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Analysis of Functional Responses in Experimental Design

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THESIS

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Abstract

The growth of sensor streamed data in recent years increases the demand for an analytical technique to properly address data measured continuously. The design and analysis of experiments (DOE) of U.S. Air Force assets are based off of sensor streamed data. Functional data analysis (FDA) is an approach of analyzing data existing over a continuum. This research aids in filling the intersection of FDA and DOE by examining a case study of an experimental design with a functional response in addition to insight on software capabilities in FDA. The case study considers a functional linear model of a whole-plot from a split-plot experimental design compared to multivariate methods and an approximated functional linear model. Initial results indicate no significant main effects were detected in the case study using FDA. However, a comparison between the different methodologies indicate similar behaviors for main effect estimates. An examination of software packages reveals the R software as most compatible with FDA methodology. Recommendations include another case study evaluation of FDA and future work in alignment of response curves.

To the people who have helped me throughout my entire life. The lessons learned from you are invaluable and I dedicate this work to you

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I would like to express my sincere gratitude to my advisor Dr. Hill. I could not be where I am now without your guidance. Thank you and I look forward to our future academic endeavors.

Matthew E. Scherer

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ANALYSIS OF FUNCTIONAL RESPONSES IN EXPERIMENTAL DESIGN

I. Introduction

This chapter serves as an introduction to the analysis of a functional response in an experimental design. It begins with the motivation for the problem by identifying current gaps in existing methodologies of experimental design with a functional response and then addresses the problem through several research questions.

1.1 Motivation and Background

The advancement in technology over the recent decades have led to precise observations being taken in quick succession to each other. Measurements can now be recorded beyond human perception in research areas such as audiology, biology, ergonomics, economics, meteorology, and physiology (Zhang, 2013). Approximating these sources of measurement in aggregate statistics greatly reduces the information given from the data itself and present poor data to models in machine learning, experimental design, stochastic processes, etc. In experimental design, the response can be measured at a high enough frequency to create a functional response. This capability to measure at such a high frequency implies the assumption of an underlying curve to be approximated. Based on this assumption, functional data analysis (FDA) methods are implemented to take advantage of the assumed curvature presented in the response (Ramsay and Silverman, 2005).

This research focuses on implementing a FDA methodology into an experimental design to show FDA as a useful methodology for analyzing response curves. Responses are generally examined through use of aggregate statistical methods and lose

possible information gained in the experimental design. The design and analysis of experiments is advantageous due to its design run structure to efficiently create a factorial design. However, information is lost in analysis by summarizing an entire design run duration into a single statistic. By integrating a FDA approach, more precise effects can be measured in designed experiments with longitudinal data.

This research also examines the capability of software packages available to USAF operations research analysts and correct implementation of FDA methods into testing and evaluation tactics, techniques, and procedures (TTP). The software packages are compared based upon their capabilities, ease of use, as well as other considerable features. The software packages examined are based on their accessibility to an United States Air Force Operations Research Analyst. Some resources included are open-source and require further discussion from a data sensitivity point of view. However, this research focuses only on the implementation of a FDA methodology.

A case study is used to provide insight between different methodologies used for experimental design and FDA. The data are based upon a split-plot design with 1 whole plot and 6 subplot factors. A single whole plot is analyzed to avoid discrepancies in the error structure. The response is the oxygen percentage measured across the duration of the entire test. In the test examined, oxygen percentage is a physiological demand that must be maintained to remain vigilant and not succumb to hypoxia. A functional linear model is an appropriate test for this design. For comparison, the mean of each response curve is examined as well as the mean of each response curve at each second of the response curve.

1.2 Problem Statement

The primary objective of this work is to find characterizations of experimental design response data using functional data analysis through smoothing methods uti-

lizing popular software packages. In addition, different software packages capabilities and insights are compared.

1.3 Research Questions

This study addresses the following research questions on correct implementation of functional responses into current testing and evaluation methodologies.

Question 1

What is an effective way to characterize functional response data in an experimental design?

Question 2

How do different available software packages compare in being able to handle functional response data?

1.4 Organization of the Thesis

This thesis is comprised of 5 chapters including chapter 1 as the introduction. Chapter 2 is a literature review of prominent procedures used in experimental design and functional data analysis in a military context. Chapter 3 is an organized description of the methodology implemented as a factorial design with a functional response. Chapter 4 provides insights on software packages with a short discussion and chapter 5 puts these results into final conclusions and recommendations for decision makers. Chapter 5 also contains future research possibilities.

II. Literature Review

This chapter provides background on seminal and subsequent work in the domains of experimental design and functional data analysis, creating a basis for understanding this research and its goals. Sections one and two explain the general concepts of experimental design and in particular its applications in military systems. Sections three, four, and five provide general concepts of functional data, the methods for the analysis of functional data, and FDA's implementation into military systems, respectively. Section 6 depicts a combination of the two spheres with experimental design with a functional response.

2.1 Concepts of Experimental Design

Design and analysis of experiments (DOE) began with the pioneering work of Sir Ronald A. Fisher (Box, 1980). Experimental design originates in the scientific method by correctly implementing an experiment to find causation of a factor to a measurable response. One traditional experiment involves manipulating a single factor and observing the effect on a designated response while holding all other factors constant. This technique of one-factor-at-a-time (OFAT) testing is not an efficient use of resources for an experiment because it ignores interactions among factors. Czitrom (1999) compares DOE to OFAT experiments. The benefits of DOE over OFAT experiments include less resources used to produce factor effect estimates with higher precision and the ability to estimate factor interactions. Finally the factor space is larger resulting in lower variance in the response and therefore optimized test building process.

The use of factorial experiments is an advantage of DOE because it creates an improved feature space with higher precision at a lower resource cost. The use of

three main principles of DOE contribute to the strength of DOE over OFAT experiments. The basic principles of experimental design are randomization, replication, and blocking (Kirk, 2012). Randomization of the experimental runs helps to validate the assumptions of independent, normally distributed errors with equal variance while also reducing the effects of any error due to extraneous factors (Montgomery, 2017). Replication provides improved precision estimates of factor effects and estimates of noise, or error, to help distinguish the signal in an experiment from the error. Blocking is a technique to reduce the effects of nuisance factors that create variability between groups. Experimental design has had significant impacts on multiple fields from life sciences to engineering or even the taste testing of a new soft drink. Montgomery (2017) provides a basis of the overview of design and analysis of experiments for full and fractional factorial designs with multiple resolutions.

Fractional factorial designs are a subset of factorial designs that provide cause and effect relationships associated with lower-order effects with fewer observations (Montgomery, 2017) when compared to the full factorial experiment. However, the fractional factorial design suffers from a lower resolution and therefore aliasing between interactions can cause ambiguity on the interpretation of interactions and their effect on the response. The resolution determines how many factors in an interaction are aliased with each other. In general a higher resolution test contains less aliasing and therefore distinguishable factor interaction effects. The use of fractional factorial designs allows general cause and effect relationships associated with lower order effects to be discovered and then explored in greater detail using a sequential design approach.

The myriad experimental designs to help manage and expend test resources efficiently, such as the split-plot design. The origin of the split-plot design comes from an agricultural setting containing factors extremely difficult to change quickly (hard-

to-vary) compared to other easy-to-vary factors (Yates, 1978). The randomization paterns are such that the hard-to-vary factors do not change as frequently as the easy-to-vary factors. This means there are two estimates of error, the whole plot and the sub plot error (Bisgaard and de Pinho, 2004). The convenience of the split-plot design compromises with the randomization constraint to create less power for detecting effects in the hard-to-vary factors. This design creates a convenient randomization process but in exchange for less efficiency and power. The split-plot design does require specialized analytical methods as the randomization restrictions create the sources of error.

Myers et al. (2016) provides methodologies for different response surfaces in experimental design as catalyzed by Box and Wilson (1951). Response surface methodology (RSM) is used to find an approximation of the optimal response by systematically adjusting the factors in the design. Typically, a second-degree polynomial is used as an approximation that requires a three level factorial experiment. However, the central composite design (CCD) introduced by Box and Wilson (1951) provides the benefit of using the center points collected in the experimental design to estimate the second-degree polynomial. RSM in DOE often uses sequential experimentation beginning with a possible screening model followed by optimization and gradient ascent to move the experimental design region into an area of having an estimated optimum operating condition. Therefore, RSM is usually used after a smaller subset of factors have been found as significant and insignificant factors are not examined in the optimization phase.

Freeman et al. (2013) provide a framework of how to conduct an experimental design and explain the basic procedures of planning experiments within the context of the scientific method. Similar step-by-step tutorials have been generated by (Coleman and Montgomery, 1993). In these descriptions, the following steps are summarized

as:

1. Define the Problem
2. Select Response Variables
3. Identify Sources of Variation
4. Choose the Experimental Design
5. Train Experimenter/Conduct the Experiment
6. Analyze the Data
7. Conclusions/Recommendations

The main focus of this research is how to analyze the data from an experimental design with a functional response.

2.2 Experimental Design in Military Systems

The United States Department of Defense (DoD) has been using experimental design to test weapons capabilities, logistic designs, and even human subject experiments. However, there is significant re-emphasis of the method for DoD testing. The DoD created the Scientific Test and Analysis Techniques (STAT) Test & Evaluation (T&E) Center of Excellence (COE) to provide assistance across the DoD to properly conducting experimental designs (of Defense, 2012). The benefits of factorial designs, and other non-standard experimental designs, such as higher precision with less resources used are useful to the DoD. These benefits make factorial designs common as well as split-plot design in order to be flexible in resource use (e.g., see Cohen, 2009; Lee, 2010). The range of applications of DOE to the DoD is immense. For example the United States Army used a fractional factorial design to discover factors

that made Military Operations in Urban Terrain (MOUT) teams most effective Herl et al. (2005). In the United States Air Force (USAF) there exists two main branches in the test and evaluation community. Operational Test and Evaluation (OT&E) has a focus on determining how well a system would do in a realistic setting. Developmental Test and Evaluation (DT&E) is less focused on performance and instead tries to discover and learn about the system (Freeman and Warner, 2018).

Science and engineering create many applications for DOE and therefore the DoD. In the USAF specifically, a large portion of USAF assets are advanced technology developed through contracts that require complete testing to validate. Johnson et al. (2012) gives an excellent overview of the correct implementation of DOE into the DoD. There exists a large volume of general tutorials of other implementations of DOE (e.g., see Freeman et al., 2013; Simpson et al., 2013). These overviews include the different types of factorial designs, the motivation to using them, how to pursue optimal conditions using RSM, and several case studies. The research also suggests that the new era of designed experiments involves using computer simulation as the system being examined compared to traditional tangible systems as examined in wind tunnels (Leggio, 2009). Two examples of this new era include Hill et al. (2015) as an example of using metamodels of simulations to discover significant factors in a complex repair network for the F-15 and F-16. Another example includes Hodson and Hill (2014) where live, virtual, and constructive (LVC) simulation is used to facilitate weapon systems testing at a significantly lower cost compared to using live assets.

2.3 Concepts of Functional Data Analysis

Functional data analysis (FDA) use has grown recently at a significant rate. High frequency measurements are recorded implying an assumed function exists as Ramsay

and Silverman (2005) suggest instead of a typical one to one mapping structure in cross-sectional data. Even data not measured at high frequencies are also functional through a transformation from discrete to continuous such as growth studies. Smoothing techniques are typically used for the transformation, particularly basis functions such as the Fourier basis transform, spline basis, or the wavelet transform (e.g., see Ramsay and Silverman, 2005, 2007). The different basis functions are unique to the data being examined but account for information within the raw data compared to interpolation techniques. Ramsay and Dalzell (1991*a*) present several practical reasons to consider FDA:

- Functional observations are appearing more often in applied contexts than previously envisioned because of advancements in research.
- Some problems are more natural as functions even though their observations exist as a finite count.
- Functional data has the advantage of differentiability to conduct analysis.
- FDA takes into account smoothness that effects sequential analysis.

FDA has several advantages compared to multivariate data analysis (MDA). In time series data for example, high correlations existing between measurements in MDA disrupts key assumptions to MDA techniques such as the assumption of stationarity in autoregressive integrated moving average (ARIMA) models. However FDA treats the entire curve as a function therefore erasing the issue of autocorrelation as explained in Ramsay (1982) and Ramsay et al. (1988). In addition Zhang (2013) provides difficulties in MDA situations including:

- The number of sampling time points in a curve are not the same across different curves. An example would be comparing a curve based off of 100 time points compared to 10 time points.

- The sampling time points are not homogeneous. The difference of when a sample is collected does not have to be exactly the same for each sample.
- The number of sampling time points is more than the number of observations. An example would be the stock prices collected every second for the 500 stocks in the S&P 500 in a day (23,400 seconds).

All of these scenarios can be handled using FDA techniques such as data smoothing, curve registration, and functional dimensionality reduction.

To handle a problem with FDA, the methodology outlined in Ramsay et al. (2009) and Ramsay (2003) is summarized as:

1. Convert the data from a discrete form to a functional form.
2. Align the curves if necessary using data registration.
3. Graph the functional data (may include phase-plane plots).
4. Explore variability in the functional data.
5. Create a model based off of desired goal.

The conversion of data from discrete to a functional form is done through two methods. Interpolation is used if the observations are assumed to be errorless. However if there is an observational error then a smoothing technique is required. The smoothing technique is performed in a basis expansion such as

$$x(t) = \sum_{k=1}^{K} c_k \phi_k(t) \tag{1}$$

where $\phi_k(t)$ is a vector containing the k basis functions and $c_1, c_2, \ldots, c_K$ are the coefficients of the expansion. Popular basis functions from Ramsay and Silverman (2005) suggest splines (regression splines, polynomial splines, B-splines, P-splines)

for non-periodic data, the Fourier basis for periodic data, and wavelet basis for data with rapid changes and/or discontinuities. Ullah and Finch (2013) reviewed 84 FDA articles and found that B-spline basis were most prevalent due to their ability to handle non-cyclical data. A popular example of functional data is growth studies, in particular the Berkeley growth study conducted by Tuddenham (1954) recorded the heights of 54 girls and 39 boys from ages 1 to 18. To convert the data to a functional form, an 6^{th} order penalized b-spline basis with 31 knots and roughness parameter $\lambda = 10^{-0.5}$ are fit to the 54 observations of girls recorded as recommended in Ramsay and Silverman (2005) and Kokoszka and Reimherr (2017). The resulting curves are shown in Figure 1.

Data registration is the process of aligning the records to have important features in a curve at similar argument values. There are two separate axis for this alignment to occur. Registration in vertical amplitude variation and in horizontal or phase variation. Two registration methods from Ramsay (2003) use landmark features in a curve or use continuous registration. An example of a functional dataset requiring registration is examining the acceleration curves of the Berkeley growth study shown in Figure 2a. In these acceleration curves both amplitude and phase variation are present. To address both variations Kokoszka and Reimherr (2017) recommend continuous registration using warping functions to align the curves so they are closer to their mean curve, shown as the black curve in Figure 2a. The final resulting curves are shown in Figure 2b. The phase variation is noticeably reduced but there is a definitive amount of amplitude variation still present.

Graphing the functional data is the equivalent of exploratory data analysis found in multivariate methods. A general plot of the curves across their varying input t in Equation 1 is a typical starting point. Other graphical techniques include the phase-plane plot. Phase-plane plots are used to show the interactions between derivatives

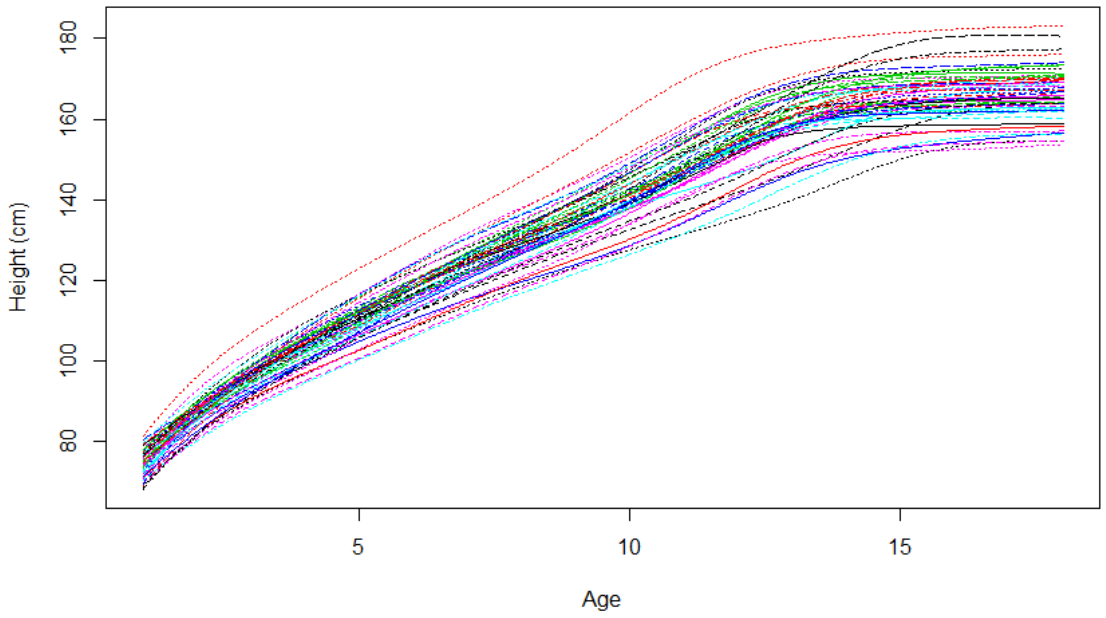
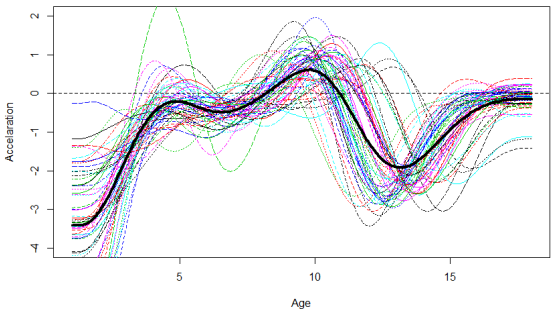
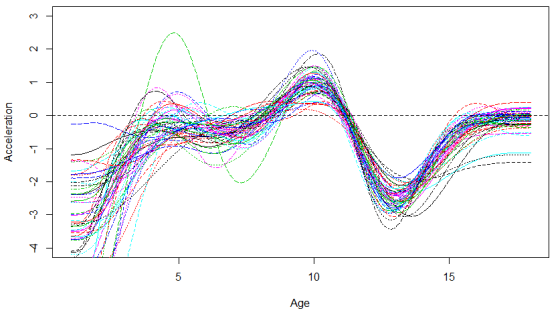


Figure 1. Smoothed Growth Curves of 54 Girls Using Penalized B-spline Basis



(a) Acceleration Curves of 54 Girls Heights Without Registration



(b) Continuously Registered Acceleration Curves of 54 Girls Heights

Figure 2. Acceleration Curves of the Girls in the Berkeley Growth Study, With and Without Registration

in a function. They are typically used as a descriptive technique to gain initial insight to how features interact within the curves examined. In the Berkeley growth study the phase-plane plot for the first 10 girls without regularization is shown in Figure 3.

Exploring the variability in the data gives insight on what factors are the main sources of variation present in the curves. Functional principal components analysis (FPCA) is a popular technique, but there are other methods such as functional canonical correlation analysis (FCCA) or functional principal differential analysis (FPDA). Functional principal component analysis behaves similarly to the multivariate case of principal component analysis (PCA). Overall FPCA examines the covariance structure within the data which may indicate a lower dimension set of principal components can explain the majority of the variation contained in the data. Silverman et al. (1996) has a detailed methodology of using smoothed FPCA to simultaneously estimate the principal components and the smoothing parameter.

The final portion of an FDA methodology is to fit the functional data to some model. Functional models may exist with functional input to discrete output, discrete input to functional output, or functional input to functional output. A brief overview of how to handle each of these combinations is covered in Kokoszka and Reimherr (2017). Similar to multivariate analysis, linear models are a conventional approach to inference and prediction. Popular methods examined by Ullah and Finch (2013) and Matsui et al. (2008) include functional linear models. Functional linear models are used to find significant effects on the functional response. In addition, functional generalized linear models have been examined in James (2002). Functional multilayer perceptrons are even proposed in Wang et al. (2019). The particular method in this study is analysis of variance (ANOVA) for functional data. Hypothesis tests are developed and explained by Zhang (2013) by explaining constant and heteroskedastic ANOVA. This analysis is also performed, primarily in MATLAB, which gives another

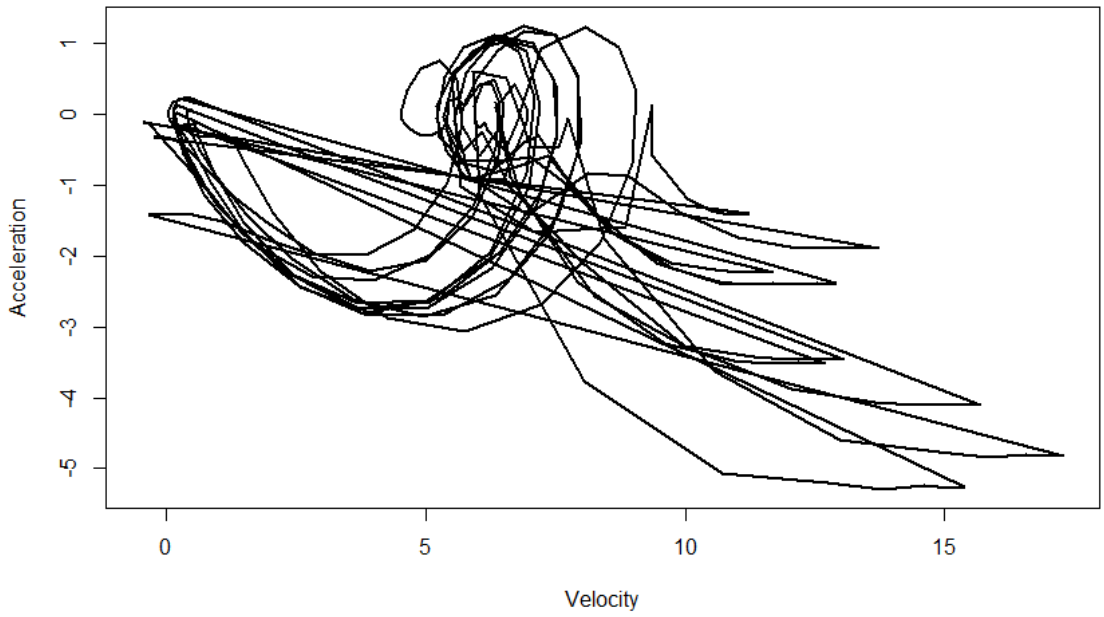


Figure 3. Phase-plane Plot for Girls in Berkeley Growth Study

software package for exploration in this domain. Febrero Bande and Oviedo de la Fuente (2012) provides an overview of the packages available within the R software.

2.4 Functional Data Analysis in Military Systems

It seems a large amount of military functional data has not been examined in functional methods. In particular, functional data is prevalent with weather data, testing and evaluation measurements, personnel data, etc. However the literature applying FDA methods to such a military system is sparse . For example, in Din et al. (2011) FDA is applied to gait data of Malaysian military personnel carrying additional loads. This research examined the weight bearing effects on the personnel by using a B-spline, curve registration, and permutation test. The research also concluded that FDA is a superior technique for gait analysis. Similar examples are examined in Ramsay and Silverman (2007).

Sensor streamed data for a turbofan aircraft engine are examined in Liao and Sun (2011) indicates their findings using FDA have value in military applications. In the research, a two-staged approach is applied where the functional principal component analysis (FPCA) is applied to determine functional principal component scores as inputs into a functional regression model. The research highlights the advantages of using FDA over artificial neural networks in sensor data as examined by Guo and Nurre (1991).

2.5 Experimental Design with a Functional Response

Functional data is used in a multitude of settings. The breadth and depth of the different functional data techniques are similar to multivariate analysis. Each technique is specific to the goal and form of the data. To remain at a superficial level, functional models only pertaining to experimental design are examined. The use of functional analysis of variance (FANOVA) is popular in experimental design because it allows for multiple comparisons between experimental groups. Experimental designs exhibit discrete inputs in the factor levels and can contain a functional response. Faraway (1997) proposes the use of a L^2-norm-based test with a bootstrap resampling method to approximate the null distribution. In addition, Faraway (1997) discusses the use of regression models for inference, prediction, and residual analysis of a functional response. FANOVA is discussed in Ramsay and Silverman (2005), who adopt the pointwise F-test. Zhang (2013) summarizes the pointwise, L^2-norm-based, F-type, and bootstrap tests. Each test is best suited for the shape of the distribution or number of observations. In each test the general hypothesis for the main effect test of a one-way FANOVA is:

$$y_{ij}(t) = \eta(t) + \alpha_i(t) + \nu_{i,j}(t), j = 1, 2, \ldots, n_i; i = 1, 2, \ldots, k \tag{2}$$

where $\eta(t)$ is the overall mean function of the k treatments, $\alpha_i(t)$ is the main effect of treatment i, and $\nu_{i,j}$ is the error function for each observation n.

Extensions of FANOVA models have been examined such as Zhang (2013) describing a heteroskedastic FANOVA model by using an extension of the Behrens-Fisher problem detailed in Zhang et al. (2010). The approach is more computationally expensive then using a pooled covariance function estimate because it requires a separate calculation of each covariance function.

Other models besides FANOVA in DOE exist such as the functional mixed-effects model. Mixed effect models are comprised of fixed and random effects and are used in split-plot experimental designs. Saleh (2015) describes how to build an D-optimal experimental design to conduct analysis on a functional response when using a mixed-effects model. An early example of smoothing the response with a b-spline basis and then estimating the regression coefficients using a mixed-effects model is proposed in Del Castillo et al. (2012). In addition, the mixed-effects model is discussed through the methodology of examining a split-plot design as seen in Zhang and Großmann (2016).

III. DOE with a Functional Response Case Study

3.1 Introduction

Interest in the analysis of functional data has grown significantly recently due to the large influx of sensor-streamed data. Data are considered functional in nature if they can be represented as a continuous curve instead of discrete observations. Functional data can be from sparse or densely collected data frequencies across a continuum. Common areas of FDA include economics, growth studies, weather analysis, behavioral sciences, and other time-series based data. The monograph by Ramsay and Silverman (2005) provides an overview of typical analytical tools used in functional data analysis.

FDA provides several distinct benefits compared to traditional multivariate statistical techniques. Wang et al. (2016) explains the key differences between the two areas of statistics. Multivariate analysis only handles finite-dimensional random vectors while functional data are inherently infinite-dimensional. Functional data are assumed to be smooth functions compared to multivariate where smoothness is not even a consideration. Functional data analysis benefits include examining sparsely observed data using its nonparametric techniques. Smoothing is handled through basis expansions which may include penalization, local polynomial kernel smoothing, and functional principal component analysis. Proper smoothing translates discrete data into a functional data object. A functional data object can then be manipulated to conduct exploratory data analysis by examining its derivatives, conducting functional principal component analysis Rice and Silverman (1991), and curve registration Gervini and Gasser (2004).

After converting into a functional data object and conducting initial analysis, functional modeling techniques can be applied. While the literature of functional

models is rich, Kokoszka and Reimherr (2017) provide a baseline introductory level of the main three broad categories of functional regression models.

To begin, the fundamental linear regression model (3) is examined with x_{ij} are the discrete data points and β_j are the effect estimates.

$$y_i = x_{i1}\beta_1 + x_{i2}\beta_2 + \cdots + x_{ij}\beta_j + \epsilon_i \quad i = 1, 2, \ldots, N \tag{3}$$

Functional linear models have a similar structure but the variables and coefficients can exist as a function. In the case of scalar-on-function regression (4), the scalar response Y_i contains a functional regressor $X_i(s)$ and effect estimate $\beta(s)$.

$$Y_i = \int \beta(s)X_i(s)ds + \epsilon_i \tag{4}$$

Function-on-scalar regression is the case of the regressors as discrete vectors X_{ij} while the effect estimates $B_j(t)$ are curves (5).

$$Y_i(t) = \sum_{j=1}^{p} x_{ij}\beta_j(t) + \epsilon_i(t) \tag{5}$$

The third main category of functional regression models is function-on-function regression, where the regressors $X_i(s)$, the effect estimates $\beta(t, s)$, and the response $Y_i(t)$ are curves (6).

$$Y_i(t) = \int \beta(t, s)X_i(s)ds + \epsilon_i(t) \tag{6}$$

This work examines use of an experimental design applied to a functional response, inferring a function-on-scalar regression model. A functional regression model is used to estimate effect estimates and find statistically significant factors effecting the response curve. In addition, this model undergoes a residual analysis to validate model

assumptions.

A majority of the literature of functional data analysis involves its influence in observational studies but the analytical techniques can be extended into a designed experiment. Faraway (1997) provides the basis for a full analysis of a scalar-on-function regression model with model creation, hypothesis testing, and residual analysis for an ergonomic case study. Saleh (2015) provides key insights into the design of optimal experimental designs with a functional response but the focus is on creating an optimal design and not on the analysis. Zhang (2013) explains the functional ANOVA (FANOVA) model and describes a case study of a split-plot design in Zhang and Großmann (2016). The FANOVA model is of interest in experimental design when handling categorical factors. The use of continuous factors provides prediction capabilities at values between the observed levels of a factor. Therefore a functional regression model is examined in this case study.

The particular methodology examined to perform functional data analysis is based on Ramsay and Silverman (2005). The model is generated by first creating a functional object for the response curves. The particular details for this process are explained in Ramsay et al. (2009) but models are typically fit with a basis such as a Fourier basis for periodic data or a b-spline basis. The basis is then smoothed by using a penalty function on the model to encourage a smoother fit to reduce noise within the data. This smoothing parameter is determined by examining the generalized cross validation score of a grid search approach to basis fitting with different penalty values. Finally, the process of curve registration is used to reduce unwanted variation between response curves. Once a functional object is created for each of the response curves, exploratory data analysis involves the use of functional principal component analysis or summary statistics. The response curves are fit to a functional response model with the desired covariates included in the model. This final model is

examined compared to a permutated null distribution to estimate its significance and the functional principal component scores of the residuals are examined to validate model assumptions. The explanation of these diagnostics of the model are found in Chiou and Müller (2007) while the test statistic is explained in Ramsay and Silverman (2005). This work is an example of functional data analysis and how it relates to the analysis of designed experiments in a multivariate setting.

3.2 Case Study

3.2.1 Introduction

This work examines the effect of different factors on the oxygen percentage of an United States Air Force (USAF) piloted flying asset. Oxygen percentage is an important characteristic to examine in USAF assets to avoid hypoxia. In flight testing oxygen percentage is examined across time for the duration of each test conducted. Different methods are examined to characterize the response curves. Initially the response curves are aggregated into an average, followed by examining the response curves at discrete time steps, then finally examining each response curve as a function. Of the six factors, only one factor is statistically significant in the aggregate model at the $\alpha = 0.1$ level. The other methods examined coincided with this result when examining the effect estimates but did not find any statistically significant results effecting the oxygen conditions for the pilots. This case study provides an overall approach of how to handle designed experiments with a functional response by different levels of model complexity.The models are compared based on their results, efficiency, and ability to handle all the information present within the response curves.

3.2.2 Background

Hypoxia is a physiological condition where not enough oxygen is being delivered to tissues within the body. A shortage of oxygen supply in a pilot creates hazardous flying conditions. On-Board Oxygen Generating Systems (OBOGS) exist to create an reliable oxygen supply for pilots. This study examines the reliability of the OBOGS to find its behavior under multiple flying conditions. The oxygen percentage reported is measured for the entire duration of the flight. 16 flights are used to screen to whether any of the six factors are statistically significant. Each of the 16 response curves are shown in Figure 4

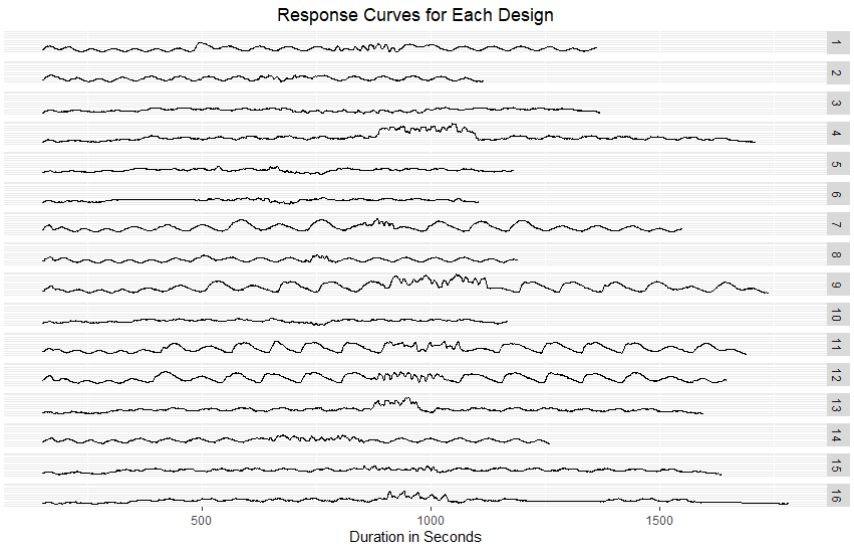


Figure 4. Response Curves for Each of the 16 runs in the Design

3.2.3 Multivariate Linear Regression

Traditional multivariate Analysis of Variance (ANOVA) tests are conducted to find the statistically significant factor affecting the aggregate response. The mean response is selected but other aggregate statistics are possible. Figure 5 is an example of a single test run and the characteristics of its response curve. In addition the effect

estimates for the main effects of the six factors are examined for comparison to the other techniques examined.

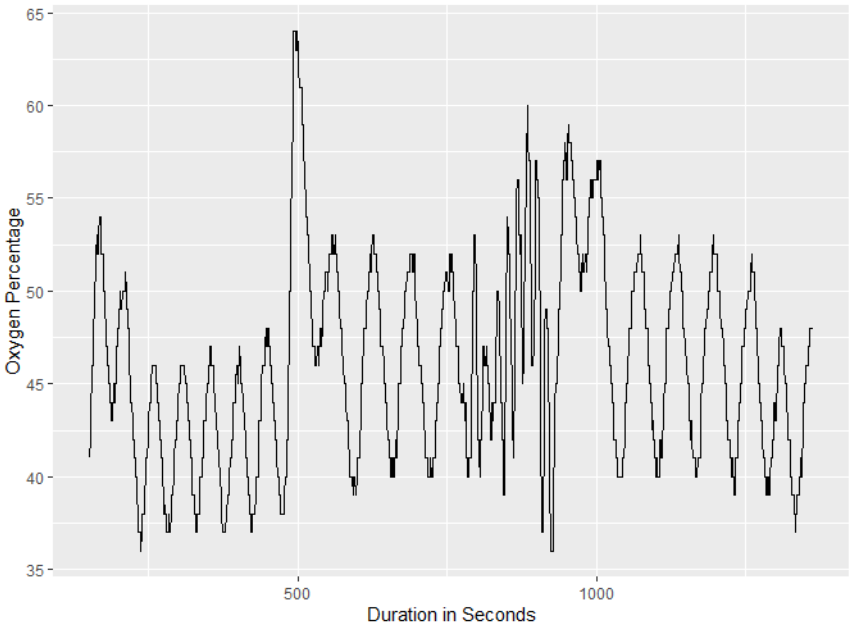


Figure 5. First Design Run Response Curve

The initial ANOVA model examined including the main effects is:

$$Y_i j = \mu + \tau_i + \epsilon_{ij} \quad i = 1, 2, \ldots, a \;\; j = 1, 2, \ldots, n \tag{7}$$

with the appropriate hypotheses:

$$H_0 : \tau_1 = \tau_2 = \ldots \tau_a = 0 \tag{8}$$

$$H_1 : \tau_i \neq 0 \quad \text{for at least one i,} \tag{9}$$

where a is the number of factors, n is the number of observations for each factor, μ is the overall mean, τ_i is the i^{th} factor effect, and ϵ_{ij} is error. The overall F-test did not find any statistically significant evidence of a significant model at the $\alpha = 0.05$. To compare the main effect estimates between models, the ANOVA table found in

Table 1, indicates factor C is statistically significant at an $\alpha = 0.10$ with no other factors providing any evidence of a significant effect on the response.

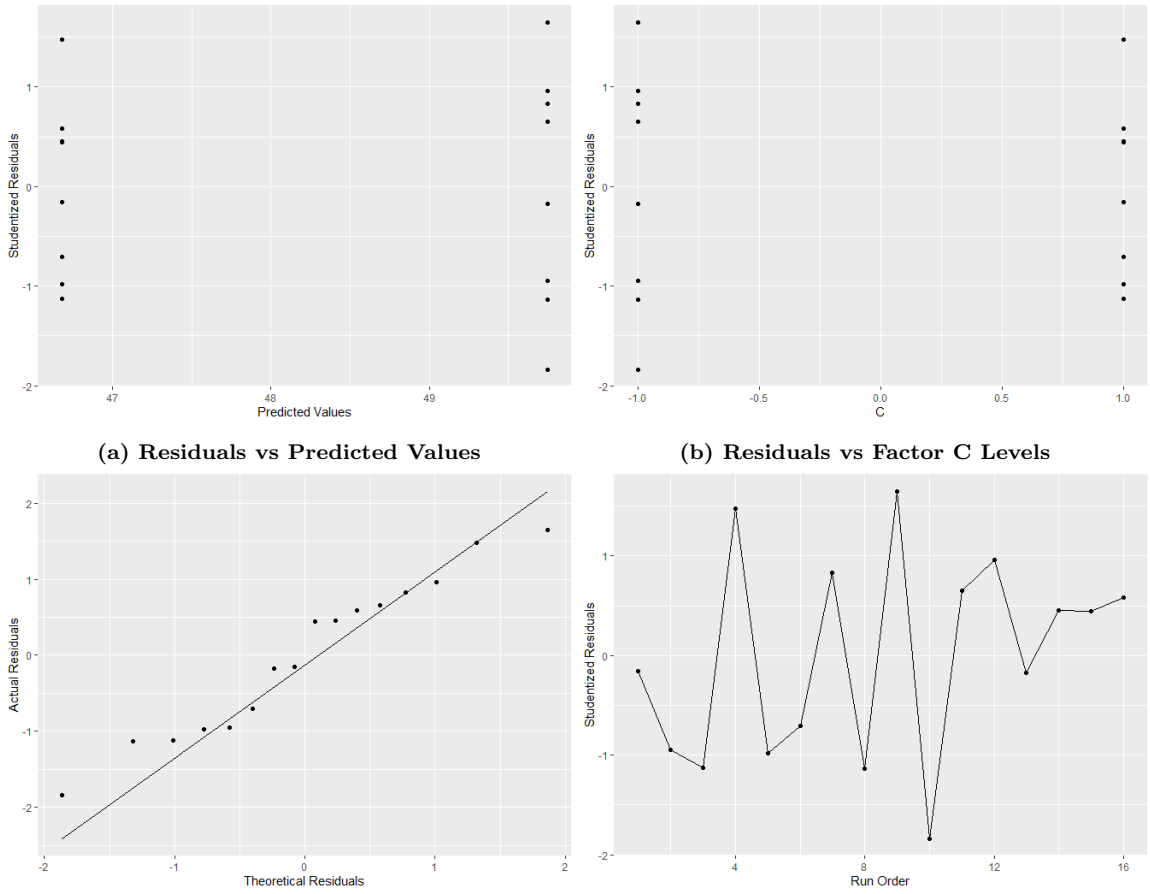
Table 1. ANOVA Table for Mean Response

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
A	1	6.32	6.32	0.46	0.5137
B	1	14.33	14.33	1.05	0.3329
C	1	53.39	53.39	3.90	0.0797
D	1	0.12	0.12	0.01	0.9276
E	1	12.77	12.77	0.93	0.3593
F	1	0.04	0.04	0.00	0.9561
Residuals	9	123.16	13.68		

The final model $Y = \mu + \tau_c$ included only factor C with an estimated effect of -1.5% (90% C.I. [-3.08,-0.01]). The assumptions of the linear regression model are validated through visualization of the calculated errors. Figure 6 illustrates the model assumptions of independent errors with constant variance and following a well behaved distribution. The assumption of constant variance is validated by examining Figures 6a and 6b. The two plots are the studentized residuals plotted against the predicted values and the studentized residuals against the factor levels included in the final model. The normal probability plot in Figure 6c indicates the errors follow a normal distribution by the lack of evidence of non normal residuals. Finally the assumption of independence is not violated as illustrated by Figure 6d and the random behavior between observations. Overall there is no evidence of violations of the assumptions of the linear regression model.

3.2.4 Approximated Functional Regression

To estimate the effect curves across a continuum, an approximated functional regression model is implemented. The model is composed of a sequence of discrete linear models formulated at each time step t. The effect estimate curves are approximated by gathering the effect estimates at each time step t. The estimated effect



(a) Residuals vs Predicted Values

(b) Residuals vs Factor C Levels

(c) Normal Probability Plot of Residuals

(d) Residual vs Run Order

Figure 6. Validation of Model Assumptions of Constant Variance (6a,6b),Well Behaved Distribution (6c), and Independence (6d)

curves provide inference regarding behavior of the response curve at any discrete moment and are evidence for a model with functional covariate estimates. However, the ability to examine statistical hypothesis testing is hindered by inconsistent error estimates between each discrete time step. This approximated functional regression model serves to help bridge the connection between a functional regression model and a strictly scalar linear regression model.

$$Y(t) \approx \sum_{j=1}^{P} \beta_{tij} X_{tij} + \epsilon_t \quad t = \{1, 2, \ldots, n\} \tag{10}$$

The model included only the main effects of the factors. Figure 7 illustrates the

approximated effect estimates. The visualization depicts the approximated curves as continuous functions but they exist as discrete values stringed together for closure. Estimating the effect at a non-discrete multiple of t requires linear interpolation. In this particular case, the time step is one second and only the overlapping time segments of each design run are examined. The pattern for each effect estimate appears irregular but also exhibits a sinusoidal behavior similar to Figure 4. A closer examination of the effect estimate compared to the null hypothesis of no effect detailed by the solid black line reveals evidence of nonzero effect estimates. For example in Factor C a negative effect is evident for the majority of the examined time span.

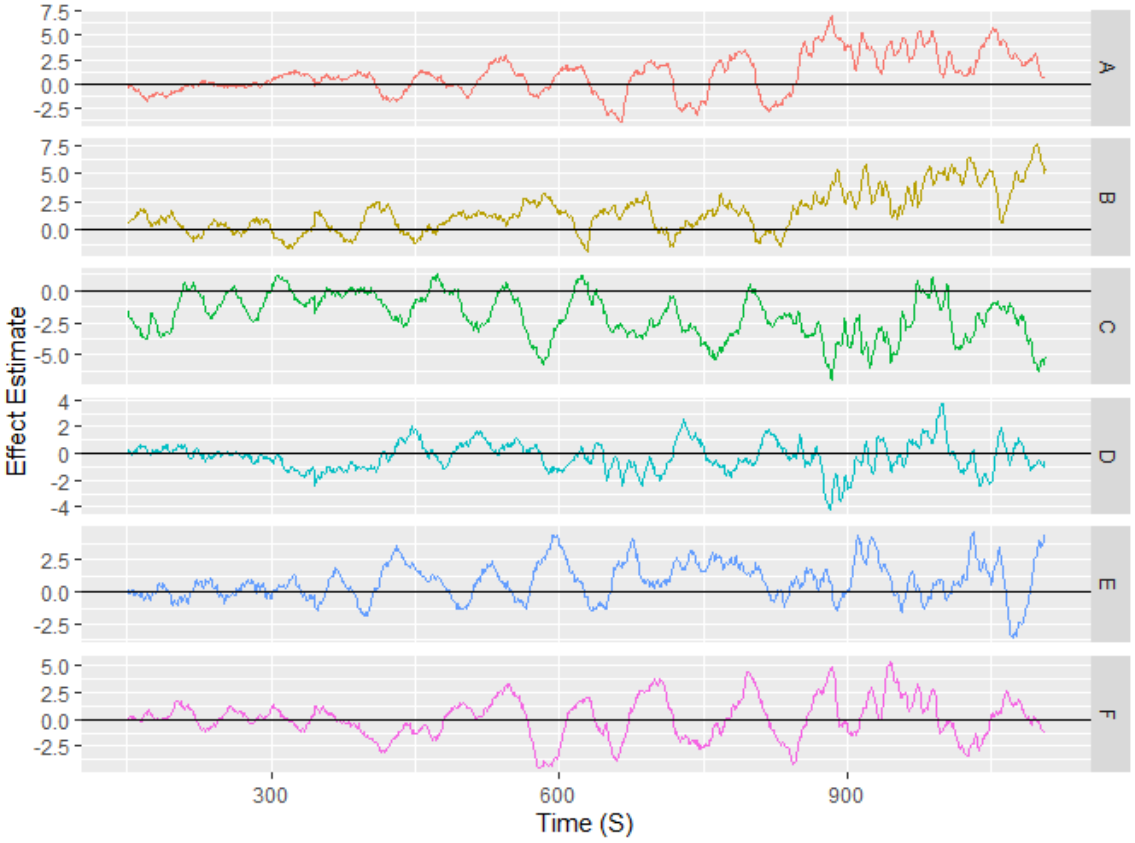


Figure 7. Approximated Effect Estimates

Validation of the linear regression assumptions through residual analysis in the approximated functional regression case is unexplored. The residual analysis previously

examined is performed through visual representations and inspecting for patterns. An issue occurs because the approximated functional regression model is comprised of t regression models with each model having their own set of assumptions that need to be examined. Recreating Figure 6 for each discrete time step t is impossible to visualize and inspect. An alternative solution is to perform a series of statistical tests for the assumptions of independence, constant variance and following a well-behaved distribution within the model errors. For example a Durbin-Watson test with a $t-1$ auto-correlation recorded at each time step t for the assumption of independence. However this process is still flawed because the response curves contain a repeating pattern and cannot be corrected using a $t-n$ lag. In conclusion, the lack of validity of residual analysis in the approximated model stresses the importance of utilization of a functional model.

3.2.5 Functional Regression

The functional regression model methodology from Ramsay and Silverman (2005) and Ramsay and Silverman (2007) is the basis for this analysis. The approach is related to generalized additive models examined in Hastie and Tibshirani (1990) since only main effect estimates are included. The main effect estimates provide inference on the response curve behavior and a pointwise F-statistic described in Zhang (2013). Residual analysis is conducted through processes described in Chiou and Müller (2007). To begin, the model examined includes all main effects as:

$$Y(t) = \beta_0 + \beta_1(t)x_1 + \beta_2(t)x_2 + \beta_3(t)x_3 + \beta_4(t)x_4 + \beta_5(t)x_5 + \beta_6(t)x_6 + \epsilon. \quad (11)$$

To effectively estimate the main effect curves, a 6^{th} order b-spline basis with a knot for every time step is fit to the response curve. The resulting curve is then truncated

for comparison to the approximated functional regression model. This truncation serves as a registration technique by aligning the curves for the 16 design runs. Curve registration reduces the noise between observations to distinguish the signal present for each of the design runs. The six effect estimate curves were constructed with 6^{th} order b-spline basis to allow for the curvature present in the approximated regression model. A Fourier basis is another alternative but does not perform as well if the starting and ending value is different as expected with the case study examined. Other basis functions are possible, and are elaborated in Ramsay and Silverman (2005), including penalized methods or local polynomial kernel smoothing.

The functional effect estimates are plotted in Figure 8 and have a irregular behavior similar to the approximated effect estimates in Figure 7. These effect estimates are generated from a 6^{th} order b-spline basis with 100 knots. Increasing the knots to a higher frequency such as in the response curve drastically increased the computational efficiency of generating the effect estimates. The distinguishable patterns are a minor effect on the response in the initial portion of the test then much larger effect estimates as time progresses. Factors B, C, and E show a large negative effect for the ending portion of the test while factor A provides a positive effect. These patterns are consistent with the approximated model except that factor B provided a positive effect as seen in Figure 7.

A pointwise F-statistic is calculated for the response curves. The null hypothesis for the test is:

$$H_0: \quad \beta_1(t) = \beta_2(t) = \beta_3(t) = \beta_4(t) = \beta_5(t) = \beta_6(t) = 0. \tag{12}$$

For each time step t, an F-statistic is computed. The hypothesis test is shown in Figure 9. The collection of these F-statistics form a function $\hat{F(t)}$ (represented by the blue/darker line). The distribution of $\hat{F(t)}$ is unknown and is approximated

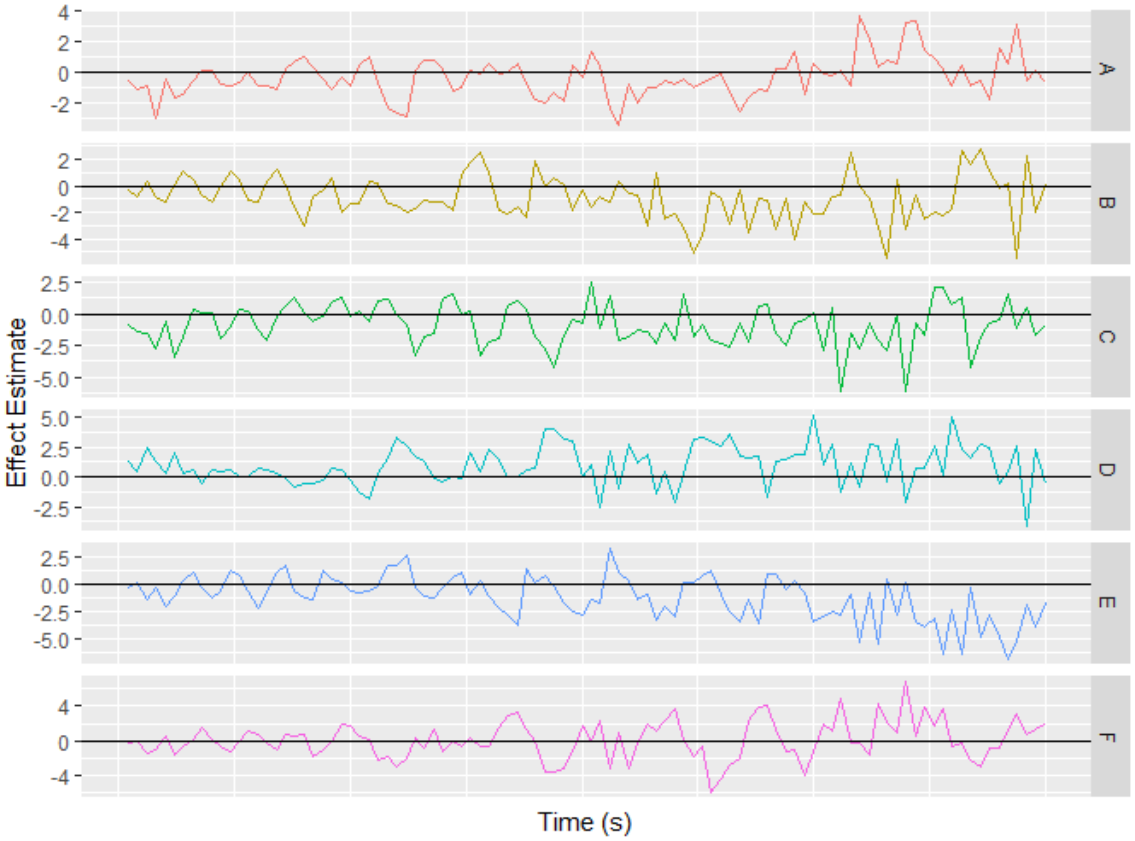


Figure 8. Functional Effect Estimates

through a permutation of the treatment combinations. The gray lines in Figure 9 are the $F\hat{(}t)$ functions for the approximated distribution. $F\hat{(}t)$ does not cross the critical value represented by the red dotted line in Figure 9. Therefore, there is no evidence of a significant effect on the response for any of the effect estimates.

A residual analysis is conducted to show the process for a functional case. Zhang (2013) outlines the assumptions of a functional linear model which include that the error function is a Gaussian process. The other assumptions listed are related to whether the functions evaluated are L^2-integrable and are finite. These assumptions were initially shown in Faraway (1997) but are also explained in detail in Chiou and Müller (2007). These diagnostics are synonymous to a multivariate regression residual analysis by examining the functional principal component (FPC) scores of the fitted

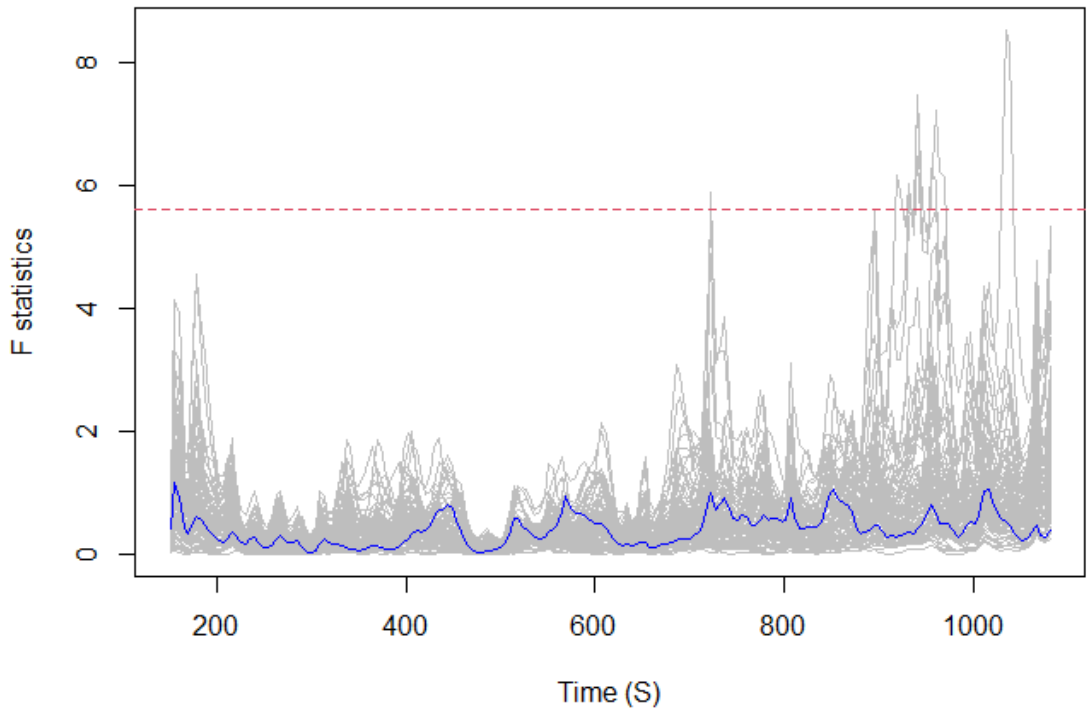


Figure 9. F-Statistic for the Hypothesis of a Significant Effect Present in the Main Effects Model

residuals vs the predicted response values. The number of functional principal components selected is based off of the cumulative proportion of the variance explained. For the fitted values, 94% of the cumulative variance is explained in the first functional principal component while three functional principal components were needed to explain 77% of the cumulative variance. Figure 10 shows the functional principal component scores for the residuals vs fitted values. Included are the labels for each observation to indicate potential influential points. The three plots do not show any evidence for patterns of violate the model assumptions. However, the large deviation of FPC scores for observations four and nine is alarming. Chiou and Müller (2007) provide further analysis on functional Cook's D influence, based off Cook (1977), to

detect influential observations present in the model.

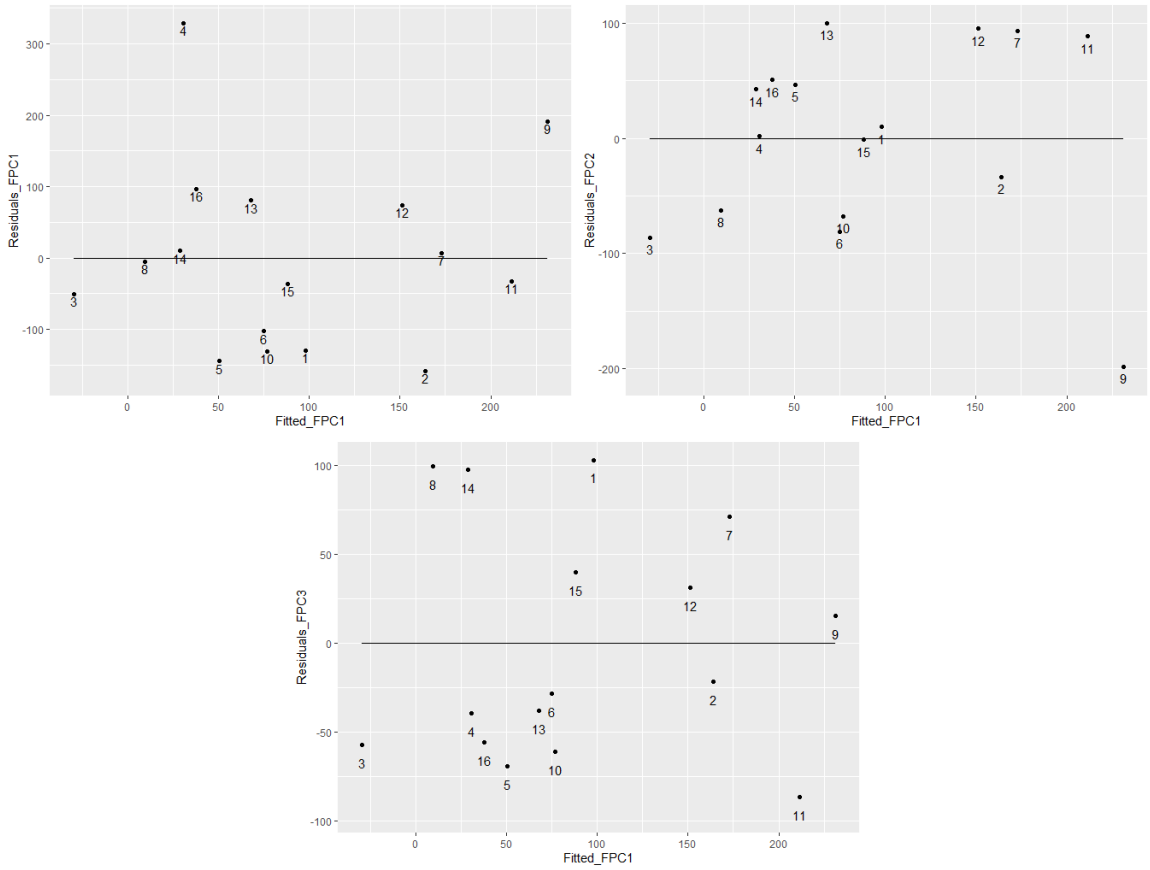


Figure 10. Validation of Functional Model Assumptions Through Inspection of Functional Principal Component Scores

3.3 Discussion

The three methods examined provide different competing analytical perspectives. The differentiating portion of each method is how to handle a functional response. The first method examined contains a response for each design run uses an aggregation method and then calculated a linear regression model. In the case study, the mean is considered but other aggregation statistics could include the maximum, minimum, etc. This strategy is subject to Type I error by erroneously creating response values to characterize the response curves. The second method uses the multivariate linear

regression model at discrete time steps and then approximates the continuous time steps by interpolating a straight line between observations. This method is approximating a functional regression model but is lacking a true continuous relationship by not containing functional data structures within it. The functional regression model does not require evaluating the model at every time step, compared to the approximated functional model, and instead utilizes the smoothness of the response curve to provide a continuous effect estimate and test statistic to examine the statistical significance of the model.

The analysis conducted provides similar conclusions in the case study examined. In all three cases the main effects model acts as a screening design. The experiment conducted had 16 observations across six factors. In the mean response model, none of the main effects are statistically significant at the $\alpha = 0.05$ level of confidence and only factor C is statistically significant at the $\alpha = 0.1$ level of confidence. Residual analysis is conducted to validate the assumptions of the error structure in the multivariate model. In the approximated functional regression the effect estimates are calculated by interpolating the effect estimates between each discrete time step. Significance tests are not conducted due to the ambiguity in the error structure between each time step model. In addition, the residual analysis for this model is not well defined. Finally, the functional regression model is calculated by creating B-spline basis functions for each design run and then fitting B-spline basis effect estimates for the main effects model. Permutation testing is used to calculate F-statistics as defined in Reiss et al. (2010). The average of the F-statistics show no evidence of a statistically significant functional regression model. Residual analysis is conducted to check if any abnormalities exist within the error structure. The diagnostics are explained in Chiou and Müller (2007), Zhang (2013), and Kokoszka and Reimherr (2017). They are analogous to the multivariate model but there are no normal probability plots

and functional principal component scores are required to inspect the error structure.

The multivariate model did not find any statistically significant main effects at the $\alpha = 0.05$ level but factor C provides some evidence at the $\alpha = 0.1$ level as shown in Table 1. The factor is included in a final model to see its estimated effect on the aggregated response. It is expected to decrease the response by -1.5% on average by changing factor C from its low to high setting. Comparing this effect estimate to the approximated functional regression and functional regression model the effect estimate curves in Figure 11 exhibit similar behaviors. For example, both effect estimate curves exhibit an overall negative trend and only diverge in behavior near the end of the test duration. However, in the functional regression model the F-statistic shown in Figure 9 did not contain any evidence of statistically significant effects in the model. The approximated functional regression and functional regression effect estimate curves inconsistencies are due to the construction of the functional models effect estimate curves from an 6^{th} order B-spline basis with 100 knots. This advantage results in a reduction in the total number of calculations by using the B-spline basis at each knot instead of each discrete second in the approximated case. In addition, the functional case provides the utility of derivatives of the response curves and their functional principal components to fully extract information from the smoothness in the curves. Another source of differentiation may be the use of a b-spline basis to create the effect estimate curves while the approximated functional model is interpolating a convex combination from point to point.

A majority of FDA methodology has subjective elements for choosing a basis, its penalization for smoothing, line registration, model selection, and number of functional principal components to select. Ramsay and Silverman (2005) and Ramsay and Silverman (2007) provide objective statistics to aid in methodology, such as the generalized cross validation score for selecting a smoothing penalty or the cumulative

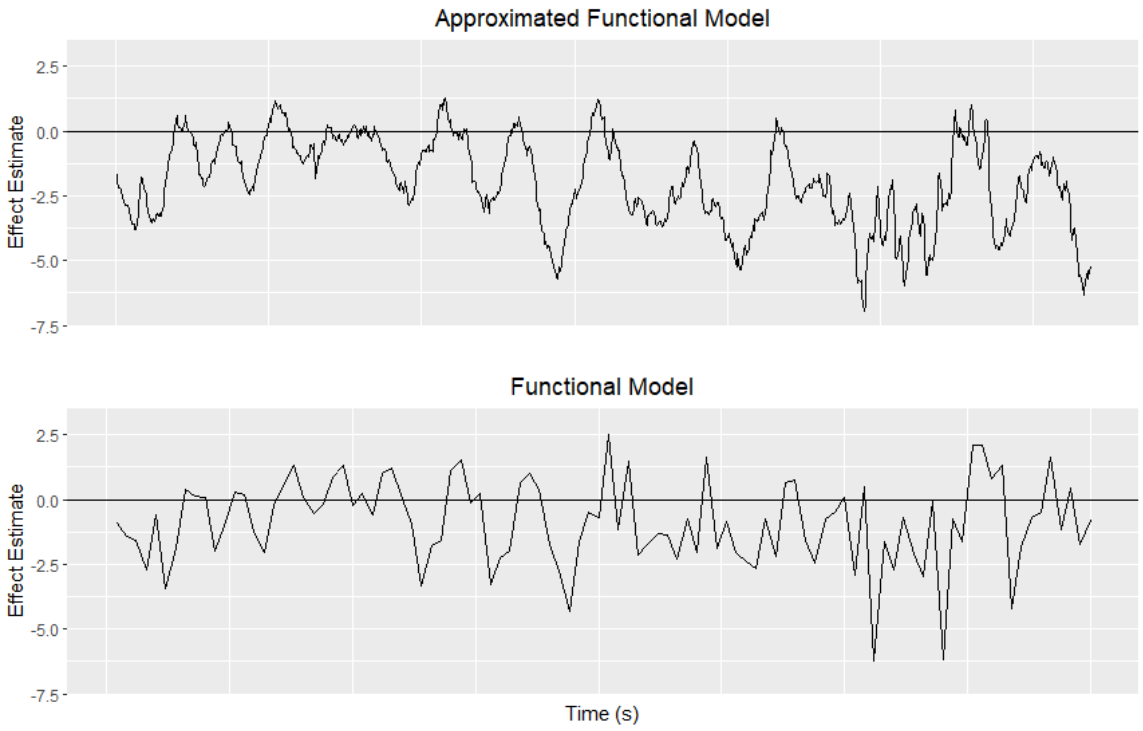


Figure 11. Comparison of the Effect Estimate Curve for Factor C of the Approximated Functional Linear Model and Functional Linear Model

proportion of variance explained for functional principal components, but there are still interpretations subjectively selected by the analyst. These minor adjustments in analysis did not make any significant changes to the analysis conducted in this case study. However, it does exemplify the uniqueness of a particular solution obtained.

3.4 Conclusion

The various methods examined provide insight on the difference of analysis for a designed experiment. While the literature in this intersection of functional data analysis and experimental design is sparse, there are broad extensions originating with Faraway (1997) and Ramsay and Silverman (2005). The use of linear regression models to approximate effect estimates and determine statistically significant effects are explained fully in Montgomery (2017). The approximated functional regression

model examined is not discussed explicitly in literature but is the underlying process occurring in functional regression but with basis objects instead of discrete observations in the calculations. The approach used in this study examined all three methods to provide insight in a sequential manner. Initially, a multivariate aggregated statistic is examined to screen for statistically significant main effects, then an approximated model is examined to find trends occurring in the effect estimates across time, and finally a functional model is fitted to provide a complete analysis of the response curves examined.

In this case study specifically, for all methods explored, only the aggregate model contained a statistically significant model. Besides this, there is no evidence of the factors providing an effect on the oxygen percentage of a pilot. Residual analysis is discussed in each section and provides connections between methodologies. While no particular results were found in this study, the methods explored and their similarities and differences are shown. The functional approach is recommended because it utilizes the entire curve without misrepresenting a response curve through an aggregate statistic. However the functional data analysis methodology requires a demanding methodology in comparison to a multivariate case. The adoption of FDA methodology in popular software packages such as R, Python, or JMP®, provide a degree of capability to assist in the FDA methodology.

IV. Functional Data Analysis within Software Packages

4.1 Introduction

FDA has grown significantly in the 21^{th} century due the influx of sensor streamed data and its extension of multivariate data analysis. Compared to multivariate data, functional data are assumed to contain smooth functions over a continuum. Multivariate data consists of observations of finite sets while functional data are represented as infinite dimensional curves. Ramsay and Dalzell (1991*b*) coined the term FDA while providing different techniques for FDA methodology. Examples of functional data include sparse measurements along a time span such as growth studies and quarterly econometric data or more dense observations such as sensor data for weather or engineering systems. A meta-analysis of different applications of FDA and the specific FDA features used for each application are shown in Ullah and Finch (2013). The monograph by Ramsay and Silverman (2005) describes an overall approach to implementing FDA and Ramsay and Silverman (2007) accompanies it with an applied approach through examining multiple examples. Kokoszka and Reimherr (2017) is an introductory text with R code provided. Other texts are complementary into specific topics within FDA such as Ferraty and Vieu (2006) for a theoretical perspective of FDA, Zhang (2013) for functional ANOVA (FANOVA), or Horváth and Kokoszka (2012) for inference within FDA.

FDA methodology typically follows a sequence of calculations to form a functional data object then perform exploratory, descriptive, and prescriptive analysis. Ramsay et al. (2009) provides a skeleton of an FDA methodology. The methodology begins with converting discrete data into a functional data object using a basis expansion. If a large degree of noise is present within the functional data curves, a roughness penalty (λ) is included based on the norm of the second derivative of the curve. The

value for λ is selected by finding the maximum of the generalized cross validation score with a grid-search selection of λ (Ramsay and Silverman, 2005). After converting to a functional data object, curve alignment (manipulating functional data curves positioning along the continuum) within each curve is required to reduce unwanted variation between observations. The functional data curves are examined using exploratory data analysis such as graphs of the curves or of their derivatives to gain initial insights. Phase-plane plots are also useful to explore relationships between derivatives as well as covariance plots if multiple functional covariates are being examined. Functional principal components analysis is another exploratory technique that generally provides more information than in a multivariate setting. Descriptive statistics are also accessible from the calculated basis functions. Finally, a functional model is tailored for the goal of the analysis. Other overviews found in Cuevas (2014) and Wang et al. (2016) give similar perspectives. The FDA methodology mimics the multivariate setting, but contains nuances that make FDA a unique methodology.

Enacting FDA methodology requires software to calculate linear combinations of basis functions, penalize the basis functions to reduce deviation due to noise, curve alignment, functional principal components, functional models, and other FDA techniques. Ramsay (2003) is a surface level introduction to functions elaborated in Ramsay et al. (2009) which describes the **fda** package for MATLAB or R. Kokoszka and Reimherr (2017) discuss introductory methodology and additional packages such as the **refund** package (Goldsmith et al., 2016) or **fda.usc** package (Febrero-Bande et al., 2013) within R. The **scikit-fda** package (Ramos-Carreño et al., 2019) within Python replicates the tools in Ramsay et al. (2009) with a few additions for other machine learning algorithms. The JMP® Pro 15 software includes a functional data explorer within its specialized modeling apparatus.

In the R software specifically, recent developments create an efficient approach to

functional data analysis. The original software package **fda** creates a **fdata** object within R. Febrero Bande and Oviedo de la Fuente (2012) give an in depth description of the **fda.usc** package which provides exploratory and descriptive analytic as well as a variety of scalar response functional models. Goldsmith et al. (2016) expands upon this utility and provides regression models for scalar-on-function regression, function-on-scalar regression, and function-on-function regression. The **refund** package provides hypothesis tests beyond a limited pairwise comparison only offered in the **fda** package. Wrobel et al. (2016) created an interactive R Shiny web application for functional data. The web application provides exploratory data analysis through different visualizations of functional data and functional principal component analysis without requiring as many granular details.

The **tidyverse** package suite (Wickham et al., 2019) has become a popular set of analytical tools within the R software. The **tidyverse** package suite includes data importing, tidying, manipulation, visualization, and programming. Modeling is under development in the **tidymodels** package, but the **caret** package (Kuhn et al., 2008) covers a similar array of models. The notion of tidy data is defined in Wickham et al. (2014). Tidy data consists of three items:

1. Each variable forms a column
2. Each observation forms an row
3. Each type of observational unit forms a table

Advancements are being developed to aid in the FDA toolkit include a **tidyfun** package to assist in functional data manipulation within the structure of the **tidyverse** package suite. The **tidyverse** verbs are intuitive and require low-level grammar and data structures to perform common analytical tasks.

The remainder of this work examines each software in a detailed fashion beginning

with R, followed by MATLAB, Python, and JMP® Pro 15. Comparisons between each software are made and recommendations for potential methodologies are explained. Finally a summary of the software examined and the recommended software for a functional data analysis methodology is revisited.

4.2 Software Features

4.2.1 R

The **fda** package within the R software is the foundation for the subsequent packages mentioned and is detailed in Ramsay et al. (2009). The package provides analytical tools for all portions of the FDA methodology with restrictions in some domains. The **fda** package creates a *basisfd* object, with a basis function to represent a curve. The two most popular basis functions, the Fourier basis for periodic data and a b-spline basis for non-periodic data, are available as well as constant, monomial, exponential, polygonal, and power basis. Bases may also be defined empirically by estimating the functional principal components of the data. A linear combination of the bases and a set of coefficients form a functional data class (*fd*). The *fd* class contains specific attributes such as the basis object and the basis coefficients. An advantage of FDA is the use of derivatives, stored as a linear differential operator class (*Lfd*). The **fda** package includes data smoothing, introducing a roughness penalty for noisier data. The smoothing parameter λ is chosen by finding a minimum through a grid-search of the generalized cross validation score. This results in a *fdPar* class representing a *fd* class with a roughness penalty. These classes form the foundation of FDA by converting data from a discrete to continuous form and storing them as distinct objects. These objects are accessible from other FDA packages within R.

After converting the data to a functional data object, descriptive statistics and visualizations are available within the **fda** package such as the mean function, the

covariance function, and phase-plane plots. Other FPCA to explain the primary sources of variation present in the data structure. Similar to multivariate analysis, the functional principal component analysis is conducted through calculating orthogonal eigenfunctions of the covariance function and finding respective eigenscores for each observation. The **fda** package stores all of this calculated information as a *pca.fd* class for use for subsequent analysis.

The final data manipulation strategy before modeling is curve registration. Curve registration is used to remove phase or amplitude variation between observations. The **fda** package provides landmark and continuous registration methods. Landmark registration is accomplished through the user selecting a moment along the continuum while continuous registration requires dynamic time warping to align the curves.

Modeling the functional data is subject to the goal of the overall analysis. In the **fda** package, the only models available are functional linear models with scalar and functional responses. However, the **fda.usc** package provides an expansion of the FDA architecture by providing several supervised and unsupervised functional models such as generalized functional models and k-means models with hypothesis tests and diagnostics. The **fda.usc** package is limited to only scalar response models while the **refund** package provides models for scalar-on-function, function-on-scalar, and function-on-function models. In addition, the **refund** package allows penalized regression methods proposed in Goldsmith et al. (2011).

The development of an R Shiny web application allows users to perform functional data analysis without knowing the granularity of coding such as syntax, variable manipulations, etc. Wrobel et al. (2016) describes the capabilities of the **refund.shiny** package. In essence, the application creates interactive plots with basic functionalities such as visualizing functional principal component analysis and visualizing the effect estimates with function-on-scalar regression. The R Shiny app is a visualized expe-

rience through the FDA methodology similar to the functional data explorer within the JMP® Pro 15 software.

4.2.2 MATLAB

Integration of function data analysis into MATLAB is provided through the **fda** package. The **fda** package in MATLAB contains the same set of capabilities as the R software version. The only differences are in software conventions such as calling functions within R is *create.bspline.basis()* while *create_bspline_basis()* is used in MATLAB. The explanations for these differences are explained in Ramsay et al. (2009). The **fda** package is designed to minimize the differences between R and MATLAB when conducting an FDA methodology. Other packages exist within MATLAB for FDA but were not relevant to the analysis conducted and were not explored in depth.

4.2.3 Python

Python is a powerful tool for data analysis due to large progresses within its open source framework. Recent FDA work in python has been accomplished through Ramos-Carreño et al. (2019) in providing a package suite with basis creation, smoothing, curve registration, exploratory data analysis, and modeling. The features available are also being developed for further expansion to mimic capabilities found within the R software. The package includes most of the techniques explained in Ramsay and Silverman (2005). An expansion of techniques are included, such as different machine learning models for classification, regression, and unsupervised methods in a functional setting. However, all these models are limited to only a scalar response with functional predictors.

4.2.4 JMP®

The JMP® software package provides a set of analytical tools with a spreadsheet design allowing for easier access to analytical techniques without the need for extensive coding technique. In contrast to the earlier software packages, JMP® has a graphic user interface for creating models through a "drag and drop" simplicity while generating complicated models. In JMP® Pro 15, the functional data explorer specialization is added to the repertoire. The capabilities within the functional data explorer include basis fitting with penalization for smoothing, curve registration, and functional principal components for exploratory analysis. The basis systems include b-spline bases and Fourier bases but are limited on the number of knots and the degree of the splines. Helpful visualizations for selecting an appropriate basis are generated based off of fit criteria such as the Bayesian Information Criterion (BIC). For further details of the functional data explorer, consult Chapter 15 of SAS Institute Inc. (2019).

4.3 Discussion

This portion of the research compares software package capabilities for conducting functional data analysis methodology. All of the software packages mentioned have the potential to create extensive functional data analysis methodologies but the expertise required is beyond the scope of this research. The focus is to address already developed tools within different software to assist in the FDA methodology and then compare these capabilities between each other. The software is evaluated based on subjective measures for its ease of use, access to additional resources, and the extent of its FDA capabilities.

The R software provides an extensive set of FDA tools to perform a variety of FDA techniques. The basis is the **fda** package. The package mimics all the FDA topics

reviewed in Ramsay and Silverman (2007) for comparison. This package is expanded upon through the **fda.usc** package and are the two most popular for conducting FDA. Other capabilities such as diagnostics and penalized regression methods are added in the **refund** package. Other packages exist for specialized FDA techniques such as the **fpca** package (Peng et al., 2011) for functional principal component analysis and the **fdANOVA** package (Górecki and Smaga, 2019) for functional analysis of variance (ANOVA). These packages are evidence of the power of open source collaboration to enhance FDA capabilities within R.

In addition to the volume of the R software's technical capabilities, R provides a full documentation for many of the packages mentioned above. The Comprehensive R Archive Network (CRAN) contains a library of vignettes for each package. The vignettes are descriptions of the package, the functions available within the package, details on the arguments required for a function, the output for a function, and typically an example of the function. In addition to these vignettes, Ramsay et al. (2009) and Kokoszka and Reimherr (2017) explicitly state lines of code to use to perform FDA. The combination of these sources of documentation bridge the mathematical aspects of FDA in Ramsay and Silverman (2005) and the technical aspects of coding.

The largest barrier within R is that some level of coding experience is a requirement to successful use of R. Due to the vast collection of packages available for analysis, there is not a standardized data workflow between packages. The **refund.shiny** package Wrobel et al. (2016) attempts to alleviate the issue by providing an intuitive graphic user interface only requiring a functional data input, but the R shiny web application is limited to exploratory analysis and function-on-scalar regression. The only coding experience needed is for possible data manipulation and creating the correct functional data object to implement into the R Shiny application. If the FDA technique is beyond the scope of the **refund.shiny** package, then the analy-

sis requires understanding of the software packages mentioned before to conduct the analysis.

MATLAB is properiety software developed by Mathworks with a focus on matrix manipulation and calculations. The **fda** package (Ramsay et al., 2009) within R is identical to that within MATLAB. The conventions of the functions are subject to the software being used but the capabilities are matched. In MATLAB 8 different basis are offered for constructing a functional data object. Penalization methods, curve registration, functional principal components, and functional modeling are all included. Any analytical techniques discussed within Ramsay and Silverman (2005) and Ramsay and Silverman (2007) are possible within MATLAB. The main restriction is that MATLAB does not contain any additional packages, like the R software does, for recently developed techniques. For example, penalized functional regression, functional ANOVA models, or clustering models are not accessible within MATLAB.

Python is a popular open source object oriented programming language. The vast libraries from developers in Python are powerful for data analysis, such as **Pandas** (McKinney et al., 2011), **Numpy** (Walt et al., 2011), and **Scikit-Learn** (Pedregosa et al., 2011). The **scikit-fda** package (Ramos-Carreño et al., 2019) is tailored for FDA and contains numerous functionalities comparable to R package **fda**. The package includes additional models for unsupervised techniques such as functional clustering, but all of the models are scalar responses only. The documentation is thorough and provides examples from Ramsay and Silverman (2007). The **scikit-fda** is a recently developed package, indicating it might be expanded upon in later versions and contain other modeling architectures for function-on-scalar and function-on-function models. The package contains the baseline for other software packages to build off of. The*FDataGrid* , *FBasis*, and *FData* classes are defined within this package and provide an organization for future developments. The restriction is this single resource

is the only complete package dedicated to functional data analysis. Therefore the capabilities are limited to whatever is addressed within this single package.

JMP® Pro 15 is a set of computer programs combined in an easy to use interface to perform statistical analysis. The platform has functionalities for data manipulation, experimental design, analysis, and visualization. Additionally, the data are displayed in a spreadsheet format. This creates a low barrier to entry for advanced analytical techniques. In terms of functional data analysis, the functional data explorer in JMP® Pro 15 is a powerful tool for finding a correct basis, curve registration, and exploratory data analysis. The basis systems included are a Fourier basis, a B-spline basis, and a penalized B-spline basis. These basis can be fit to the curve simultaneously with a comparison of their fits based on a scoring criteria. The number of knots and their specific placement are adjustable through the interface, but the total number of knots is limited by computational efficiency. A basis expansion with 1000 knots is possible within R, MATLAB, or Python but is severely handicapped in JMP® Pro 15. The software is lacking in functional modeling. JMP® does provide FPCA and uses the functional principal component (FPC) scores on the FPC profiler. The FPC scores are used as inputs to a linear regression model to configure the FPC profiler. In a similar manner, the factor profiler is used to analyze the effect estimates for an experimental design. An example of an optimal design based off of a desirability function is shown in Figure 12. The FPC profiler does not support as much inference as a factor profiler in a multivariate experimental design because the different inputs.

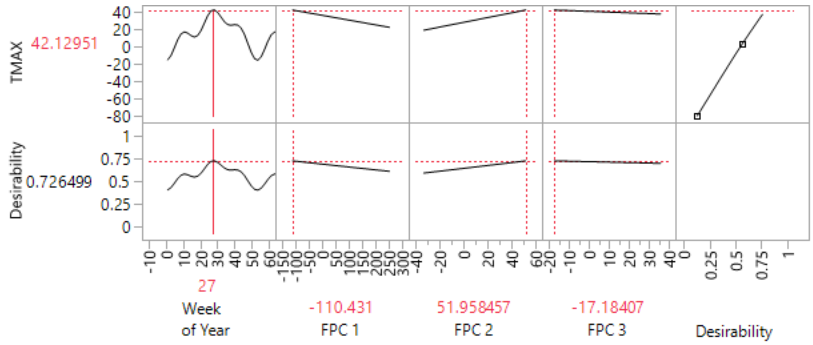


Figure 12. Example of FPC Profiler in JMP® Pro 15

4.4 Recommendations

After examining a variety of software implementations for functional data analysis, a methodology is recommended through these software packages. The areas of interest include the scope of the software, its ease of use, and the dependencies the package requires. In terms of the scope of the software, R has the largest and most updated implementation of FDA methodologies. Unfortunately, these methodologies are covered in multiple packages rather than one central package. The JMP® Pro 15 software package provides the lowest barrier to entry from a coding perspective. The interface combined with its documentation improve its accessibility. The **refund.shiny** application in R attempts to compete in this domain, but the required dependent packages and coding for data manipulation make it tedious for analysis. Finally, the dependencies of the packages must be addressed due to the confidentiality of the data examined. The open source programming languages such as Python or R are of concern when handling sensitive data. A proprietary product with a standing reputation for working with sensitive data is advantageous such as the JMP® software. JMP® is already used across confidential systems to conduct analysis and has an established relationship. The functional data explorer within the JMP® Pro 15 software is recently developed and has potential for improvements. These improvements combined with the ease of use of the JMP® infrastructure make it a

competitive choice for functional data analysis. Until the JMP® software has more capabilities added, the R software is the leading competitor in the FDA domain. The majority of the methodology should be carried out within R due to the depth of its capabilities and its documentation.

4.5 Conclusion

In conclusion, the software packages examined provide a diverse and overlapping techniques for functional data analysis. The power of open source collaboration makes the R software a competitive package for FDA but is a nuisance to track all the extra packages for specialized modeling. Recent developments make Python attractive since it is already a familiar programming language for data analysis. MATLAB is limited to only an original package with functionalities identical within R. The JMP® Pro 15 software is easily accessible to a variety of modeling architectures, but its lacking in capabilities related to FDA to be competitive. The software is useful as an exploratory tool to examine data or learn FDA techniques. After these considerations, the recommended software is R due to its depth of capabilities through a variety of software packages. The packages discussed in this work provide a foundation for a full FDA methodology of data manipulation, transformation, basis expansion, smoothing, curve registration, functional modeling, and diagnostics. The recommended software package to perform this FDA methodology is R due to its advantages in each sequence of an FDA methodology. In addition, R contains an archived documentation source and R packages are in development to assist in functional data analysis.

V. Conclusions and Recommendations

The remainder of this work discusses the contributions and recommendations to continue this research. To begin, the methodology and conclusions from the case study are reinstated. Additionally, recommendations from the case study and potential software packages are summarized for the sponsor of interest. Finally, any future research is discussed for continuity.

5.1 Conclusions

The adaptation of sensor streamed data in experimental test of USAF aircraft provides a rich influx of data. Current methodologies consist of using aggregated statistics or feature engineering to create response values for curves measured along a time continuum. Introducing techniques from functional data analysis, the entire response curve is analyzed instead of using multivariate methods. In addition, a functional linear model is able to examine the statistical significance of main effects or possible higher order interactions within a designed experiment.

The dense supply of sensor data within an experimental design creates a demand for an analytical technique other than the use of multivariate methods of linear regression or ANOVA. To meet this demand, this research aims to answer the following questions:

Question 1

What is an effective way to characterize functional response data in an experimental design?

Question 2

How do different available software packages compare in being able to handle functional response data?

The first question is examined in the case study presented in Chapter III. The case study consists of an experimental design with 16 observations across 6 main effects. The methodology is predominantly adopted from Ramsay and Silverman (2005) and computed in the R software. To summarize, a functional data object is created from each of the design runs by adopting a b-spline basis. The functional data object is used a response curve with each having a determined factor combination for the six factors. After aligning all the curves through landmark registration, a function-on-scalar regression model is fitted. The effect estimates for the six main effects are shown in Figure 13 and the overall F-statistic is computed to test for statistical significance shown in Figure 14. Finally the residual behavior is examined for validation of assumptions for the functional linear regression model.

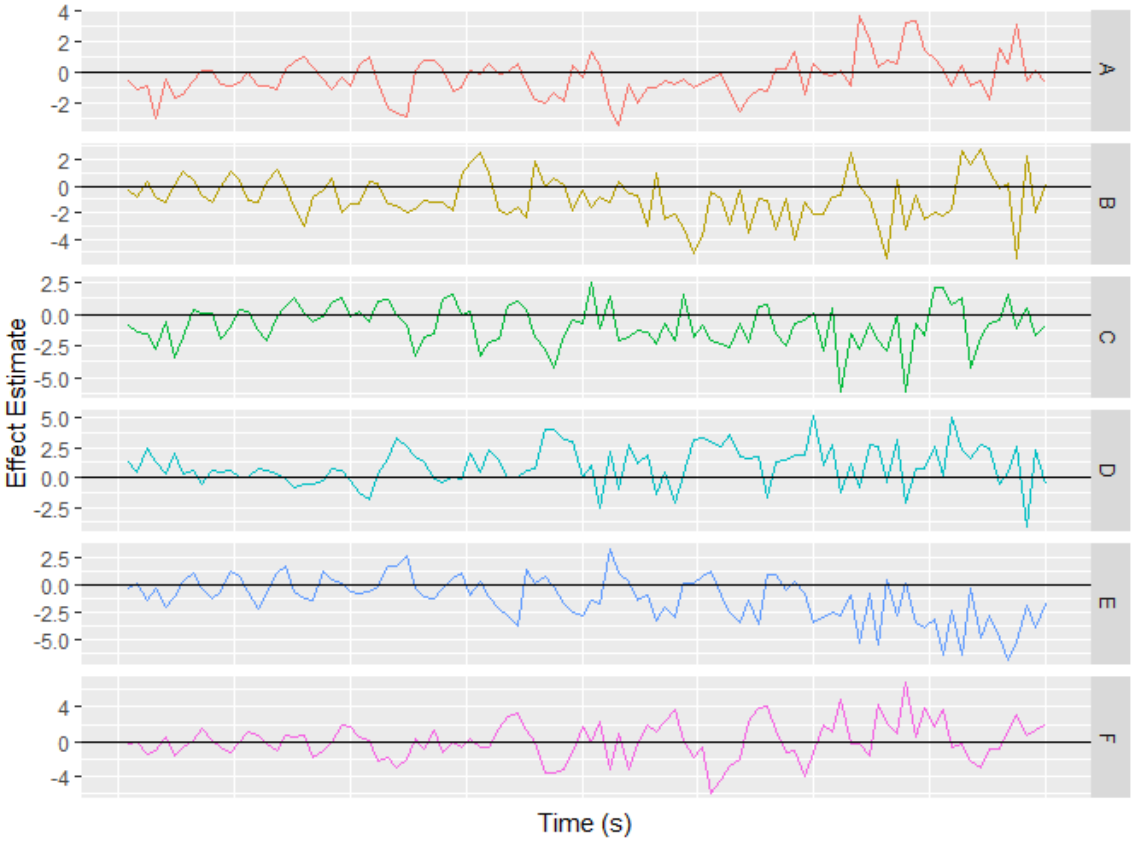


Figure 13. Effect Estimates for Main Effects of Functional Linear Model

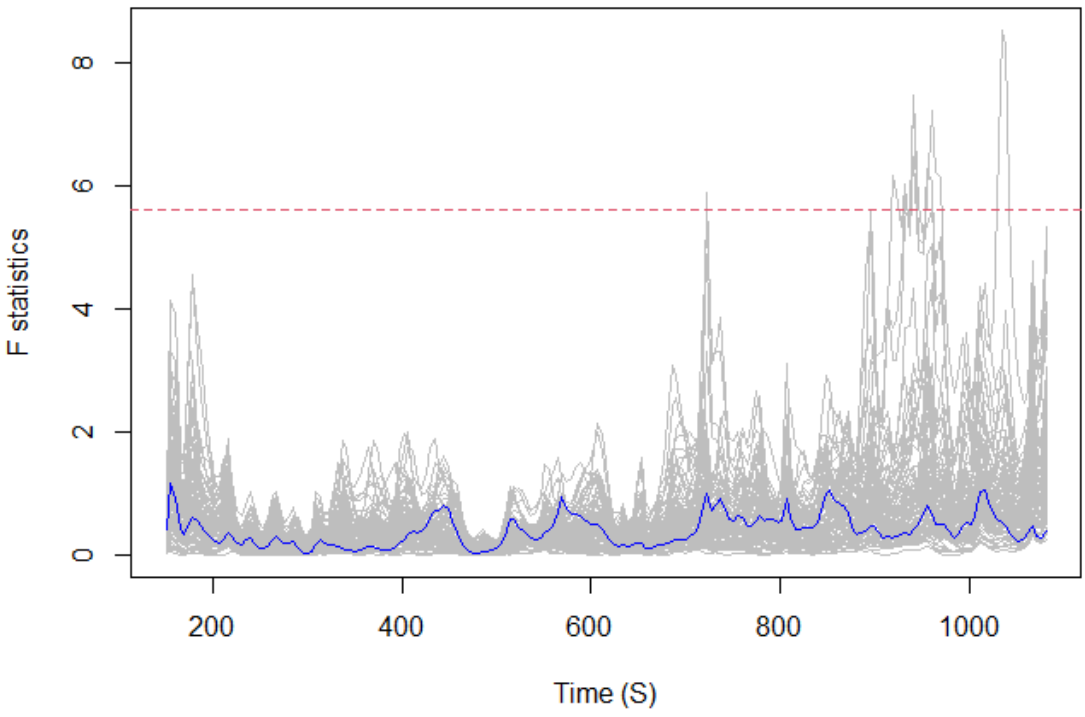


Figure 14. Overall F-Statistic for Main Effects of Functional Linear Model

For comparison, multiple aggregate response values are calculated for the 16 response curves and examined in a linear model. In addition, a linear model is fitted at each time unit to create an approximated functional linear model. In all of the cases mentioned there were no statistically significant main effects at the 95% confidence level. Factor C is only statistically significant at the 90% confidence level if the response is the mean of the response curve.

The comparisons serve to bridge different methodologies for characterizing a response curve. The aggregated response values are computationally preferred but are poor characterizations of an entire response curve. These values are subject to outliers, noise, and influential points within a curve. In addition, creating multiple test statistics increases the likelihood of type 1 error. The approximated functional linear model attempts to use the entirety of the response but is easily subject to amplitude and phase variation between observations. Correct alignment before examining the response curves aides in the FDA methodology for a functional linear model. Another possible methodology could examine the effect of data registration through dynamic time warping, but this might also generate a type 1 error by forcing the response curves to inaccurate behavior.

The case study reveals it is evident that functional data analysis is the correct methodology to undertake to analyze an experimental design with the response being a curve. However, in the case study examined, no statistically significant evidence was found. There does appear to be a relationship between the different models examined for comparison. For example, the approximated functional linear model did have similar effect estimates as the functional linear model as seen in Figure 15. However at the end of the effect estimate the directions of the effect estimates diverge. This contrast may exist for a variety of reasons. A difference may exist because the effect estimates generated in the functional linear model are created from a B-spline

basis while the approximated functional linear model is a sequence of discrete effect estimates with interpolated continuities. Neither models found any significant factors, complicating the comparison between the two methodologies.

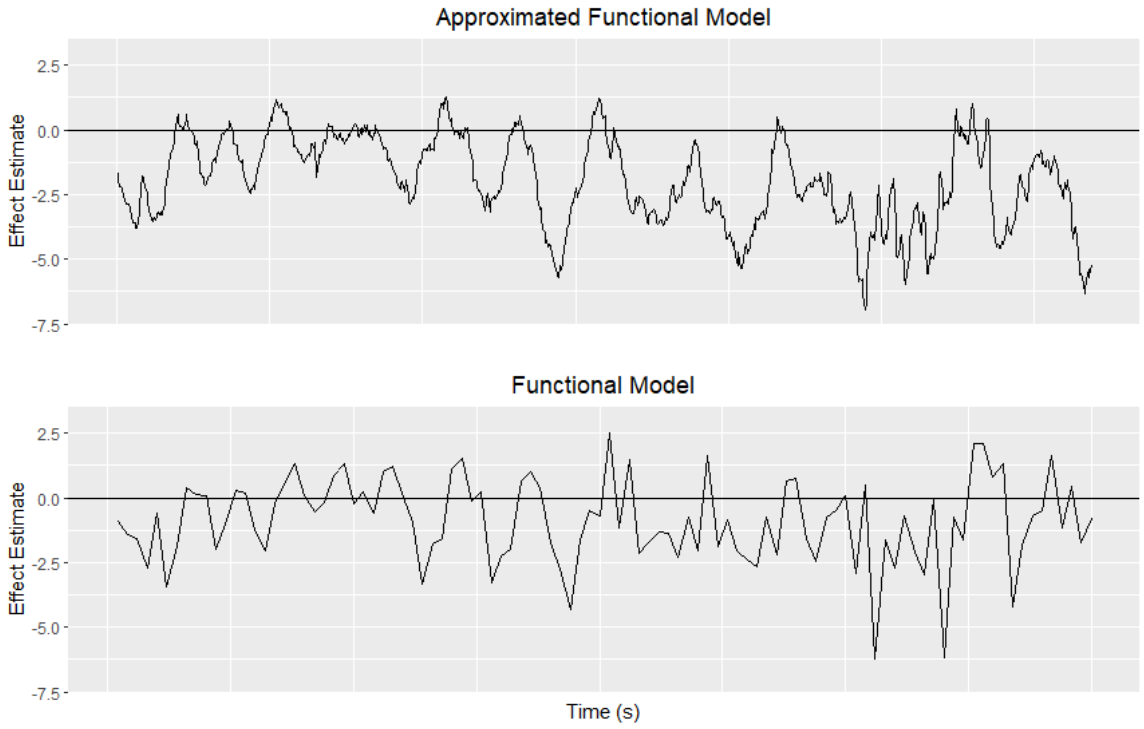


Figure 15. Comparison of the Effect Estimate Curve for Factor C of the Approximated Functional Linear Model and Functional Linear Model

The second research question addresses the tools to perform functional data analysis. The variety of software packages evaluated included the R software, JMP® Pro 15, Python, and Matlab. Of all these tools, the R software appeared to be the most capable in terms of handling a variety of FDA methodologies. However, JMP® Pro 15 is capable of some functional data analysis with a much lower barrier to entry from a technical perspective. MATLAB and Python both have FDA capabilities as well and may be better suited for familiar users. Developments are ongoing for both R and Python, and the functional data explorer with JMP® Pro 15 is a new feature. Therefore, it is likely that future expansions will be added to each software to advance their capabilities. A recommended source for assistance in the methodology

used in this analysis can be found in Chapter 5 of Kokoszka and Reimherr (2017) and Chapter 10 of Ramsay et al. (2009).

JMP® Pro 15 contains the simplest interface for an individual new to FDA. The documentation, examples, and capabilities are useful. The commercial software contains useful functionalities, such as in Figure 16. The visual provides an intuitive comparison of the fit of different order splines and different number of knots based off of the Bayesian Information Criterion (BIC). The main constraint within the JMP® Pro 15 software package is its computational limits. Fitting a functional data object with a large volume knots is intractable. By comparison, MATLAB, Python, and the R software were capable of fitting over 1000 knots in the case study examined with higher order B-spline bases.

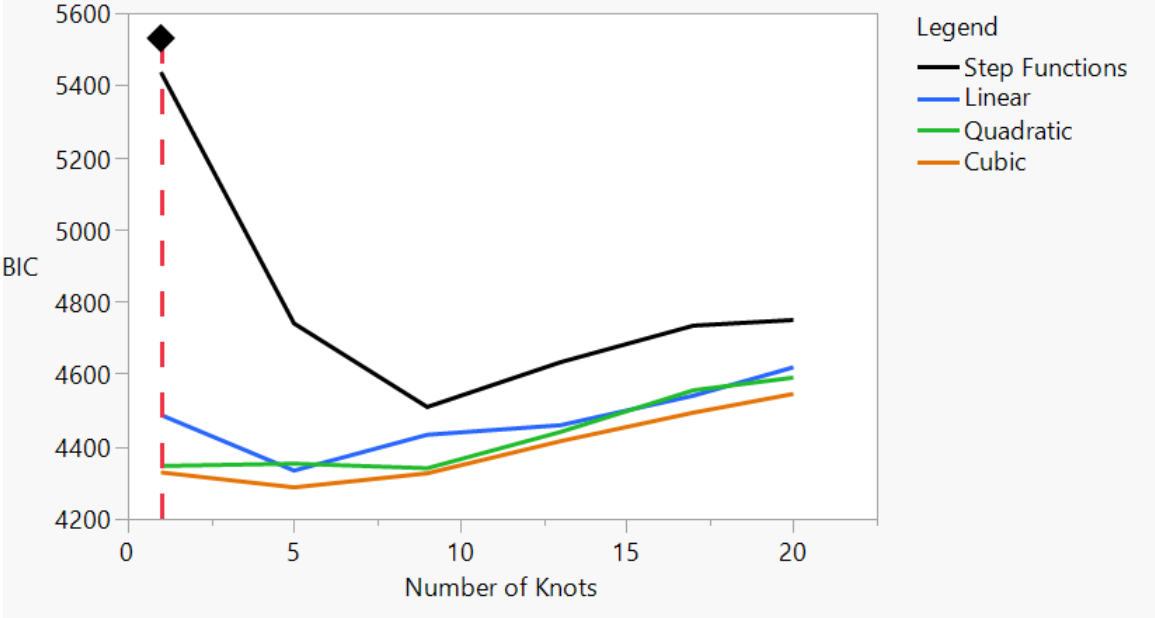


Figure 16. Example of Comparison of Different Order B-Spline Basis on Functional Data

5.2 Recommendations

This work examines an experimental design with a functional response with the intention of creating a deliverable methodology for the Scientific Test and Analysis Techniques (STAT) Test & Evaluation (T&E) Center of Excellence (COE). The adoption of a functional data analysis methodology presented in Chapter III gives a robust analytical procedure without neglecting potential information present within an experiment. In addition, the use of the R software to perform the majority of the analysis is recommended due to its depth and accessibility in FDA. Implementing this methodology does introduce a computational burden compared to an aggregated response model as well as technical nuance when performing the analysis. In spite of these issues, the use of functional data analysis provides a powerful advantage to the analyst in finding potential signals present in a noisy experiment.

Future research in this domain is recommended to fully exploit the potential benefits from FDA. In the case study examined, only main effects were estimated while a higher order model may be suggestive of different behaviors created by the manipulated factors. In addition, the case study examined a split-plot design but focused on only a whole plot. An introduction of a functional model tailored for the split-plot design can be augmented from the split-plot design shown in Montgomery (2017). Zhang and Großmann (2016) provides an example using a split-plot design including the calculations for the sources of error for an ANOVA table as well as the appropriate degrees of freedom.

An examination of the case study in Chapter III alludes to several other augmented methodologies. FDA methodologies have a significant amount of analyst based decisions rather than objective measures. In the case study, an inverse relationship exists for computational time and the fidelity of the basis expansion chosen. A B-Spline basis was chosen with a knot at every time segment, compared to having

a sparse knot scheme. The concentrated knot selection provides an extremely flexible basis expansion but introduces computational demands. Penalization methods were also examined to improve the robustness of the basis expansion and reduce unwanted fitting due to error, but objective methods such as the generalized cross validation score indicated these were negligible and were therefore ignored.

Including all whole plots in the original design may have helped in the basis expansion, curve registration, or model fitting portions of the methodology. However their introduction of non-desirable error for the subplots creates further complications. Curve registration was performed based on the initial climb in oxygen percentage present in each observation, but a robust approach such as dynamic time warping may prove beneficial by aligning the sinusoidal waves present throughout the duration of the design runs. It it hypothesized that these non-uniform peaks and troughs in the design run curves disrupt potential signals in the differences of the design runs.

In terms of fitting the functional linear model, higher order effects may prove significant but are unlikely due to the principle of sparsity of effects. Other additions include changing the basis expansion for the effect estimates. A higher order B-spline basis may be used with more knots but a computational burden is imposed through this process. Other basis could be used such as the Fourier basis but the B-spline basis is recommended because it is not constrained to periodic functions.

In terms of software packages to perform FDA methodology, the open source architecture of the R software and Python creates a near limitless potential. It is impossible to mention all the potential packages to use for FDA, but the packages mentioned in Chapter IV are baseline introductions for each software. The demand for rigorous FDA techniques requires additional packages or user developed applications. Limitations exist within software such as JMP® Pro 15 based on the memory required for computations. In terms of the case study examined, MATLAB, the R software,

and Python were all capable of fitting a functional data object to the data but were limited on the subsequent methodology as mentioned in Chapter IV.

Overall, this work provides a methodology for characterizing a functional response of a designed experiment as well as an introduction to different software packages to perform different portions of the methodology. Results indicate that no significant main effects were found present within the functional linear model. The R software is best tailored for this methodology but other software packages have potential capabilities in development or not discussed in this work. Further work exists within this methodology for different designed experiments in the United States Air Force to test its rigor and usefulness as an analytical technique in the experimental design domain.

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14. ABSTRACT

The growth of sensor streamed data in recent years increases the demand for an analytical technique to properly address data measured continuously. The design and analysis of experiments (DOE) of U.S. Air Force assets are based off of sensor streamed data. Functional data analysis (FDA) is an approach of analyzing data existing over a continuum. This research aids in filling the intersection of FDA and DOE by examining a case study of an experimental design with a functional response in addition to insight on software capabilities in FDA. The case study considers a functional linear model of a whole-plot from a split-plot experimental design compared to multivariate methods and an approximated functional linear model. Initial results indicate no significant main effects were detected in the case study using FDA. However, a comparison between the different methodologies indicate similar behaviors for main effect estimates. An examination of software packages reveals the R software as most compatible with FDA methodology. Recommendations include another case study evaluation of FDA and future work in alignment of response curves.

15. SUBJECT TERMS

functional data analysis, experimental design, split-plot design, multivariate data analysis, functional linear model

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