curve from the TIR library. The curves for each cluster have been shifted and stretched randomly from the base.

the consideration of the special properties of functions such as LRR and k-means would be inferior. In this test, 2 to 8 clusters were created consisting of twenty 1-D curves of length 100. The curves in each cluster were sine waves, with each cluster corresponding to a unique frequency from 0.1 to 40Hz. Within each cluster we applied progressive amounts of warping. See Figure 2 for an example of data from three synthetically generated clusters. For each number of clusters setting, we repeated the experiment 50 times with new data generated each time to obtain basic statistics of SAC.

Results are reported using subspace clustering accuracy and can be found in Table 1 and Figure 3. Note that in Table 1 and the following ones, the number besides rFMC indicates the number of clusters tested, and $\bar{T}$ in the tables is the average run time for the algorithms in the tests. This is a challenging dataset due to a large amount of distortions. However in this experiment rFMC achieves very high clustering accuracy in terms of the statistics of accuracy values. From Figure 3, it is clearly seen that rFMC outperforms other methods in terms of SAC mean and median. When the number of clusters grows, the performance decreases due to increasing difficulty. Note that when the number of clusters reaches 8, the clustering accuracies of all methods drop below 50%, which is not informative. Moreover, some methods like Bayesian become unstable for some reason. So we set 8 as the maximum number of clusters in all tests. In the following experiments, we test 3, 5, and 8 clusters to observe the behaviour of different methods in terms of both clustering accuracy and the trends when the number of clusters vary.
<table>
<thead>
<tr>
<th>Method</th>
<th>Mean</th>
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<th>Max</th>
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</tr>
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<td><strong>78.8%</strong></td>
<td>7.0%</td>
<td>658.50</td>
</tr>
</tbody>
</table>

Table 2: Thermal Infrared Results
5.2 Semi-Synthetic Thermal Infrared Spectra Clustering

We assemble semi-synthetic data from a library of pure infrared hyperspectral mineral data [30]. For each cluster we pick one spectral sample from the library as a basis. Each curve basis is then randomly shifted and stretched in a random portion. This random warping is performed 20 times to produce the curves for each cluster. See Figure 4 for an example of data used in this experiment. Again as in the previous experiment we repeated the test 50 times.

Results are reported in Table 2. The results show that non-functional based methods cannot accurately cluster data with this sort of structural contamination, which is commonly found in this type of data due to impurities in the mineral samples. On the other hand, rFMC almost perfectly clustered the data with superb consistency across all cases. The closest competitor was the Bayesian method, which also performed well by clustering accurately most of the time at the cost of extremely high computation load. However in some cases the clusters produced were of poor quality, which can be observed in the minimum accuracy and standard deviation statistics. Therefore, rFMC is far more reliable and efficient at clustering this data than other methods.

5.3 Handwriting Character Velocities

In this experiment a real world dataset consisting of a collection of pen tip trajectories of handwritten English characters were used to evaluate performance. The dataset consists of pen position data collected by a digitisation tablet at 200Hz, which is then converted to horizontal and vertical velocities [47, 48]. These 2-D trajectory curves are normalised such that the mean of each curve is close to zero. See Figure 5 for some examples of this data. Figure 6 shows the example plots of curves used in this experiment.

For each run of this test, twenty characters were randomly selected from 3, 5 and 8 random character classes. The data as originally released have been carefully produced and processed so that trajectories for each characters are extremely similar. Far more so than is realistic. For example the start time for each character has been aligned furthermore the writing speed, character size and variance in velocity over time is extremely consistent. Therefore to make the data more realistic we randomly globally shift each character so that their start times vary. Furthermore we randomly globally stretch and shrink each trajectory to account for different writing speeds, we also scale the trajectories by applying constant factors to ac-
Figure 5: Example data from the character velocity dataset. The top row plots the x and y pen tip velocities over time for three sample characters. The bottom row shows the corresponding character reconstruction by integrating the pen tip velocity data (for visualisation only).
Figure 6: Example plots of curves used in the character velocity experiment. Each cluster consists of randomly selected characters from each class that are then subject to a combination of shifting, warping, stretching or shrinking and scaling. The top row shows the curves from the pen tip velocity in the X direction over time and the bottom row shows the same but for the Y direction.
<table>
<thead>
<tr>
<th>Method</th>
<th>Mean</th>
<th>Median</th>
<th>Max</th>
<th>Min</th>
<th>Std</th>
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<td>77.5%</td>
<td>43.8%</td>
<td>7.7%</td>
<td>163.35</td>
</tr>
</tbody>
</table>

Table 3: Character Velocity Results
Figure 7: Example data from the character classification dataset. Note that the writing style and typeface varies within each character class. There is also variance in size and position of the characters.

count for character size and we lastly perform local warping (as done in the semi-synthetic experiment) to account for variance in speed over time.

Results can be found in Table 3. RFMC shows excellent performance with a median accuracy of 86% for the case of 3 classes on this extremely challenging dataset. The closest competitors only reach a median clustering accuracy of 50%. Similar comparison can be observed in other cases. It is clear to see that rFMC outperforms other methods in all metrics in all cases of various numbers of classes.

5.4 Handwriting Character Trajectories

In this experiment we used the Chars74K [49] dataset, which consists of pen tip positions (different from trajectories) of handwritten English characters. The dataset consists of 62 character classes with 55 samples per class. Different from the previous English character dataset, the writing style or the typeface varies within each character class. For example some people choose to close the top of the character “4” while others leave it open or they choose to write their characters with differing amounts of serifs as can be seen with the character “1”. See Figure 7 for visual examples. This creates a significant problem for clustering as the shape of the data within a class vary significantly and it is actually best to treat these different font faces as separate classes for greater accuracy. However we do not divide the classes into separate font faces.

Similar to the previous experiment for each run of this test twenty characters were randomly selected from 3, 5 and 8 random character classes and 50 runs were performed. However, different from the previous experiment, we do not apply any further post processing to reduce alignment since this
dataset is relatively unprocessed. Results can be found in Table 4. In spite of the aforementioned challenges with this dataset, rFMC leads by a significant margin. Notably bayesian clustering suffered many clustering failures leading to very poor accuracy. This was due to implementation limitations in the original code provided from [29]. We also have to exclude LRR for the cases where the number of classes is more than 3, because it failed on most random samples.

5.5 Sign Language Word Clustering

In this final experiment we use the Australian Sign Language (Auslan) Signs (High Quality) dataset [50]. This dataset consists of a single native Auslan signer performing 91 different signs (the classes) with 27 samples per sign. The signer wore motion capture gloves that captured the position (x, y, z), roll, pitch and yaw of each hand along with finger bend measurements. This data was captured at 100Hz and no post processing was applied. The signs were collected three at a time over a period of nine weeks so there is noticeable variation within each class.

As with the previous experiments, for each run, twenty data points

<table>
<thead>
<tr>
<th></th>
<th>Mean</th>
<th>Median</th>
<th>Max</th>
<th>Min</th>
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Table 4: Character Trajectory Results
Table 5: Sign Language Results

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</table>

(signed words) were randomly selected from 3, 5 and 8 random word classes and 50 runs were performed. Only the position, roll, pitch and yaw channels were used since the finger bend measurements were far too noisy and unreliable to be of use. We also performed a parallel test to determine the effectiveness of smoothing as a first attempt for noise handling. A multi-channel total variation based smoothing method was used [51]. Results can be found in Table 5 and 6. Overall rFMC performed slightly better than or similar to Bayesian clustering and significantly better than the baseline methods. We noticed that smoothing the data actually decreased clustering performance of all methods, which indicates non-triviality of noise removal.

6 Conclusions

In this paper, we proposed an algorithm called robust functional manifold clustering (rFMC) to reliably and accurately cluster functional data in term of their subspaces. This is a highly challenging problem as functional data
<table>
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<th>Max</th>
<th>Min</th>
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Table 6: Smoothed Sign Language Results
from the same class can vary greatly due to stretching, shrinking, non-
uniformly warping and scaling. We achieved this by representing functional
data in curves manifold invariant to these distortions and addressed the
challenge of lack of vector forms. The analysis is performed in tangent
spaces of each point in the manifold via the recovery of null spaces of the
log maps of the points to solve the multiple view problem. An optimisation
scheme with convergence guarantee was also provided to realise the model.

Nevertheless this paper still leaves many areas open for further research.
Firstly we only address the data on the manifold of open curves, however
much of the data in recognition and computer vision tasks will lie on the
manifold of closed curves. Moreover our focus was on robustness against
geometric distortions. Additive noise will be carried through the trans-
formations onto curve manifold and affect the performance. However, the
mechanism is not fully understood although the proposed algorithm can
be applied in this case. Nonetheless, it is interesting to study the noise
to further improve the results. We leave solving these problems for future
research.

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