Monitoring of functional profiles combining the notion of Fréchet mean and the framework of deformation models with application in ambient air pollution surveillance

G. I. Papayiannis\textsuperscript{a}, S. Psarakis\textsuperscript{b}, and A. N. Yannacopoulos\textsuperscript{c}

\textsuperscript{a}Hellenic Naval Academy, Department of Naval Sciences, Section of Mathematics, Mathematical Modelling and Applications Laboratory, Piraeus, GR; Athens University of Economics & Business, Stochastic Modelling and Applications Laboratory, Athens, GR

\textsuperscript{b}Athens University of Economics & Business, Department of Statistics, Laboratory of Statistical Methodology, Athens, GR

\textsuperscript{c}Athens University of Economics & Business, Department of Statistics, Stochastic Modelling and Applications Laboratory, Athens, GR

Abstract

A framework suitable for monitoring functional profiles combining the notion of Fréchet mean and the concept of deformation models is developed and proposed. The generalized sense of mean that the notion of the Fréchet mean offers is employed to capture the typical functional shape of the data, while the concept of deformation models allows for interpretable parameterizations of profile’s deviations from the typical shape. Functional EWMA-type control charts are built and proposed based on shape characteristics of the functional data, allowing for (a) identifying shifts from the in-control behaviour and (b) providing causal relationships of the potential shifts with significant deviances of certain qualitative characteristics (e.g amplitude or phase deformations). The functional monitoring scheme is implemented to assess ambient air pollution. In particular, the method is implemented to a synthetic data example to assess its performance under various conditions, and to a real-world example using sensor data from an area in the city of Athens, where air pollutants profiles and their characteristics are successfully analyzed and out-of-control behaviours are identified.

Keywords: ambient air pollution; deformation models; EWMA control charts; Fréchet mean; functional profiles monitoring;

1 Introduction

Ambient air pollution levels monitoring, prediction and assessment in urban environments are of major importance for the public health, especially in big cities. According to the World Health Organization\textsuperscript{1} (WHO) air pollution causes an estimated seven million premature deaths worldwide every year while recorded data indicates that 9 out of 10 people breathe air that exceeds WHO guideline limits\textsuperscript{2} concerning the safety levels of pollutants. The recent COVID-19 pandemic outbreak, worsened the situation, especially in urban environments where higher densities of people are observed. In this work is proposed a suitable and reliable framework for the successful surveillance of air quality and air pollution levels, compatible with the functional data setting and allowing for the quantification of the intensity of possible deviant behaviours.

\textsuperscript{1}https://www.who.int/

\textsuperscript{2}https://www.who.int/news-room/fact-sheets/detail/ambient-(outdoor)-air-quality-and-health

\*Corresponding author: Hadjikyriakou Avenue, Piraeus, 18539, Greece. E-mail: g.papagiannis@hna.gr

\*arXiv:2010.02968v2 [stat.ME] 10 Sep 2022
(out of control) through appropriate parameterization. In particular, air pollution data are treated under the functional statistics setting (as curves), and not as random measurements. In urban environments, due to the people’s daily routine (traffic, working hours, etc.), the evolution of a pollutant’s concentration during the day presents certain patterns due to the chemical interactions with the other quantities (environmental or not) that appear in the local atmosphere in each period of the day depending also on the season. Describing by functional objects the daily evolution of polluters in a city’s regional atmosphere, allows to extract much more information (e.g. correlation patterns that are observed spatio-temporally), comparing to working with a dataset of discrete measurements at various time instants. In this spirit, a functional profiles’ monitoring framework appropriate for the study and surveillance of daily evolution pollutants’ profiles is developed and proposed, combining (a) the notion of Fréchet mean and the generalized sense of the mean it offers, allowing for an efficient estimation of the underlying and unknown mean pattern in terms of functional data and (b) the framework of deformation models, which allows for the allocation of deviances from the estimated reference pattern to certain shape deformation characteristics like amplitude and phase. Then, statistical monitoring schemes for such functional profiles are proposed, based on the setting of EWMA control charts. Importantly, through the proposed monitoring scheme construction, potential shifts from the in-control behaviour can be interpreted and rendered to significant changes of certain qualitative features of the observed shape comparing to the estimated typical functional pattern. Clearly, this allows for identifying the qualitative features of the observed profile which significantly contributed in producing an out-of-control observation. The developed method is implemented in two case studies, a synthetic-data example where profiles generated under various dependence structures are analysed to assess the performance of the monitoring schemes, and to a real data ambient air quality monitoring task in the city of Athens where recorded data from installed pollution sensors are used.

2 Previous Work & Preliminaries

2.1 Literature Review

Urban air pollution is a classical problem from the environmentalist’s perspective and so on, several aspects of the problem have been investigated. The problem of selecting the optimal location for installing sensors for pollution monitoring is considered in Pittau et al. (1999), while a study concerning the efficiency of air pollution detection systems in European big cities is presented in Voigt et al. (2004). Some interesting works considering the problem of air pollution prediction are the following (but not limited to): in Szpiro et al. (2010) an analysis of long-term averages of certain pollutants is presented, in Alimissis et al. (2018) Artificial Neural Networks (ANN) are employed for this task, in Bose et al. (2018) adaptive Principal Components Analysis (PCA) is performed and in Wan et al. (2021) an EM algorithm is used for the calibration of appropriate spatio-temporal models. Concerning environmental pollution monitoring, in Marchant et al. (2019) typical statistical process control tools are implemented for air pollution surveillance, while in Bersimis & Triantafyllou (2020) a state-space modeling approach has been adopted for this task. In the quite recent review Xie et al. (2017) are discussed the developments in air pollution monitoring, including both the pollution data acquisition and the pollution assessment methods. An interesting attempt in mapping air pollution to quantify health risk in a region is presented in Adams & Kanaroglou (2016) while a software package for analysing environmental data (however not employing the functional statistics setting discussed in this work) has been developed in the R language by Carslaw & Ropkins (2012).

Monitoring of functional profiles has attracted the interest of the statistical community the latter years. The development of more elaborate and complex statistical monitoring schemes is required for the statistical treatment of dynamical and functional data structures in order to
reveal and recover important information concerning the special features of the process under study. The resulting functional data (and their increased complexity) is an issue that at a first stage can be handled either by the application of non-linear models or by non-parametric or semi-parametric models (e.g. kernel-based estimators, wavelets, etc.). However, as far as statistical control is concerned, for these functional models the classical control tools may not be appropriate (partly because of their functional nature and partly because the output of such models may not be appropriately accommodated in a vector space framework). This fact imposes the need for development of new monitoring mechanisms. Particularly, in the area of functional profiles monitoring, several approaches have been proposed in the later years, through non-parametric regression or wavelets approaches (Chicken et al., 2009; Qiu et al., 2010; McGinnity et al., 2015), interpolation approaches (Moguerza et al., 2007; Fassò et al., 2016), through PCA and functional PCA (Shiau et al., 2009; Yu et al., 2012; Paynabar et al., 2016), functional regression (Centofanti et al., 2021), employing the intrinsic geometry of the data manifolds and exploiting the notion of statistical depth (Harris et al., 2020; Zhao & Del Castillo, 2021) and others. The majority of the aforementioned approaches attempt (through modifications in the modeling procedure, but still relying on the current setting of process control theory and practice) to extent the current monitoring tools to better treat the new modeling setup accommodating certain of the salient features of the data in question (such as functional dependence etc).

However, an important issue that requires further investigation is the actual definition of the typical (or the so called in control (IC)) behaviour of the object under study. The main problem here is that the standard approaches have been developed for data that can be considered as points of a finite dimensional Euclidean space (e.g. of $\mathbb{R}^d$) of suitable dimensionality related to the number of features under consideration, possibly carrying a correlation structure or displaying variability which is modelled essentially under the assumption of a probability laws similar or sufficiently close to a Gaussian one. On the context of functional data, the above setting is not appropriate for a number of reasons. To name just a few, the finite dimensionality assumption is no longer sufficient as the data in question are infinite dimensional (e.g. curves, shapes, surfaces), the dependence structure between the data may not be suitably modelled within the normality assumption and, importantly, in many cases of interest the observed data may no longer be understood as elements of a vector space but may be elements of a space with nonlinear or convex structure (e.g. elements of a general metric space like covariance matrices, curves of particular form, etc). Recently, Cano et al. (2015) initiated the development of a more appropriate framework for dealing with functional data of the above type using tools from the statistical shape theory. In this work, we emphasize on the appropriate definition of the IC behaviour of the statistical process under study, through a more general notion of mean applicable for metric space valued data, the Fréchet mean, combined with the framework of deformation models. The approach we propose and develop is quite general and can be applied to any functional object (e.g. curves, surfaces, etc.), however we restrict ourselves to the case of curves in order to properly motivate the proposed methodology. Advantages and capabilities of the proposed approach are illustrated and discussed in Section 5 and Section 6 through (a) an illustrative example with synthetic data and (b) a real world example where ambient air quality in an area of the city of Athens is monitored by applying the proposed method in past data.

2.2 Preliminaries: Deformation models and the Fréchet mean

A very natural setting for the study of functional profiles is that of deformation models. Deformation models produce metric space valued random elements which belong to some set $M = \{ f \circ T : T \in V \}$ where $f$ is a deterministic function (often to be specified) characterizing the typical (average) shape, and $T(\cdot) = T(\cdot, \omega)$ is a random deformation typically chosen from a vector space $V$ so that the composition $f \circ T(\cdot, \omega)$ generates a random element from $M$, satisfying certain qualitative features. Hence, each random element is parameterized in terms of
the realization of $T \in V$. For example, $f$ can be the curve modeling the distribution of some pollutant over the day, accounting for patterns like the mean variability of traffic or the mean variability of temperature, while $T$ accounts for specific features that may randomly happen on a particular day and may not repeat. We emphasize that in many case of interest $M$ is not endowed with a linear structure (e.g. in the case of s-shaped curves) but is rather a subset of a more general metric space. For instance, consider curves of a specific shape as those appear in medicine (e.g. intra-day blood pressure curves) or those describing the intra-day demand of electric energy in a city. Such objects do not necessarily belong to a vector space, since summing two sampled objects does not lead to an object of the underlying space.

This type of statistical modeling has found several applications in practice so far, e.g., in image and signal processing [Bigot et al. (2009, 2011), in analysing point processes Panaretos et al. (2016), in medicine Papayiannis et al. (2018), in electric energy prediction Kampelis et al. (2020), etc.). The reason behind the growing popularity of this semi-parametric approach is that although fully non-parametric approaches seem very tempting in theory, in practice they rarely can be used for statistical inference when comparisons are needed.

Restricting attention to the case where $f : I \rightarrow \mathbb{R}$ is a function from some interval of $I$ ($I = [0, 1]$ without loss of generality) is a suitable choice for the study of nonlinear profiles. Quite a general deformation model has been studied in Panaretos et al. (2016), modeling separately amplitude and phase deformation characteristics. Under this perspective, the shape relation between curves $f$ and $g$ is expressed as

$$f(t) = (\Lambda \circ g \circ \Pi^{-1})(t) + \epsilon(t) = \Lambda (g(\Pi^{-1}(t))) + \epsilon(t) \quad (1)$$

where $\Pi : I \rightarrow I$ for $I \subset \mathbb{R}$ denotes the phase operator or phase deformator (its inverse $\Pi^{-1}$ is often referred to as the time-warping function) and $\Lambda : L^2(I) \rightarrow L^2(I)$ denotes the amplitude operator or amplitude deformator and $\epsilon(t)$ the residuals, i.e. the aspects of curve $f$ that cannot be efficiently captured through a deformation of $g$ under the particular shape modeling approach. Parametric forms of $\Pi$ and $\Lambda$ are conceivable and practical and hence often used in practice (see e.g. Kneip & Engel (1995), K. Wang et al. (1997), Gervini & Gasser (2004)). The simple parametric choice $\Lambda(z) = az + b$ and $\Pi(s) = ks + c$ leads to the classical shape invariant model.

Since the output of deformation models does not produce elements belonging to a vector space, a notion of the mean which does not rely on linearity has to be adopted in order to allow for the characterization of the mean behaviour $f$ in a class of deformation models from the available data. Such a notion of the mean is the (generalized) Fréchet mean $x_F$ for a sample of random elements $\{x_1, \ldots, x_n\} \subset M$ defined as

$$x_F := \arg \min_{y \in M} \Phi(y) \quad (2)$$

where $\Phi(y) = \sum_{j=1}^n w_j d^2(y, x_j)$ is the generalized Fréchet function of the sample, $d$ is a suitable metric for $M$ and $\{w_1, \ldots, w_n\}$ is a suitable set of weights for the data (the case $w_i = 1/n$ corresponds to the standard definition of the Fréchet mean). The minimum value of $\Phi$ (achieved at $x_F$) corresponds to the variance of the sample. The Fréchet mean is a variational concept that can be obtained using techniques from the calculus of variations and optimization (see e.g. Kravvaritis & Yannacopoulos (2020)) and its theoretical properties are well documented (see e.g. Le & Kume (2000); Afsari (2011); Arnaudon et al. (2013); Petersen et al. (2019)). It has been recently used by the statistics community as an important tool in the study of data which cannot be conveniently described as elements of vector spaces (see e.g. Izem et al. (2007), Jung et al. (2012), Papayiannis & Yannacopoulos (2018), Dubey & Müller (2019), etc.). In the proposed monitoring framework, the generalized Fréchet mean is employed to capture the typical pattern or mean behaviour of an IC sample of functional profiles. However, the performance of this
approach significantly depends on the suitability of the deformation model that is chosen to model the variations around the typical pattern (in the case that a semi-parametric approach is adopted).

2.3 Contributions of the present work

In what follows, a monitoring scheme for functional profiles is developed, based on the EWMA-type control charts, employing and combining the notion of the Fréchet mean and the concept of deformation models. The generalized mean sense offered by the Fréchet mean allows for the determination of the typical behaviour of objects that are not necessarily members of a vector space, i.e. extending in this manner the applicability of the method to more complex data structures like curves, surfaces, etc. Secondly, employing certain classes of deformation models in the procedure, allows for (a) further statistical interpretations of the results since certain qualitative features of the shapes under study are quantified by certain parameters and (b) more efficient estimation of the mean patterns when the employed deformation family is suitable. Moreover, the EWMA control chart is revisited and employing the notion of Fréchet mean and the class of deformation models, is extended to be applicable for more complex data structures (functional profile data like curves) by respecting the special characteristics of the data (non-vector spaces). Note that the provided EWMA-type construction, even for the deformation model parameters, does not coincide with the typical EWMA but rather relies on the Fréchet mean between different profiles (please see Section 3). Therefore by construction, the resulting monitoring approach does not only identifies shifts from the typical (IC) behaviour, but further allows for exploring causal relations of potential shifts in the profile status with significant changes to certain deformation characteristics to explain the phenomenon. Note that the proposed method is appropriate for recovering the mean pattern and explaining deviations from it with respect to certain deformation characteristics. However, if some data (profiles) do not come from the same underlying pattern, the method should fail to provide valid connections with the estimated typical shape, but it could possibly detect the OOC behaviour due to inability of the IC data to describe the observed different in nature profile. For the better understanding of the approach, the method is presented analytically for the case of the shape invariant model (Section 4) and in Sections 5 and 6 is implemented to a synthetic data example and to a real data air pollution monitoring case study, respectively.

3 A monitoring framework for functional profiles

In this section, a monitoring approach for functional profiles employing the notion of Fréchet mean combined with the framework of deformation models is presented, by appropriately constructing EWMA-type shift detection mechanisms. Phase I of the monitoring scheme consists of characterizing the in control (IC) behaviour of the profiles under study, through estimating a semi-parametric version of the Fréchet mean where the type of parameterization depends on the family of deformation models that is employed. In Phase II of the procedure, an appropriately modified version of the EWMA control chart (in order to be compatible with the functional setting and the deformation models family) is also constructed. Finally, as a case of particular interest, the well known shape invariant model (SIM) is implemented as the modelling instrument of the deformations from the mean behaviour and appropriate numerical approaches for its implementation are proposed.

3.1 Estimation of the in control behaviour

Consider the case where \( n \) functional profiles are available, e.g. a set of curves

\[
\mathcal{F} := \{f_1, f_2, ..., f_n\} \subset M \subset V,
\]
providing evidence of IC behaviour regarding the statistical process under study, where \( M \) is a metric space and \( V \) an ambient function vector space, e.g., \( L^p(I) \) or a suitable Sobolev space \( W^{r,p}(I) \). For example, in medicine these curves could represent the daily evolution of blood pressure from subjects which have been characterized as non-hypertensives and can be estimated by some non-parametric modeling approach, e.g., kernel-based estimators [Wand & Jones (1994); Ramsay & Silverman (2007)], splines [Wahba (1990)], wavelets [Chui (2016)], etc. It is important at the first step of the monitoring task, to provide a condensed estimation regarding the typical behaviour of subjects that are characterized as IC to define a reference object suitable for comparison. The set \( F \) will be used as the training set to estimate the typical profile that represents the typical behaviour of the profiles that belong to the IC status. The notion of Fréchet mean is employed to estimate the mean pattern, since the profiles \( \{f_j\}_j \) do not necessarily belong to a vector space and as a result, the typical notion of mean is not applicable.

Depending on the application, certain assumptions regarding the underlying space of interest has to be made. The most usual approach is to consider that all objects under study are members of the ambient space. Without loss of generality set \( V = L^2(I) \) (the Lebesgue space of square integrable functions), i.e. \( f_j \in L^2(I) \) for all \( j = 1, 2, \ldots, n \), and consider the corresponding \( L^2(I) \) norm \( \|f_i - f_j\|_2 = \left( \int_I |f_i(t) - f_j(t)|^2 dt \right)^{1/2} \) as the dissimilarity between the curves \( f_i, f_j \). Therefore, to derive a fully non-parametric estimate of the mean IC behaviour within this framework, one may seek for the mean element of \( F \) within the \( L^2(I) \) framework. Although this problem is computationally tractable, the resulting mean may fail to enjoy certain important qualitative properties which must hold for the elements of \( M \), hence, this mean may not be a suitable representation of the typical IC behaviour.

To remedy this situation, the deformations modeling framework discussed in Section 2.2 is implemented, where combined with the notion of Fréchet mean provides a suitable reference object and quantifies several qualitative aspects regarding the acceptable deviations from the mean shape. These aspects are quantified by the estimation of certain deformation parameters of the employed model (representing features like oscillation in location, amplitude, phase, etc with respect to the mean shape) and are extremely useful for studying newly sampled objects. A standard assumption that is made, is that all objects under study are of the same nature, i.e. there is a certain underlying shape and each object’s shape can be expressed efficiently as a deformation of it with respect to the employed deformable model. Such approaches have been investigated in literature either from the perspective of differential geometry (see e.g. Goodall (1991); Kendall et al. (2009); Small (2012) or from the perspective of statistical shape modeling (see e.g., Kneip & Engel (1995); Gervini & Gasser (2004); Bigot et al. (2013)). However, to the best of our knowledge, such a framework has not previously been proposed to the field of statistical process monitoring.

The amplitude-phase deformation model [Panaretos et al. (2016)] discussed earlier offers a quite general deformation framework. Consider that each curve \( f_j \) in the train set \( F \) can be sufficiently modeled as a deformation of the mean curve \( f_{IC} \) (not known yet) as shown in (1) with deformation parameters \( \theta_j = (\gamma_j, \xi_j) \) and substituting \( g \) with \( f_{IC} \). Amplitude and phase distortions of the curve \( f_j \), comparing to the reference (Fréchet mean) curve \( f_{IC} \), are captured by the deformators \( \Delta_j = \Lambda(\cdot; \gamma_j) \) and \( \Pi_j = \Pi(\cdot; \xi_j) \) and quantified by their respective parameters \( \gamma_j \) and \( \xi_j \). However, the deformation parameters cannot be chosen unless the Fréchet mean is specified. Under the current modeling approach, a semi-parametric expression of the mean can be obtained through averaging. In particular, reversing the modeling of each curve as a model of the Fréchet mean with respect to each curve \( f_j \) we obtain the expression

\[
f_{IC} = \hat{f}_{IC,j}(\theta_j) + \eta_j = \Lambda_j^{-1} \circ f_j \circ \Pi_j + \eta_j
\]

where \( \eta_j := \Lambda_j^{-1} \circ \epsilon_j \circ \Pi_j \) denotes the distorted error term related to the estimation error relying on the observation from only the curve \( f_j \). The mean curve \( f_{IC} \) must be chosen in such a
manner that satisfies the barycenter property, i.e. being simultaneously so close and so far from all the elements in the set \( F \). Therefore, a standard requirement that has to be met is that the average of the residuals \( \eta_j \) among all curves, for each time instant \( t \in I \), must be zero, i.e. 
\[
\frac{1}{n} \sum_{j=1}^{n} \eta_j(t) = 0 \quad \text{for all } t \in I.
\]
As a result by properly averaging every possible model of \( f_{IC} \) as a deformation of each \( f_j \in F \) we obtain the following semi-parametric expression of \( f_{IC} \)
\[
\hat{f}_{IC}(\theta) = \frac{1}{n} \sum_{j=1}^{n} \hat{f}_{IC,j}(\theta_j) = \frac{1}{n} \sum_{j=1}^{n} \Lambda_j^{-1} \circ f_j \circ \Pi_j
\]  
(4)
where \( \theta = (\gamma, \xi)' \) with \( \gamma = (\gamma_1, ..., \gamma_n)' \) stands for the amplitude deformation parameters and \( \xi = (\xi_1, ..., \xi_n)' \) stands for the phase deformation parameters. Clearly, what is represented in (4) is not the Fréchet mean, but rather its best approximation by members of the parametric family of deformation models we consider. The optimality criterion under which the parameter vector \( \theta \) will be chosen, depends on the metric sense \( d_M \) under which we wish to derive the mean element. Keeping in mind the Fréchet function defined in (2), the optimal parameter vector \( \theta_* \) is obtained as the solution to the minimization problem
\[
\theta_* := \arg \min_{\theta \in \mathcal{D}} \frac{1}{n} \sum_{j=1}^{n} d_M^2(\hat{f}_{IC}(\theta), f_j)
\]  
(5)
where \( \mathcal{D} \) stands for the subset of \( \mathbb{R}^{np} \) in which the parameter vector \( \theta \) lies. Depending on the deformation models that are chosen, certain centrality requirements may be asked for their parameters to satisfy. In the case of the amplitude-phase model, standard requirements for the parameters may be any constraints induced by the centrality properties \( \mathbb{E}[\Lambda_j] = \mathbb{E}[\Pi_j] = Id. \)

It is evident that this semi-parametric approach provides additional advantages as compared to a fully non-parametric estimation of the mean curve. Besides the mean estimate, one can derive further information regarding the acceptable deviance levels from the typical shape that characterize the IC behaviour (in the perspective of the adopted deformation model). The latter can be represented/quantified either in terms of the deformation functions or in terms of the individual parameter values in the following manner. Let us denote by \( f_0 := f_{IC}(\theta_0) \). Then, for each \( f_j \in F \) solve the registration problem
\[
\theta_j := \arg \min_{\theta \in \mathbb{R}^{p}} \min_{(\gamma, \xi) \in \mathbb{R}^{p_A} \times \mathbb{R}^{p_L}} R_j(\theta) = \min_{(\gamma, \xi) \in \mathbb{R}^{p_A} \times \mathbb{R}^{p_L}} \frac{1}{n} \sum_{j=1}^{n} d_M^2(\hat{f}_{IC}(\theta), f_j)
\]  
(6)
Note that the parameters \( \theta_j \) obtained by solving problem (6) do not necessarily coincide (and in general do not) with the parameter values obtained by solving (5). That happens since the goal in problem (5) is to optimally register the curve \( f_j \) as a deformation of \( f_0 \), while in problem (6) is to optimally register \( f_0 \) to all curves in \( F \). Repeating the registration procedure described in (6) for each \( f_j \in F \), leads to the construction of the IC datasets \( \{\theta_j = (\gamma_j, \xi_j)'\}_{j=1}^{n} \) (or \( \{\Lambda_j, \Pi_j\}_{j=1}^{n} \) in terms of the amplitude and phase deformators as functions) which provide valuable information about the acceptable deviation levels from the mean curve. Moreover, from the IC dataset, the probability distributions for the deformation parameters are deduced, providing important information concerning the IC random behaviour of the curves under study, allowing for further statistical interpretations. In particular, these datasets are employed in the Phase II of the monitoring scheme, to provide a causal relationship of a potential shift of a profile, with potential shifts in the deformation characteristics.

### 3.2 An EWMA-type control chart for functional profiles

Following the characterization of the IC behaviour in Section 3.1, the construction of an EWMA-type chart for detecting shifts from the IC standard is proposed. We focus our interest on the
case of curves representing the evolution of a quantity in a specified time interval \( t \in I \), whose shape can be efficiently calibrated by some amplitude-phase deformation model as discussed above. The rationale behind the developed control chart, is similar to the classical EWMA charts procedure either for monitoring the process mean or variability of the statistical quantity under study (see e.g. Montgomery (2009)).

Given the set of IC data \( \{f_1, ..., f_n\} \) the typical shape \( f_0 \) is estimated through the procedure described in Section 3.1 under the assumption that any IC element is acceptably deviant from the mean shape \( f_0 \) with respect to the amplitude-phase deformation model, i.e.

\[
f_j = \Lambda_j \circ f_0 \circ \Pi_j^{-1} + \epsilon_j
\]  

where the remaining process \( \epsilon_j(t) \) is considered as white noise. Being acceptably deviant means that the aggregate deformation occurred by both amplitude and phase deformators \( \Lambda_j \) and \( \Pi_j \) does not exceed the deviance levels observed from the IC dataset. So, we need to investigate if a newly sampled element \( f_j \) is characterized as an out-of-control (OOC) one, which deformation is beyond the acceptable limits and of course to define that limits. Given the IC behaviour \( f_0 \), for a newly sampled \( f_j \), the best representation according to model (7) has to be obtained through the solution of the related registration problem which in variational formulation is stated as

\[
(\Lambda_j, \Pi_j) := \arg \min_{\Lambda, \Pi} d_M^2(f_j, \tilde{f}(\Lambda, \Pi))
\]  

(8)

where \( \tilde{f}(\Lambda, \Pi) := \Lambda \circ f_0 \circ \Pi^{-1} \) and \( \Lambda_j, \Pi_j \) are the corresponding deformation operators of \( f_j \) with respect to the IC standard \( f_0 \), i.e. the deformation model that can best represent \( f_j \) as an amplitude-phase distortion of \( f_0 \).

Then, the construction of an EWMA-type chart is possible, which in terms of functional profiles can be expressed through the general expression

\[
\tilde{f}_j = FM(f_j, \tilde{f}_{j-1}; \lambda, 1 - \lambda), \quad \lambda \in (0, 1], \quad j = 1, 2, ...
\]  

(9)

where \( \tilde{f}_0 = f_0 \) (the Fréchet mean of the IC curves), \( FM(g, h; \lambda, 1 - \lambda) \) denotes the Fréchet mean between the curves \( g \) and \( h \) with respective weights \( \lambda \) and \( 1 - \lambda \), while \( \lambda \in (0, 1) \) denotes the sensitivity parameter of the chart as usually defined in EWMA charts. The choice of \( \lambda \) depends on the user’s preferences, i.e. how sensitive desires to make his scheme in oscillations from the mean pattern, and can be set either empirically or by tuning according chart’s performance in previous data. The chart element \( \tilde{f}_j \) is decomposed to the amplitude and phase deformators \( \tilde{\Lambda}_j \) and \( \tilde{\Pi}_j \) (remember that we assume that \( \tilde{f}_j = \tilde{\Lambda}_j \circ f_0 \circ \tilde{\Pi}_j^{-1} \)) which are obtained as the minimizers of the weighted variational problem

\[
(\tilde{\Lambda}_j, \tilde{\Pi}_j) := \arg \min_{\Lambda, \Pi} \left\{ \lambda d_M^2(\Lambda \circ f_0 \circ \Pi^{-1}, \Lambda_j \circ f_0 \circ \Pi_j^{-1}) + (1 - \lambda) d_M^2(\Lambda \circ f_0 \circ \Pi^{-1}, \tilde{\Lambda}_{j-1} \circ f_0 \circ \tilde{\Pi}_{j-1}^{-1}) \right\}
\]  

(10)

for \( j = 1, 2, ... \) where \( \tilde{\Lambda}_0 = Id \) and \( \tilde{\Pi}_0 = Id \). Solving the latter problem is equivalent to solving the problem (9) since the pair of optimal deformators \( (\tilde{\Lambda}_j, \tilde{\Pi}_j) \) fully characterizes the optimizer of (9) under the deformation model (7), i.e. \( \tilde{f}_j = \tilde{\Lambda}_j \circ f_0 \circ \tilde{\Pi}_j^{-1} \). However, the resulting chart element is not just a point but a new curve and consequently, any attempt to illustrate directly the chart elements may be impractical for the monitoring purposes.

Instead, assessing the deviance of the newly observed profile from the IC standard is much more meaningful for determining the control status of the new element. A control chart with respect to the deviance of \( f_j \) from the IC profiles Fréchet mean is designed, taking into account the derived information concerning the deformation features that are employed, building on the
solution of problem (10). Let us denote by $D_j = d_M^2(\tilde{f}_j, f_0)$ where $\tilde{f}_j$ obtained from the solution of problem (9). Then, the chart elements for the variability process are calculated as

$$\tilde{D}_j = \lambda D_j + (1 - \lambda)\tilde{D}_{j-1}, \quad j = 1, 2, ...$$

(11)

where $\tilde{D}_0$ is set as the mean of the quadratic deviations of all the IC observations from the mean with respect to the metric $d_M$.

Note that the optimization problems (8) and (10) may be proved quite challenging or computationally intractable, depending on the nature of elements $f_j \in M$, the metric $d_M$ used and the required conditions on the amplitude and phase deformators (especially the second ones). Therefore, it is much more preferable in practice to use some parametric models for describing the deformators $\Lambda, \Pi$ (as already discussed in Section 3.1) both for computational efficiency and interpretation reasons. By this mean, the requirements for the deformators are transformed to certain constraints concerning some parameter vector $\theta = (\gamma, \xi) \in \mathbb{R}^p$ and the variational problem (8) is simplified to the fitting problem

$$\theta_j := (\gamma_j, \xi_j) = \arg \min_{\theta \in \mathbb{R}^p} R_j(\theta) = \arg \min_{\theta \in \mathbb{R}^p} d_M^2(f_j, \hat{f}(\theta))$$

(12)

where $\hat{f}(\theta) := \Lambda_\gamma \circ f_0 \circ \Pi^{-1}_\xi$ and $\gamma_j, \xi_j$ denote the amplitude and phase deformation parameters. Then, the vector $\theta_j$ contains the optimal deformation parameters $\gamma_j$ (amplitude) and $\xi_j$ (phase), which characterize the respective deformation functions (i.e. $\Lambda_j := \Lambda(\cdot; \gamma_j)$ and $\Pi_j := \Pi(\cdot; \xi_j)$) and $f_j$ can be best represented as a deformation of the Fréchet mean $\tilde{f}_j$ under the amplitude-phase deformation model (7). In this case, the EWMA-chart elements $\tilde{f}_j$ are calculated as the Fréchet mean between the elements $\tilde{f}_j := \hat{f}(\theta_j)$ and $\tilde{f}_{j-1} := \hat{f}(\tilde{\theta}_{j-1})$ with respective weights $\lambda$ and $1 - \lambda$ assuming that $\tilde{f}_j$ can be successfully modeled by (7). Then, the chart element estimation problem is equivalent to the weighted fitting problem

$$\tilde{\theta}_j := (\tilde{\gamma}_j, \tilde{\xi}_j)' = \arg \min_{\theta \in \mathbb{R}^p} \tilde{R}_j(\theta) = \arg \min_{\theta \in \mathbb{R}^p} \left\{ \lambda d_M^2(\hat{f}(\theta), \tilde{f}_j) + (1 - \lambda) d_M^2(\hat{f}(\theta), \tilde{f}_{j-1}) \right\}$$

(13)

The minimizers of (13) determine the deformators $\tilde{\Lambda}_j = \Lambda(\cdot; \tilde{\gamma}_j)$ and $\tilde{\Pi}_j = \Pi(\cdot; \tilde{\xi}_j)$ which are then used to estimate the element $\tilde{f}_j = \tilde{\Lambda}_j \circ f_0 \circ \tilde{\Pi}_j^{-1}$. Therefore, the procedure for the construction of a EWMA-type chart for $f_j$ based on the Fréchet mean and amplitude-phase deformation model framework can be briefly described by the following algorithm:

Algorithm 3.1. (EWMA-type scheme for functional profiles monitoring)

Phase I

I.1 Determine the Fréchet mean $f_0$ from the IC dataset following the procedure in 3.1.

Phase II

II.1 For a newly sampled $f_j \in M$, determine $\theta_j$ by solving (12).

II.2 Determine $\tilde{\theta}_j$ for $j = 1, 2, ...$ (setting $\tilde{\theta}_0$ such that satisfying the appropriate centrality conditions with respect to $f_0$) through the solution of problem (13).

II.3 Set $\tilde{f}_j := \hat{f}(\tilde{\theta}_j)$, for $j = 1, 2, ...$ with $\tilde{f}_0 = f_0$ and estimate the variability chart element $\tilde{D}_j$ according to the procedure described in (11) in order to detect significant shifts from $f_0$. For any newly sampled $f_j$, repeat the steps from II.1 to II.3 while the IC standard $f_0$ is still valid.

The minimizers of problem (13) play the most important role in the monitoring procedure since we need these to define the chart elements for every possible characteristics of interest,
i.e. parameters for phase or amplitude distortion. The minimizing vector $\hat{\theta}_j$ can be first used as a monitoring tool for the state of the process under study by paying special attention only to the deformation features. Then, EWMA-type charts can be constructed for the amplitude and phase parameters $\tilde{\gamma}_j$ and $\tilde{\xi}_j$ (or the respective deformation functions $\tilde{\Lambda}_j$ and $\tilde{\Pi}_j$) providing causal relations with potential shift detection status in the profile under study.

Remark 3.2. One may consider beginning the monitoring procedure by building EWMA on the deformation parameters and then extending this chart for the deformation processes and then at the monitoring object $f_j$. However, non-linearity of $f_j$ does not allow for such an extension. Notice that even in the case where both deformation functions $\Lambda, \Pi$ are linear, e.g. $\Lambda(z) = az + b$, $\Pi(s) = cs + d$, although one may attempt to monitor the deformation functions separately, e.g. $\tilde{\Lambda}_j = \lambda \Lambda_j + (1 - \lambda)\tilde{\Lambda}_{j-1}$ and $\tilde{\Pi}_j = \lambda \Pi_j + (1 - \lambda)\tilde{\Pi}_{j-1}$, then the resulting chart for $f_j$ through $\tilde{f}_j = \lambda \tilde{\Lambda}_j \circ f_0 \circ \tilde{\Pi}_j + (1 - \lambda)\tilde{f}_{j-1}$ does not coincide with the minimizer of equation (10).

4 An explicitly solvable case: The shape-invariant deformation model

4.1 EWMA-type charts using the shape-invariant deformation model

In this section we implement the monitoring procedure proposed in Section 3 for the particular case where the shape invariant model is employed as the deformation model with respect to which the mean pattern is estimated and the monitoring procedure refers to. This shape modeling approach has been repeatedly discussed and extended in the functional modeling literature (see e.g. Kneip & Engel (1995); Gervini & Gasser (2004); Bigot et al. (2013)) due to its applicability in many different contexts and the nice interpretation of its parameters. In this setting, each object $f_j$ is modeled as a distortion of the IC standard $f_0$ (i.e. the mean behaviour of the IC objects) through the relation

$$f_j(t) = \beta_j + \alpha_j f_0 \left( \frac{t - \zeta_j}{\kappa_j} \right) + \epsilon_j(t), \quad t \in I$$

(14)

which can be also realized as a special case of the amplitude-phase deformation model where $\Lambda_j(z) = \alpha_j z + \beta_j$ and $\Pi(s) = \kappa_j s + \zeta_j$ with $(\alpha_j, \beta_j)$ denote the deformation parameters on the scale and location on the process’ amplitude, while $(\kappa_j, \zeta_j)$ denote the deformation parameters on the scale and location on the process’ phase (please see Figure 1 for an illustration of the deformation model’s characteristics). In other words, we realize $\mathcal{M}$ as the subset of $L^2$

$$\mathcal{M} := \left\{ f \in L^2 : \exists (\alpha, \beta, \kappa, \zeta) \in \mathbb{R}^4 \text{ such that } f(t) = \beta + \alpha f_0 \left( \frac{t - \zeta}{\kappa} \right), \quad t \in I \right\}$$

Following the functional monitoring approach described in Sections 3.1 and 3.2, assuming that there is available a set of IC curves $\mathcal{F} = \{f_1, \ldots, f_n\} \in \mathcal{M} \subset L^2$, we estimate the corresponding Fréchet mean (i.e. the IC standard). By directly substituting the above linear amplitude and phase deformation parametric models to equation (4) we obtain the following semi-parametric representation of the Fréchet mean:

$$\tilde{f}_{IC}(t; \theta) = \frac{1}{n} \sum_{j=1}^{n} \left\{ \alpha_j^{-1} f_j(\kappa_j t + \zeta_j) - \alpha_j^{-1} \beta_j \right\}$$

(15)

which depends on the vector of deformation parameters

$$\theta := (\alpha, \beta, \kappa, \zeta)' = (\alpha_1, \ldots, \alpha_n, \beta_1, \ldots, \beta_n, \kappa_1, \ldots, \kappa_n, \zeta_1, \ldots, \zeta_n)' \in \mathbb{R}^{4n}.$$
The optimal parameter vector that characterize the respective Fréchet mean is chosen through the solution of the optimization problem (Fréchet function minimization)

$$\theta^* = \arg\min_{\theta \in D} \frac{1}{n} \sum_{j=1}^{n} \|f_j - \hat{f}_{\text{IC}}(\theta)\|_2^2,$$

(16)

where $D \subset \mathbb{R}^{4n}$ denotes the parametric space on which feasible solutions of (16) are contained, satisfying the centrality requirements

$$\prod_{j=1}^{n} \alpha_j^{1/n} = 1, \quad \sum_{j=1}^{n} \beta_j = 0, \quad \prod_{j=1}^{n} \kappa_j^{1/n} = 1, \quad \sum_{j=1}^{n} \zeta_j = 0$$

in order to satisfy the deformators’ centrality properties $E[\Lambda] = I_d$ and $E[\Pi] = I_d$. Then, we set as IC standard the curve $f_0 := \hat{f}_{\text{IC}}(\theta^*)$. For a newly sampled $f_j$ a registration step is performed, in order to model the curve $f_j$ as a shape-invariant deformation of $f_0$ (with respect to the formulation (14)), through the related registration problem

$$\theta_j = (\alpha_j, \beta_j, \kappa_j, \zeta_j) = \arg\min_{\theta \in \mathbb{R}^4} \|f_j - \hat{f}(\theta)\|_2^2$$

(17)

where $\hat{f}(\theta) = \beta + \alpha f_0 \left( \frac{t-\zeta}{\kappa} \right)$.

Let us denote $\tilde{f}_j := \hat{f}(\theta_j)$. Then we construct the EWMA-type chart on $f_j$ using the assumed
shape parameterization, which elements \( \tilde{f}_j \) are chosen as the Fréchet barycenter between \( \hat{f}_j \) and \( \tilde{f}_{j-1} \) with weights \( \lambda \) and \( 1 - \lambda \) respectively, i.e. through the fitting problem

\[
\tilde{\theta}_j := \arg \min_{\theta \in \mathbb{R}^4} \lambda \| \hat{f}(\theta) - \hat{f}_j \|^2 + (1 - \lambda) \| \hat{f}(\theta) - \tilde{f}_{j-1} \|^2
\]  

(18)

where \( \tilde{f}_{j-1} := \hat{f}(\tilde{\theta}_{j-1}) \) and \( \tilde{\theta}_0 = (\tilde{\alpha}_0, \tilde{\beta}_0, \tilde{\kappa}_0, \tilde{\zeta}_0) = (1, 0, 1, 0) \). Setting \( \tilde{f}_j := \hat{f}(\tilde{\theta}_j) \) we construct a EWMA-type chart for monitoring variability of the process as proposed in equation (11) under the setting of the shape-invariant model. If a shift is detected, EWMA-type charts can be constructed for the amplitude and phase deformation parameters using the minimizers of problem (18). Of course, EWMA-type charts can be also build for each deformation parameter separately since each one quantifies different aspects of deviance from the IC standard. However, potential shift detections on some of the shape distortion parameters do not necessarily lead to a shift of the corresponding curve under study. The procedure is briefly described below.

**Algorithm 4.1. (EWMA-type monitoring scheme for functional profiles under the shape invariant model)**

**Phase I: Determination of the IC behaviour and acceptable levels of deviance**

**I.1** Provide as input a set of IC curves \( \{f_1, f_2, ..., f_n\} \).

**I.2** Estimate the Fréchet mean curve \( f_0 \) from the IC data and the related IC set of deformation parameters \( \{\theta_{IC}^j = (\alpha_{IC}^j, \beta_{IC}^j, \kappa_{IC}^j, \zeta_{IC}^j)\}_{j=1}^n \).

**Phase II: EWMA-type chart construction and detection of possible shifts from the IC standard**

**II.1** Given a newly sampled curve \( f_j \) and a choice for \( \lambda > 0 \) register it to the SIM deformation model with respect to \( f_0 \) by solving problem (17) and obtain the deformation parameters \( \theta_j \) and set \( \hat{f}_j := \hat{f}(\theta_j) \).

**II.2** Calculate the component \( \tilde{f}_j \) of the EWMA-type chart through the solution of the problem (18) and then calculate the \( j \)-th component for the EWMA-type variability monitoring chart as proposed in (11). If a shift is detected, then characterize the curve as OOC and check the relevant control charts for the deformation parameters \( \tilde{\theta}_j \) for causal relations of the detected shift with potential shifts in the deformation parameters.

II.3 Repeat Steps II.1 - II.2 for any newly sampled curve.

### 4.2 Numerical Schemes for the Monitoring Procedure

In this subsection we discuss the numerical approximation of the optimization problems (16), (17) and (18) related to the proposed monitoring process for functional profiles. These problems concern the determination of the Fréchet mean of the IC curves, the modeling of newly obtained data (curves) as shape-invariant deformations of the mean curve and the estimation of the EWMA-type chart elements. We will discuss each optimization problem separately as it occurs.

First, we treat the Fréchet mean estimation problem (16) for the IC data curves. For convenience, let us denote the objective function of the problem as

\[
V(\gamma, \xi) := \frac{1}{n} \sum_{j=1}^{n} \int f_j(t) - \hat{f}_{IC}(t; \gamma, \xi))^2 dt
\]

(19)

where \( \hat{f}_{IC} \) is defined in (15), \( \gamma = (\bar{\alpha}, \beta)' \) (with \( \bar{\alpha} := \alpha^{-1} \)) denotes the vector of amplitude deformation parameters and \( \xi = (\kappa, \zeta)' \) denotes the vector of phase distortion parameters.
Splitting the parameters into two distinct groups is extremely important for the development of an efficient numerical scheme. In the absence of the parameter centrality constraints, the function $V$ depends pseudo-quadratically on the parameter vector $\gamma$ (after the substitution of $\alpha$ with $\bar{\alpha}$) while as far as the parameter vector $\xi$ is concerned, the dependence is fully non-quadratic and importantly non-convex on the parameter vector $\xi$. Treating the problem with respect to all the parameters simultaneously, results to a non-convex minimization problem which is computationally quite expensive. Alternatively, we propose an iterative two-stage minimization scheme which exploits the pseudo-quadratic nature of the problem with respect to the amplitude deformation parameters $\gamma$. Let us consider the parameter spaces $\Theta_\Lambda, \Theta_\Pi$

\[
\Theta_\Lambda = \left\{ \gamma = (\bar{\alpha}, \beta)' \in \mathbb{R}^{2n} : \prod_{j=1}^{n} \bar{\alpha}_j^{1/n} = 1, \sum_{j=1}^{n} \beta_j = 0, \bar{\alpha}_j > 0, \forall j = 1, 2, ..., n \right\}
\]

\[
\Theta_\Pi = \left\{ \xi = (\kappa, \zeta)' \in \mathbb{R}^{2n} : \prod_{j=1}^{n} \kappa_j^{1/n} = 1, \sum_{j=1}^{n} \zeta_j = 0, \zeta_j \in \left[ -\frac{1}{2}, \frac{1}{2} \right], \forall j = 1, 2, ..., n \right\}
\]

for the amplitude deformation and phase deformation parameters respectively. The following two-stage minimization scheme is proposed:

**Algorithm 4.2. Two-stage iterative numerical scheme for the Fréchet mean estimation under the shape invariant model**

**Step 0** Set $k = 1, \gamma^{(0)} = (1,1,...,1,0,0,...,0)'$, $\xi^{(0)} = (1,1,...,1,0,0,...,0)'$ and define the tolerance level ($\epsilon > 0$).

**Step 1** Solve the unconstrained quadratic optimization problem $\hat{\gamma} = \arg\min_{\gamma \in \mathbb{R}^{2n}} V(\gamma, \xi^{(k-1)})$ and then compute the projection $\gamma^{(k)} = \text{Proj}_{\Theta_\Lambda}(\hat{\gamma})$

**Step 2** Solve the unconstrained nonconvex optimization problem $\hat{\xi} = \arg\min_{\xi \in \mathbb{R}^{2n}} V(\gamma^{(k)}, \xi)$ and then compute the projection $\xi^{(k)} = \text{Proj}_{\Theta_\Pi}(\hat{\xi})$

**Step 3** If $\|\gamma^{(k)} - \gamma^{(k-1)}\| < \epsilon$ and $\|\xi^{(k)} - \xi^{(k-1)}\| < \epsilon$ stop and set $(\gamma_*, \xi_*) = (\gamma^{(k)}, \xi^{(k)})$. Else set $k = k + 1$ and go to Step 1.

Clearly, the parameter vector $(\gamma_*, \xi_*) \in \Theta_\Lambda \times \Theta_\Pi$ determines the Fréchet mean of the data under study. At Step 1, the solution of the unconstrained quadratic minimization problem can be derived explicitly and then the projection to the parameter space $\Theta_\Lambda$ can be treated effectively by any gradient-descent type scheme. At Step 2, the unconstrained nonlinear (non-convex) minimization problem is quite difficult to handle effectively by gradient-based algorithms. Therefore, the use of an evolutionary optimization method (like Simulated Annealing or Particle Swarm Optimization) is recommended here in order to avoid local minima of the problem. The projection to the parameter space $\Theta_\Pi$ can be efficiently treated as in Step 1 by any gradient-based scheme (since this problem is strongly convex with respect to $\xi$). The terminal condition in Step 3 guarantees the convergence of the problem to the minimum value of $V(\gamma, \xi)$ due to the continuity with respect to the problem parameters. The above two-stage iterative scheme generates a sequence of points $\{\theta_k\}_k$ by alternating projections between two convex sets. In fact, at Step 1 the problem is solved on the convex set $\Gamma := \Theta \times \mathbb{R}^{2n}$ generating a sequence of points $\{\theta_k\}_k \subset \Gamma$, while at Step 2, the problem is solved on the convex set $\Xi := \mathbb{R}^{2n} \times \Theta_\Pi$ generating a sequence of points $\{\theta_k\}_k \subset \Xi$. It can be shown by the alternating projections algorithm (see e.g. Bauschke & Borwein (1993, 1994)) that as $k$ grows, both sequences converge to a point $\theta_*$ in the intersection of the two sets $D = \Gamma \cap \Xi$, being the minimizer of $V(\theta)$.

Next we discuss the registration problem (17). Since the Fréchet mean have been determined as $f_0 := f_{1C}(\theta_*)$ the next crucial step for the monitoring procedure is the determination of the
deformation parameters with respect to the IC standard \( f_0 \). Assuming that the values of the phase deformation parameters \( \kappa, \zeta \) are known, the optimal values for the amplitude deformation parameters can be derived in analytical form and in particular

\[
\alpha_* (\kappa, \zeta) = \frac{\int_I f_0 \left( \frac{t-\zeta}{\kappa} \right) f_j(t) dt - \int_I f_0 \left( \frac{t-\zeta}{\kappa} \right) dt \int_I f_j(t) dt}{\int_I f_0^2 \left( \frac{t-\zeta}{\kappa} \right) dt - \left( \int_I f_0 \left( \frac{t-\zeta}{\kappa} \right) dt \right)^2} \quad (20)
\]

\[
\beta_* (\kappa, \zeta) = \int_I f_j(t) dt - \alpha_* (\kappa, \zeta) \int_I f_0 \left( \frac{t-\zeta}{\kappa} \right) dt. \quad (21)
\]

This fact, allows us to rewrite the problem \([17]\) to a reduced form depending only on the phase deformation parameters \((\kappa, \zeta)\). However, the resulting problem is a fully non-quadratic and non-convex problem with respect to the phase deformation parameters and therefore any gradient-based scheme has high chances to fail in locating the minima. As a result, any evolutionary minimization method offers an easy way out especially because the low dimension of the problem.

Finally, the EWMA-type chart element estimation problem expressed in \([18]\) can be treated similarly to \([17]\) since the optimal amplitude deformation parameters can be analytically expressed as functions of the phase deformation parameters:

\[
\tilde{\alpha}_* (\tilde{\kappa}, \tilde{\zeta}) = \frac{\lambda \left( \int_I f_0 \left( \frac{t-\tilde{\zeta}}{\tilde{\kappa}} \right) \tilde{f}_j(t) dt - \int_I f_0 \left( \frac{t-\tilde{\zeta}}{\tilde{\kappa}} \right) dt \int_I \tilde{f}_j(t) dt \right)}{\int_I f_0^2 \left( \frac{t-\tilde{\zeta}}{\tilde{\kappa}} \right) dt - \left( \int_I f_0 \left( \frac{t-\tilde{\zeta}}{\tilde{\kappa}} \right) dt \right)^2} \\
+ (1 - \lambda) \left( \int_I f_0 \left( \frac{t-\tilde{\zeta}}{\tilde{\kappa}} \right) \tilde{f}_{j-1}(t) dt - \int_I f_0 \left( \frac{t-\tilde{\zeta}}{\tilde{\kappa}} \right) dt \int_I \tilde{f}_{j-1}(t) dt \right) \quad (22)
\]

\[
\tilde{\beta}_* (\tilde{\kappa}, \tilde{\zeta}) = \lambda \int_I \tilde{f}_j(t) dt + (1 - \lambda) \int_I \tilde{f}_{j-1}(t) dt - \tilde{\alpha}_* (\tilde{\kappa}, \tilde{\zeta}) \int_I f_0 \left( \frac{t-\tilde{\zeta}}{\tilde{\kappa}} \right) dt . \quad (23)
\]

Substituting the above relations into problem \([18]\) a reduced form of the problem is obtained depending only on the phase parameters \((\tilde{\kappa}, \tilde{\zeta})\) which can be optimally chosen with the same minimization approach used in the aforementioned registration problem.

### 5 An illustrative example with synthetic data

To better study the characteristics and the shift detection capabilities of the proposed monitoring method, we design and perform a simulation study. The functional model used for creating the synthetic data is designed so as describe and mimic the intra-day evolution of environmental quantities that typically present repeated patterns, multiple periodicities and amplitude or phase shifts. In particular, we propose a functional model for the generation of the data of the form

\[
f(t; \Psi) = A_0 + A_1 \sin(B_1 \pi t) + A_2 \cos(B_2 \pi t), \quad t \in [0, 1] \quad (24)
\]

depending on the parameter vector \( \Psi = (A_0, A_1, A_2, B_1, B_2)' \in \mathbb{R}^5 \). This model, although not exactly the same, can be identified by the shape-invariant model for appropriate choices of the parameters \( \Psi \). Moreover, the parameters \( B_1, B_2 \) control various periodicities and their total effect can be related to phase shifts, while the parameters \( A_0, A_1, A_2 \) are responsible for amplitude shifts.

Using this model, a training dataset is produced by choosing parameters \( \Psi \) randomly from a distribution centered around the vector \( \Psi_0 = (40, 20, -20, 2, 4)' \). For each random choice of the parameter vector \( \Psi_j = (A_{0,j}, A_{1,j}, A_{2,j}, B_{1,j}, B_{2,j})' \) where \( \Psi_j \sim N(\Psi_0, C_\Psi) \) with \( C_\Psi \) denoting
the covariance matrix of the parameters $\Psi_j$, a new random curve $f_j$ is generated according to the model

$$f_j(t) = f(t; \Psi_j) = A_{0,j} + A_{1,j} \sin(B_{1,j} \pi t) + A_{2,j} \cos(B_{2,j} \pi t). \quad (25)$$

The perturbations of the parameters' vector can be understood as perturbations on: (a) location ($A_{0,j}$), (b) amplitude ($A_{1,j}, A_{2,j}$) and (c) phase or periodicity ($B_{1,j}, B_{2,j}$) of the curve $f_j$. Using the above consideration, a sample of random curves has been generated which will form our synthetic dataset upon which we will test the performance of the proposed monitoring scheme.

5.1 Training data generation

Sequential data (each data point is a whole random curve $f_j$) are generated according to the model (25) by sequentially sampling different parameter vectors $\Psi_j$. These parameter vectors are not necessary independent samples from the distribution $N(\Psi_0, C_{\Psi})$. In fact, in order to stress the capabilities of the proposed monitoring scheme, we choose to introduce correlations between the various parameters choices $\Psi_j$, which in turn introduce correlations between the corresponding functional profiles $f_j$. The correlation patterns in the parameters are introduced according to the following scheme:

$$\Psi_j | \Psi_{j-1} \sim N(\tilde{\Psi}_j, \tilde{C}_{\Psi}) \quad (26)$$

where $\tilde{\Psi}_j = \Psi_0 + C_B C_{\Psi}^{-1} (\Psi_{j-1} - \Psi_0)$, $\tilde{C}_{\Psi} = C_{\Psi} - C_B C_{\Psi}^{-1} C_B$ and $C_B = SRS$ with $S$ being the diagonal matrix with the standard deviations for each parameter in $\Psi_j$ in the diagonal, $R = \rho I$ with $\rho \in (-1,1)$ denoting the correlation index and $I$ denoting the identity matrix. As previously mentioned, the latter will allow for assessing the performance of the discussed method under different correlation intensities between the sampled curves. It is important to know that our training data that is the IC data are generated by correlation pattern presented in (26) and one of the interesting questions posed in this simulation study is whether the performance of the proposed monitoring scheme is affected by the possible existence of dependence structures in the datasets.

5.2 Test dataset generation

The test dataset is created in the same manner as above, but with the following twist: with probability 80% the curves are generated as in the previous section, whereas with probability 20% the curves are generated by a parameter vector $\tilde{\Psi}_j = \Psi_j + u_j$ where the first component is sampled according to (26) while the second component is a uniform perturbation where $u_j \sim U([a,b])$ for appropriate choices for $a,b$. The curves corresponding to the parameter vectors $\tilde{\Psi}_j$ will be considered as OOC curves.

5.3 Performance of the functional monitoring scheme

Using the methodology presented in the previous two subsections we generate two synthetic datasets, a training and a test dataset. We assume the composition of the test dataset in terms of IC and OOC samples is not known to us, as also the exact functional model that generated the data. Our intention in this section is to check whether the proposed functional profiles monitoring scheme, based on the shape-invariant model, is capable of distinguishing the IC from the OOC samples in the test dataset after being trained using the training dataset. This choice of experiment will test: (a) the robustness of the proposed scheme for data not exactly generated from the shape-invariant model itself and (b) the effects of correlations in data to the monitoring ability.
The generated datasets (train and test) are illustrated in Figure 2. This sequential data generation mechanism is able to simulate functional objects that are often observed in environmental applications like the one discussed in the next section, i.e. intra-day concentration and evolution of pollution levels.

We choose to use as a functional model for the observed curves the shape-invariant model. Based on this characterization, each randomly generated curve \( f_j \) can be modelled by appropriately selecting the deformation parameters of the shape invariant model if the typical curve \( f \) was known (which for the needs of the application is considered as unknown). The proposed approach is expected to efficiently capture the mean shape of the mechanism that generated the curves, and allocate the variations to the deformation parameters of the shape invariant model. For the sake of simplicity, we omit the phase deformation parameter \( \kappa \) from what follows, but it is quite straightforward to include it if one desires to do so. Therefore, the version of the shape invariant model that is used here, is the 3-parameter version, i.e. \( f_j(t) = \beta_j + \alpha_j g(t - \zeta_j) \) where \( f_j \) denotes the modelled curve and \( g \) the reference one.

| Correlation | Classification Accuracy | Classification Errors |
|-------------|------------------------|-----------------------|
|             | True (%) | False (%) | Type I | Type II |
| No correlation | 91.00    | 9.00       | 0.00   | 9.00    |
| Low         | 95.00    | 5.00       | 0.00   | 5.00    |
| Medium      | 96.00    | 4.00       | 0.00   | 4.00    |
| High        | 98.00    | 2.00       | 0.00   | 2.00    |

Table 1: Nonparametric f-EWMA charts performance

| Correlation | Classification Accuracy | Classification Errors |
|-------------|------------------------|-----------------------|
|             | True (%) | False (%) | Type I | Type II |
| No correlation | 93.00    | 7.00       | 0.00   | 7.00    |
| Low         | 95.00    | 5.00       | 0.00   | 5.00    |
| Medium      | 95.00    | 5.00       | 3.00   | 2.00    |
| High        | 98.00    | 2.00       | 0.00   | 2.00    |

Table 2: Semi-parametric f-EWMA charts performance

From the derived results, it seems that the method displayed a quite robust performance in detecting the OOC shifts, regardless the correlation intensity between the sampled curves. The percentage of true classification, regardless of higher correlations, was slightly improved when moving to higher correlations. In general, the shifts were detected with accuracy higher than 91%. It is also remarkable
the very low type-I errors that are observed. In Tables 1 and 2 are illustrated the correct classification percentages and the error rates for the cases studied with the "nonparametric" version of the functional EWMA-type chart (f-EWMA), i.e. taking directly the deviance of \( f_j \) from the mean estimated curve under the shape-invariant model (SIM), and the SIM-dependent version of the chart as stated in equation (11). Both versions of the chart (illustrated in Figure 3) provide quite close results with the nonparametric version having slightly higher type-II errors and also slightly better total accuracy. However, these minor differences in the performance of the two approaches, motivate the use of the semiparametric version of the chart since allows for further interpretation concerning the shifts in the special features that are taken into account by the employed deformation model (in our case: location, amplitude and phase) which led to the shift of the curve. In Figure 4 are illustrated the deformation parameters charts accompanying the f-EWMA based on the shape-invariant model. From these charts, causal relations to the shifts observed in the deviance f-EWMA charts can be recovered.

Figure 3: f-EWMA control charts for deviance from the mean shape (upper panel) and total deviance (lower panel).

Figure 4: f-EWMA control charts for location parameter (upper panel), amplitude parameter (middle panel) and phase parameter (lower panel).
6 Studying air quality profiles for potential polluters in the area of Athens

In this section, the functional monitoring methodology presented in Section 4 is employed in studying air pollution data collected from atmospheric pollution sensors installed in the area of Athens, by the Ministry of Environment and Energy. Specifically, the study concerns the monitoring of air pollution in the area of Patission Street for the time period 2001-2007. The available data consist of daily measurements (mean values per hour for the duration of a day, i.e. 24 measurements) regarding the concentration of quantities considered as potential polluters and specifically the concentration of: carbon monoxide (CO), nitrogen dioxide (NO₂), ozone (O₃) and sulfur dioxide (SO₂). Certain safety concentration thresholds for the human health have been set according to the directions of the World Health Organization (WHO) (Table 3) which violation consists high risk for the human health. As a result, from the scope of WHO, a day which at least one of the thresholds has been violated is considered as an OOC day, while if none has been violated is considered as an IC day.

| Polluter               | Time Interval | Unit         | Maximum Average Concentration Threshold |
|------------------------|---------------|--------------|-----------------------------------------|
| Carbon Monoxide (CO)   | 1 hr          | mg/m³        | ≤ 35                                    |
|                        | 8 hrs         | mg/m³        | ≤ 10                                    |
|                        | 24 hrs        | mg/m³        | ≤ 4                                     |
| Nitrogen Dioxide (NO₂) | 1 hr          | µg/m³        | ≤ 200                                   |
|                        | 24 hrs        | µg/m³        | ≤ 25                                    |
| Ozone (O₃)             | 8 hrs         | µg/m³        | ≤ 60                                    |
| Sulfur Dioxide (SO₂)   | 24 hrs        | µg/m³        | ≤ 40                                    |

Table 3: Safety concentration thresholds of the pollutants under study for human health according to the World Health Organization

This threshold approach is maybe not the better strategy for the efficient monitoring of air quality, since the actual data are of functional form while the threshold is defined pointwise (with respect to time and space). The discussed monitoring approach offers an alternative tool for assessing and measuring the status of such phenomena that evolve simultaneously with similar manner (maybe with small fluctuations from a specific standard). Moreover, employing deformation models in the modelling task might reveal and quantify special characteristics that cannot be captured by pointwise monitoring approaches. To illustrate the capabilities of the discussed method, we use as train dataset the measurements from the time period 2001-2004 and as test dataset the measurements from the time period 2005-2007 for the term October-December. Note that we focus on this period of year in our analysis since it is considered as the "peak period" for the concentration of polluters in the atmosphere (i.e. it is more interesting in terms of identifying the OOC days). Moreover, in these three months no major differences in the environmental conditions are observed and the median levels of the polluters are quite the same (similar median estimated curves) and as a result seasonality effect is not an issue. However, even in the case that such stationarity issues may arise, a possible way out as a preparation step for the discussed method, is applying the modelling approach and the relevant software presented and discussed in [Y. Wang et al. (2021)].

The phase I of the monitoring procedure is performed at first using as train dataset the IC observations from the time period 2001-2004, where the typical behaviour for the intra-day concentration of each polluter is estimated (i.e. the typical shape of the daily evolution of each polluter) and the empirical distributions of the deformation parameters indicating the...
acceptable levels of deviation from the mean pattern. The shape invariant model is employed as a particular deformation model, presented and discussed in Section 4, however we omit the phase scaling parameter $\kappa$ in order to simplify the analysis. Clearly, the parameterization of certain characteristics of the data allows for a more careful and meaningful monitoring of the changes that could possibly affect the air pollution status of each day (IC or OOC) in the region of interest. In Figure 5 are illustrated the IC daily curves from the train dataset and the estimated IC intra-day mean behaviour under the Fréchet mean notion for each pollutant under consideration. Clearly, the data shapes (intra-day polluter concentration curves) seem to be successfully calibrated by the shape invariant model and the calculated Fréchet means are plausible representations of the typical behaviour of the pollutants’ daily distribution curves.

Next, the Phase II of the functional monitoring scheme is performed and the test dataset concerning the time period 2005-2007 is studied. Following the described procedure, the f-EWMA charts for the sampled curves deviance from the IC standard are constructed to detect significant shifts. The resulting EWMA-type charts are illustrated for each polluter under study in Figures 6, 7, 8 and 9. In the upper panel, the deviance related charts are displayed. The first in the row refers to the typical deviance from the mean shape chart under which the OOC identifications are performed. The second chart in the row, refers to the residuals deviance chart in which curves that display quite a disturbed shape comparing to the estimated Fréchet mean are expected to be characterized as OOC from this chart (however this may not result to an OOC characterization for the curve status since this concerns only the ability of the employed deformation model to describe this day’s data). The third one in the row, is the nonparametric version of the deviance chart and is illustrated for comparison reasons. The second panel of charts concerns the monitoring of the features taken into account by the shape-invariant model (location, amplitude and phase). Note that the Fréchet mean is employed according to the $L^2$-metric sense ($q = 2$), while the exponential weighting parameters that have been tested are $\lambda = 0.01, 0.05, 0.10, ..., 0.90, 0.95, 0.99$ where the optimal choice was selected per case (by optimality we mean to seek the value of $\lambda$ for which less OOC observations are classified as IC and less IC observations are classified as OOC, i.e. minimizing both type-I and type-II
Clearly, investigating more cautiously the optimal choice for $\lambda$ could further improve the performance of the method. Perhaps, a better strategy is to occasionally alternate the weighting parameter value depending on the application. Such a task could be done by separating the train set to further parts and cross-validating for the better choice of $\lambda$ in different train sets. However, we feel that is beyond the scopes of this work and therefore we use a constant value for each polluter for the whole monitoring task.

| Polluter | # of cases | Classification Accuracy | Classification Errors | Polluter | # of cases | Classification Accuracy | Classification Errors |
|----------|------------|------------------------|-----------------------|----------|------------|------------------------|-----------------------|
|          |            | True (%) | False (%) | Type I | Type II | True (%) | False (%) | Type I | Type II |
| CO       | 266        | 96.24 (256) | 3.76 (10) | 2.63 (7) | 1.13 (3) |
| NO$_2$   | 264        | 90.53 (239) | 9.47 (25) | 0.76 (2) | 8.71 (23) |
| O$_3$    | 266        | 93.98 (250) | 6.02 (16) | 0.00 (0) | 6.02 (16) |
| SO$_2$   | 266        | 96.99 (258) | 3.01 (8)  | 0.00 (0) | 3.01 (8)  |

Table 4: Nonparametric f-EWMA charts performance

| Polluter | # of cases | Classification Accuracy | Classification Errors | Polluter | # of cases | Classification Accuracy | Classification Errors |
|----------|------------|------------------------|-----------------------|----------|------------|------------------------|-----------------------|
|          |            | True (%) | False (%) | Type I | Type II | True (%) | False (%) | Type I | Type II |
| CO       | 266        | 91.73 (244) | 8.27 (22) | 0.00 (0) | 8.27 (22) |
| NO$_2$   | 264        | 88.64 (234) | 11.36 (30) | 1.14 (3) | 10.23 (27) |
| O$_3$    | 266        | 90.60 (241) | 9.40 (25)  | 0.00 (0) | 9.40 (25)  |
| SO$_2$   | 266        | 97.74 (260) | 2.26 (6)   | 0.00 (0) | 2.26 (6)   |

Table 5: Semi-parametric (SIM) f-EWMA charts performance

In Tables 4 and 5 are illustrated the performance diagnostics for the shape-invariant based and the nonparametric version of the method concerning the true detection of the OOC observations (per polluter) and the related error rates. Similar findings with the synthetic data experiment are also observed here, i.e. SIM-based chart leads in general to slightly higher type-II errors, slightly lower type-I errors and slightly worse accuracy comparing to the non-parametric version. However, the high accuracy rate (around 90-95%) and the interpretability of the parametric version of the chart with respect to meaningful geometrical features of the observed processes, make it a better choice for analysing in more depth such type of data. The deformation parameters charts for the four polluters indicate that the phase deformation characteristic in general is not important (in terms of what WHO considers as OOC), the amplitude deformation feature seems to be significantly affected by OOC curves (in most cases OOC days lead the chart beyond the IC zone for all polluters) while the location deformation feature seems to be affected in some extreme cases. In general, for these type of data it seems that amplitude deformation level is a nice proxy for the status of the curve under study.

7 Conclusions

In this work a framework for the statistical monitoring of functional data by combining the notion of the Fréchet mean and the framework of deformation models is proposed and is implemented to the important environmental problem of air quality monitoring in cities. In particular the amplitude-phase deformation model has been studied as a modeling approach of the respective functional profiles to represent each one as a distortion of the typical profile that should be observed, i.e. the Fréchet mean of the profiles that are considered as in control. The combination of these frameworks offers (a) a computationally effective way to estimate the Fréchet mean since the computational cost is significantly reduced by transforming the related optimization problem from a variational one to a fitting one, and (b) the approach of deformation models allows for allocating the deviance of complex objects like functional profiles to significant deviations of certain geometric features setting also as a reference standard the Fréchet mean.

The important case of the shape invariant model is discussed in detail and applied in two case
studies: (a) a synthetic data experiment where the performance of the method was assessed under different conditions and, (b) in monitoring ambient air quality in the city of Athens with very interesting findings.

Acknowledgements

Two of the authors wish to acknowledge for financial support from the research program DRASI II, funded by the AUEB Research Center.

References

Adams, M. D., & Kanaroglou, P. S. (2016). Mapping real-time air pollution health risk for environmental management: Combining mobile and stationary air pollution monitoring with neural network models. *Journal of environmental management, 168*, 133–141.
Figure 8: EWMA-type charts for monitoring the status of pollutant O$_3$

Figure 9: EWMA-type charts for monitoring the status of pollutant SO$_2$

Afsari, B. (2011). Riemannian $l^p$ center of mass: existence, uniqueness and convexity. *Proceedings of the American Mathematical Society, 139*(2), 655–673.

Alimissis, A., Philippopoulos, K., Tzanis, C., & Deligiorgi, D. (2018). Spatial estimation of urban air pollution with the use of artificial neural network models. *Atmospheric environment, 191*, 205–213.

Arnaudon, M., Barbaresco, F., & Yang, L. (2013). Medians and means in Riemannian geometry: existence, uniqueness and computation. In *Matrix information geometry* (pp. 169–197). Springer.

Bauschke, H. H., & Borwein, J. M. (1993). On the convergence of von Neumann’s alternating projection algorithm for two sets. *Set-Valued Analysis, 1*(2), 185–212.

Bauschke, H. H., & Borwein, J. M. (1994). Dykstra’s alternating projection algorithm for two sets. *Journal of Approximation Theory, 79*(3), 418–443.
Bersimis, S., & Triantafyllopoulos, K. (2020). Dynamic non-parametric monitoring of air-pollution. *Methodology and Computing in Applied Probability, 22*(4), 1457–1479.

Bigot, J., Charlier, B., et al. (2011). On the consistency of Fréchet means in deformable models for curve and image analysis. *Electronic Journal of Statistics, 5*, 1054–1089.

Bigot, J., Gadat, S., & Loubes, J.-M. (2009). Statistical M-estimation and consistency in large deformable models for image warping. *Journal of Mathematical Imaging and Vision, 34*(3), 270–290.

Bigot, J., Gendre, X., et al. (2013). Minimax properties of Fréchet means of discretely sampled curves. *The Annals of Statistics, 41*(2), 923–956.

Bose, M., Larson, T., & Szpiro, A. A. (2018). Adaptive predictive principal components for modeling multivariate air pollution. *Environmetrics, 29*(8), e2525.

Cano, J., Moguerza, J. M., Psarakis, S., & Yannacopoulos, A. N. (2015). Using statistical shape theory for the monitoring of nonlinear profiles. *Applied stochastic models in business and industry, 31*(2), 160–177.

Carslaw, D. C., & Ropkins, K. (2012). Openair – an R package for air quality data analysis. *Environmental Modelling & Software, 27*, 52–61.

Centofanti, F., Lepore, A., Menafoglio, A., Palumbo, B., & Vantini, S. (2021). Functional regression control chart. *Technometrics, 63*(3), 281–294.

Chicken, E., Pignatiello Jr, J. J., & Simpson, J. R. (2009). Statistical process monitoring of nonlinear profiles using wavelets. *Journal of Quality Technology, 41*(2), 198–212.

Chui, C. K. (2016). *An introduction to wavelets*. Elsevier.

Dubey, P., & Müller, H.-G. (2019). Fréchet analysis of variance for random objects. *Biometrika, 106*(4), 803–821.

Fassò, A., Toccu, M., & Magno, M. (2016). Functional control charts and health monitoring of steam sterilizers. *Quality and Reliability Engineering International, 32*(6), 2081–2091.

Gervini, D., & Gasser, T. (2004). Self-modelling warping functions. *Journal of the Royal Statistical Society: Series B (Statistical Methodology), 66*(4), 959–971.

Goodall, C. (1991). Procrustes methods in the statistical analysis of shape. *Journal of the Royal Statistical Society: Series B (Methodological), 53*(2), 285–321.

Harris, T., Tucker, J. D., Li, B., & Shand, L. (2020). Elastic depths for detecting shape anomalies in functional data. *Technometrics, 1–11.*

Izem, R., Marron, J. S., et al. (2007). Analysis of nonlinear modes of variation for functional data. *Electronic Journal of Statistics, 1*, 641–676.

Jung, S., Dryden, I. L., & Marron, J. (2012). Analysis of principal nested spheres. *Biometrika, 99*(3), 551–568.

Kampelis, N., Papayiannis, I. G., et al. (2020). An integrated energy simulation model for buildings. *Energies.*

Kendall, D. G., Barden, D., Carne, T. K., & Le, H. (2009). *Shape and shape theory* (Vol. 500). John Wiley & Sons.
Kneip, A., & Engel, J. (1995). Model estimation in nonlinear regression under shape invariance. *The Annals of Statistics*, 551–570.

Kravvaritis, D. C., & Yannacopoulos, A. N. (2020). *Variational methods in nonlinear analysis: With applications in optimization and partial differential equations*. Walter de Gruyter GmbH & Co KG.

Le, H., & Kume, A. (2000). The Fréchet mean shape and the shape of the means. *Advances in Applied Probability*, 101–113.

Marchant, C., Leiva, V., Christakos, G., & Cavieres, M. F. (2019). Monitoring urban environmental pollution by bivariate control charts: New methodology and case study in Santiago, Chile. *Environmetrics, 30*(5), e2551.

McGinnity, K., Chicken, E., & Pignatiello Jr, J. J. (2015). Nonparametric changepoint estimation for sequential nonlinear profile monitoring. *Quality and Reliability Engineering International, 31*(1), 57–73.

Moguerza, J. M., Muñoz, A., & Psarakis, S. (2007). Monitoring nonlinear profiles using support vector machines. In *Iberoamerican congress on pattern recognition* (pp. 574–583).

Montgomery, D. C. (2009). *Statistical quality control* (Vol. 7). Wiley New York.

Panaretos, V. M., Zemel, Y., et al. (2016). Amplitude and phase variation of point processes. *The Annals of Statistics, 44*(2), 771–812.

Papayiannis, G. I., Giakoumakis, E. A., et al. (2018). A functional supervised learning approach to the study of blood pressure data. *Statistics in medicine, 37*(8), 1359–1375.

Papayiannis, G. I., & Yannacopoulos, A. N. (2018). A learning algorithm for source aggregation. *Mathematical Methods in the Applied Sciences, 41*(3), 1033–1039.

Paynabar, K., Zou, C., & Qiu, P. (2016). A change-point approach for phase-I analysis in multivariate profile monitoring and diagnosis. *Technometrics, 58*(2), 191–204.

Petersen, A., Müller, H.-G., et al. (2019). Fréchet regression for random objects with euclidean predictors. *The Annals of Statistics, 47*(2), 691–719.

Pittau, M. G., Romano, D., Cirillo, M. C., & Coppi, R. (1999). An optimal design for air pollution monitoring network. *Environmetrics: The official journal of the International Environmetrics Society, 10*(3), 351–360.

Qiu, P., Zou, C., & Wang, Z. (2010). Nonparametric profile monitoring by mixed effects modeling. *Technometrics, 52*(3), 265–277.

Ramsay, J. O., & Silverman, B. W. (2007). *Applied functional data analysis: methods and case studies*. Springer.

Shiau, J.-J. H., Huang, H.-L., Lin, S.-H., & Tsai, M.-Y. (2009). Monitoring nonlinear profiles with random effects by nonparametric regression. *Communications in Statistics: Theory and Methods, 38*(10), 1664–1679.

Small, C. G. (2012). *The statistical theory of shape*. Springer Science & Business Media.

Szpiro, A. A., Sampson, P. D., Sheppard, L., Lumley, T., Adar, S. D., & Kaufman, J. D. (2010). Predicting intra-urban variation in air pollution concentrations with complex spatio-temporal dependencies. *Environmetrics, 21*(6), 606–631.
Voigt, K., Welzl, G., & Brüggemann, R. (2004). Data analysis of environmental air pollutant monitoring systems in Europe. *Environmetrics: The official journal of the International Environmetrics Society, 15*(6), 577–596.

Wahba, G. (1990). *Spline models for observational data* (Vol. 59). SIAM.

Wan, Y., Xu, M., Huang, H., & Xi Chen, S. (2021). A spatio-temporal model for the analysis and prediction of fine particulate matter concentration in Beijing. *Environmetrics, 32*(1), e2648.

Wand, M. P., & Jones, M. C. (1994). *Kernel smoothing*. Chapman and Hall/CRC.

Wang, K., Gasser, T., et al. (1997). Alignment of curves by dynamic time warping. *The annals of Statistics, 25*(3), 1251–1276.

Wang, Y., Finazzi, F., & Fassò, A. (2021). D-stem v2: A software for modeling functional spatio-temporal data. *Journal of Statistical Software, 99*, 1–29.

Xie, X., Semanjski, I., Gautama, S., Tsiligianni, E., Deligiannis, N., Rajan, R. T., . . . Philips, W. (2017). A review of urban air pollution monitoring and exposure assessment methods. *ISPRS International Journal of Geo-Information, 6*(12), 389.

Yu, G., Zou, C., & Wang, Z. (2012). Outlier detection in functional observations with applications to profile monitoring. *Technometrics, 54*(3), 308–318.

Zhao, X., & Del Castillo, E. (2021). An intrinsic geometrical approach for statistical process control of surface and manifold data. *Technometrics, 63*(3), 295–312.