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Application of Functional Data Analysis for the Prediction of Maximum Heart Rate

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ABSTRACT Maximum heart rate (MHR) is widely used in the prescription and monitoring of exercise intensity, and also as a criterion for the termination of sub-maximal aerobic fitness tests in clinical populations. Traditionally, MHR is predicted from an age-based formula, usually 220 − age. These formulae, however, are prone to high predictive errors that potentially could lead to inaccurately prescribed or quantified training or inappropriate fitness test termination. In this paper, we used functional data analysis (FDA) to create a new method to predict MHR. It uses heart rate data gathered every 5 seconds during a low intensity, sub-maximal exercise test. FDA allows the use of all the information recorded by monitoring devices in the form of a function, reducing the amount of information needed to generalize a model, besides minimizing the curse of dimensionality. The functional data model created reduced the predictive error by more than 50% compared to current models within the literature. This new approach has important benefits to clinicians and practitioners when using MHR to test fitness or prescribe exercise.

INDEX TERMS Maximum heart rate prediction, functional data analysis, machine learning, low intensity sub-maximal test.

I. INTRODUCTION

Heart rate (HR) is one of the most widely used measures in clinical medicine and exercise physiology to evaluate a person's cardiovascular fitness. Two key reasons for this are its non-invasive ease of measurement and its low cost. Together, these two factors mean it has great utility being used in the control of exercise intensity [1], the detection and monitoring of fatigue and over-stimulation states [2], [3] and even in clinical settings to detect heart problems e.g. angina [4], [5]. These uses of HR are dependent of having a known value for maximum HR (MHR). A true MHR can only be accurately derived from a maximal effort, usually in a cardiac stress test. In these tests, heart rate will increase gradually as work rate increases, with the objective of pushing the body to its physical limit. However, a direct measurement is not always feasible because of the elevated risk of adverse events in some clinical populations [6], limited access to suitable facilities and equipment, or the disruption to an athlete's training [7].

To circumvent the issues associated with obtaining a true MHR, a number of predictive equations have been developed [8]. These predictions take account of the fact that MHR declines with age [9]. The most popular of these age-predicted maximal heart rate methods is the formula: 220 − age (years). Despite its near pandemic use by practitioners, this formula is based upon observation rather than statistically derived from experimental data and is prone to large predictive errors [8]. Some multivariate approaches have also been developed trying to better model the variability in MHR prediction. However, they do not improve the predictive power of univariate models.

The increasing capacity of electronic devices to collect data at a high sampling frequency is facilitating new insights into human physiology. Numerous smart watches now record HR in real time [10]. One benefit of this is that HR demonstrates

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a strong, linear relationship with oxygen uptake (VO_2) [11], a key determinant of physical capacity and energy expenditure [12]. With its comparative ease of measurement compared to VO_2, many wearable devices use HR to quantify exercise into HR zones, provide a score reflecting the training load or difficulty of an activity or even predict VO_2 max. All of these functions incorporate the use of a value for MHR that is often derived from an age predicted formulae. However, the errors associated with these predictions compromise the accuracy of these functions. A drawback of these approaches is that they do not incorporate important aspects of the structure of the data and, thus, do not fully exploit the potential of the information gathered during exercise tests to better understand the heart's response to external stress. The high dimensionality of data and the high correlation between nearby observations are important issues to achieve this aim. The amount of data needed to generalise a model accurately (with statistical significance) grows exponentially (curse of dimensionality) if we do not group data in objects with similar properties. However, in high-dimensional data, all objects appear to be sparse and dissimilar, which prevents common data organization strategies from being efficient.

In this paper we propose a new method for predicting MHR based on functional data analysis (FDA), which minimizes the aforementioned issues. FDA is a mathematical technique able to express the discrete observations arising from time series in the form of a function as a single observation. The idea behind FDA is that data collected (usually a dense sampling) over time reflect the influence of a smooth function in the generation of the observations. FDA uses this function to predict information from the collection of functional data. This abstraction allows FDA to take advantage of additional information from this function, contrary to classical multivariate statistical techniques.

The proposed method predicts MHR from the observations captured during the sub-maximal stages of a maximal and incremental exercise test, specifically a treadmill exercise stress test starting at 6 $km \cdot h^{-1}$ increasing by 0.25 $km \cdot h^{-1}$ every 15 seconds until exhaustion. Predictive errors obtained by this method have been compared with more traditional uni and multivariate approaches. In addition, results have also been compared with other traditional machine learning regression methods, obtaining similar scores in terms of error, but with the advantage that we know the significance of the variables introduced in the model.

Finally, a predictive module has been developed and integrated in the Athletes Management System (AMS) of the High Performance Center of Pontevedra (Spain). The MHR predictions are currently used to improve training planning, as well as for medical supervision. The developed module is also integrated with the athletes database, and is programmed to update monthly the training database used to generate the predictive model.

The paper is structured as follows: In Section II we analyse the main approaches to MHR prediction. In Section III we define the main concepts of FDA and functional regression. In Section IV we detail the experimental approach to predict MHR from sub-maximal exercise tests. In Section V we show the results obtained by the proposed method, as well as from other regression methods. In Section VI we discuss the primary findings of this study. In Section VII we describe the system architecture and its integration with the AMS of the High Performance Center. Finally, in Section VIII we summarize the benefits of our approach as well as the future work.

II. RELATED WORK

Numerous attempts have been made to derive a formulae for MHR from experimental evidence. Table 1 summarises the main studies that only take into account the effect of age. Identified papers (*i*) are indexed in scientific journals, (*ii*) contain both male and female participants, (*iii*) have no participant age limit, (*iv*) contain a prediction based on a maximal exercise test, and (*v*) have more than 5 participants per group. As we can see, formulas have different slopes and intercepts, which reflects the great disparity of results obtained when adjusting a simple regression model. The σ^* column shows the standard deviation of the error obtained with the dataset used in this paper with the formulas proposed by the different authors, while the r^2 column shows the coefficient of determination published by authors. The standard deviation of residuals is very similar in all cases, although the best result was obtained by Tanaka equation [13].

As most of age-based methods produce unacceptably large predictive errors [8], subsequent multivariate equations to predict MHR have been developed. Multivariate approaches are represented in Table 2. These approaches add explanatory variables that include, but are not limited to: ethnicity, data that can be extracted from treadmill or cycle ergometer tests, the participant's level of habitual activity and the protocol used [14]. Despite the additional variables, the predictive power of multivariable equations is no better than univariate equations, as we can see in the σ^* column.

The above proposals, both univariate and multivariate, are intended to be easily interpretable by clinicians or practitioners. This is why more complex regression approaches have not been applied in this context, e.g., support vector machines or multilayer perceptron. However, nowadays, we can apply better and more complex strategies to predict MHR thanks to technological advances in measuring devices.

It should be mentioned that high dimensionality of data also hinders the use of these methods from the interpretability perspective, in addition to the significance of the adjusted model and variables. In this context, they need to be combined with a dimensionality reduction method, such as Principal Components Analysis (PCA) or selection variable techniques [15]. PCA may change the data-space drastically and ignore dimensions with lower variance/information, thus affecting the performance of the regression method. Accordingly, the application of PCA requires an important knowledge of data [15]. On the other hand, variable selection methods, such as Lasso, often work poorly in high collinearity

TABLE 1. Univariate equations for MHR prediction.

Study	Ref.	N	Pop.	$\overline{\text{Age}}$(range)	MHR=	r^2	σ^*
Robinson	[20]	92	Healthy Men	30(6-76)	$212.0 - 0.775 \cdot A$	0.00	7.339
Lester	[9]	48	Women & Men Trained	N/A	$205.0 - 0.410 \cdot A$	0.34	7.431
Lester	[9]	148	Women & Men Untrained	43(15-75)	$198.0 - 0.410 \cdot A$	N/A	9.140
Bruce	[21]	2091	Healthy Men	44(36-54)	$210.0 - 0.662 \cdot A$	0.19	7.357
Bruce	[21]	1295	Hypertension	52(44-60)	$204.0 - 1.070 \cdot A$	0.24	13.256
Bruce	[21]	1295	Coronary heart disease	52(44-60)	$204.0 - 1.070 \cdot A$	0.13	13.256
Bruce	[21]	2091	Hypertension + CHD	44(36-54)	$210.0 - 0.662 \cdot A$	0.10	7.357
Cooper	[22]	2535	Healthy Men	43(10-80)	$217.0 - 0.845 \cdot A$	N/A	9.150
Ellestad	[23]	2583	Healthy Men	42(10-60)	$197.0 - 0.556 \cdot A$	N/A	11.553
Sheffield	[24]	95	Women	39(19-69)	$216.0 - 0.880 \cdot A$	0.58	8.225
Astrand	[25]	100	Healthy Men	50(20-69)	$211.0 - 0.922 \cdot A$	N/A	7.247
Hossack	[26]	104	Healthy Women	(20-70)	$206.0 - 0.597 \cdot A$	0.21	7.147
Hossack	[26]	98	Healthy Men	(20-73)	$227.0 - 1.067 \cdot A$	0.40	13.930
Londeree	[14]	N/A	National Level Athletes	N/A	$206.3 - 0.711 \cdot A$	0.72	7.487
Hammond	[27]	156	Heart Disease	53.9	$209.0 - 1.000 \cdot A$	0.09	8.656
Rodeheffer	[28]	61	Healthy Men	(25-79)	$214.0 - 1.020 \cdot A$	0.45	7.159
Jones	[29]	100	Healthy Women & Men	(15-71)	$202.0 - 0.720 \cdot A$	0.52	9.916
Jones	[29]	60	Healthy Women	(20-49)	$201.0 - 0.630 \cdot A$	N/A	9.540
Ricard	[30]	193	Treadmill Women & Men	N/A	$209.0 - 0.587 \cdot A$	0.38	7.491
Ricard	[30]	193	Women & Men	N/A	$200.0 - 0.687 \cdot A$	0.44	10.967
Morris	[31]	1388	Heart Disease	57(21-89)	$196.0 - 0.900 \cdot A$	0.00	17.621
Morris	[31]	244	Healthy Men	45(20-72)	$200.0 - 0.720 \cdot A$	0.30	11.412
Whaley	[32]	754	Women	41.3(14-77)	$209.0 - 0.700 \cdot A$	0.37	7.064
Whaley	[32]	1256	Men	42.1(14-77)	$214.0 - 0.800 \cdot A$	0.36	7.921
Miller	[33]	89	Women & Men Obese	42	$200.0 - 0.480 \cdot A$	0.12	8.629
Inbar	[34]	1424	Healthy Women & Men	46.7(20-70)	$205.8 - 0.685 \cdot A$	0.45	7.508
Graettinger	[35]	114	Healthy Men	(19-73)	$199.0 - 0.630 \cdot A$	0.22	10.980
Froelicher	[36]	1317	Healthy Men	38.8(28-54)	$207.0 - 0.640 \cdot A$	0.18	7.100
Fernhall	[37]	276	Mental Retardation	9-46	$189.0 - 0.560 \cdot A$	0.09	18.582
Fernhall	[37]	296	Healthy Women & Men	N/A	$205.0 - 0.640 \cdot A$	0.27	7.528
Schiller	[38]	53	Women Hispanic	46(20-75)	$213.7 - 0.750 \cdot A$	0.56	8.201
Schiller	[38]	93	Women Caucasian	46(20-75)	$207.0 - 0.620 \cdot A$	0.44	7.091
Tanaka	[13]	285	Sedentary Women & Men	N/A	$212.0 - 0.700 \cdot A$	0.66	7.821
Tanaka	[13]	229	Endurance Women & Men	N/A	$205.0 - 0.600 \cdot A$	0.66	7.340
Tanaka	[13]	514	Healthy Women & Men	(18-81)	$208.0 - 0.700 \cdot A$	0.66	7.081
Gellish	[39]	132	Healthy Women & Men	(27-78)	$207.0 - 0.700 \cdot A$	N/A	7.238
Gellish	[39]	132	Healthy Women & Men	(27-78)	$192.0 - 0.007 \cdot A^2$	N/A	9.965
Shargal	[40]	20691	Healthy Men	N/A	$208.609 - 0.716 \cdot A$	0.47	7.056
Shargal	[40]	7446	Healthy Women	N/A	$209.273 - 0.804 \cdot A$	0.55	7.144
Arena	[41]	4796	Healthy Women & Men	43(31-55)	$209.2 - 0.720 \cdot A$	0.61	7.053

$\overline{\text{Age}}$ = mean age; σ^* = standard deviation in this study; MHR = maximum heart rate; A = age.

TABLE 2. Multivariate equations for MHR prediction.

Study	Ref.	N	Pop.	$\overline{\text{Age}}$(range)	Regression (MHR=)	r^2
Londeree	[14]	23K+	N/A	(5-81)	$196.7 + 1.986 \cdot C2 + 5.361 \cdot E + 1.490 \cdot F4 + 3.730 \cdot F3 + 4.036 \cdot F2 - 00006 \cdot (A^4/1000) - 0.542 \cdot A^2$	0.77
Londeree[1]	[14]	23K+	N/A	(5-81)	$199.1 + 0.119 \cdot A \cdot E \cdot F4 + 0.112 \cdot A \cdot E + 6.280 \cdot E \cdot F3 + 2.468 \cdot C2 + 3.485 \cdot F2 - 0.00006 \cdot A^4 - 0.591 \cdot A$	0.78
Londeree[2]	[14]	23K+	N/A	(5-81)	$205.0 - 3.574 \cdot T1 + 8.316 \cdot E - 7.624 \cdot F5 - 0.00004 \cdot A^4 - 0.624 \cdot A^2$	0.85
Londeree[3]	[14]	23K+	N/A	(5-81)	$205.0 - 0.116 \cdot A \cdot E \cdot F3 - 0.223 \cdot A \cdot F5 + 0.210 \cdot A \cdot E + 6.876 \cdot E \cdot F3 + 2.091 \cdot C2 - 3.310 \cdot T1 - 0.0005 \cdot (A^4/1000) - 0.654 \cdot A$	0.86
Londeree	[14]	23K+	N/A	(5-81)	$202.8 - 0.533 \cdot A - 00006 \cdot (A^4/1000)$	0.73
Mahon	[43]	52	Children	(7-17)	$166.7 + 0.460 \cdot RHR + 1.160 \cdot MOF$	0.29
Mahon	[43]	52	Children	(7-17)	$158.4 + 0.440 \cdot RHR + 0.680 \cdot A$	0.26
Gelbart	[44]	627	Athletes	13.7(9-17.8)	$168.0 + 0.259 \cdot RHR - 0.156 \cdot BM + 0.891 \cdot MET + 0.256 \cdot BFP$	0.25
Gelbart	[44]	627	Athletes	13.7(9-17.8)	$186.0 + 0.250 \cdot RHR - 0.140 \cdot BM$	0.21

[1] Prediction of interaction MHR
[2] Prediction of cross sectional MHR
[3] Prediction of cross sectional-interaction MHR
$\overline{\text{Age}}$ = mean age; MHR = maximum heart rate; a=age; C2=continent (if European, then C2=1, otherwise C2=0); E=ergometer (if treadmill, then E=1, if bicycle then E=0); F#=fitness level (if sedentary, F2=1, otherwise F2=0; if active, then F3=1, otherwise F3=0; if endurance trained, then F4=1, otherwise F4=0; if collegiate athlete, then F5=1, otherwise F5=0); Type# =type of exercise protocol (if continuous and incremental, then T1=1, otherwise T1=0); MET = metabolic equivalent of task; MOF = maturity offset; RHR = resting HR; BFP = body fat percent; BM = body mass (kg).

contexts [16] and, moreover, are difficult to interpret. Moreover, it is often difficult to carry out an inferential process on the true significance of the selected variables (the problem of post-selection inference). Although there has been much research on this topic, models are currently limited to linear [17] or Lasso [18] regressions, and not for universal approximators such as neural networks or support vector machines.

In this paper, we use FDA to reduce the error in the MHR prediction, avoiding the aforementioned problems of collinearity and high dimensionality and, at the same time, establishing the significance of the introduced variables. FDA is better suited to this task, since it allows the analysis of dense sampling of observations over time, on the assumption that the generation of these observations is influenced by certain smooth functions. This should be the case of MHR prediction since that heart rate increase in exercise of curvilinear way with changes in different zones of metabolic exchange [19].

III. FUNCTIONAL DATA ANALYSIS

Finite discrete time series are usually treated as multivariate data. However, this approach ignores important information about the stochastic process that generated the data. Thus, it is sometimes useful to consider a more general object as the unit of measurement under study. FDA provides the techniques to analyse, model, and predict time data series when the intrinsic structure of the data is functional, i.e. when there is an underlying function that gives rise to the observed data. In this paper we worked under the hypothesis that several observations of cardiac stess test may have a functional structure.

A. FUNCTIONAL REPRESENTATION

FDA considers each observation as a function (or curve) $X_k(t)$, on a compact interval $I = [0, T]$ on the real line. These functions can be viewed as the realizations of a one-dimensional stochastic process, often assumed to be in a Hilbert space, such as $L^2(\mathcal{I}) = \{f : I \to \mathbb{R} \text{ such as } \|f\|_I < \infty\}$, where $\|f\|_I$ is the norm induced by the following inner product $\langle f, g\rangle_I = \int_I fgdx$.

In this context, high-dimensional functions such as $X_k(t)$ are modelled using a low-dimensional approximation. One approach is to use a set of basis functions $\{\phi_i\}_{i=1}^m$ to characterize the functional space, where m is the number of data recorded for the observation. Thus, each observation $X_k(t)$ can be transformed in an estimated function $\hat{f}_k = \sum_{i=1}^m \hat{c}_{ik}\phi_i(t)$, where $\hat{c}_{ik}$ are the coefficient for the k-th observation. Coefficients are usually calculated using the minimum square criterium, while basis functions are orthonormal basis by which the maximum of variance of the data can be described, such as Fourier bases, B-splines, or functions obtained from functional principal components analysis [42].

B. LINEAR REGRESSION MODEL

Traditional linear models with scalar response $Y \in \mathbb{R}$ and vector covariate $X \in \mathbb{R}^p$ can be expressed as:

$$Y = \beta_0 + \langle X, \beta\rangle + \epsilon = E(Y|X) + \epsilon \tag{1}$$

using the inner product in the Euclidean vector space, where β_0 and β are the regression coefficients (intercept and slope of each covariate). The error ϵ is assumed to be a gaussian random variable with mean zero.

In this paper, we assume $X(\cdot) \in L^2(\mathcal{I})$ and use the $L^2(\mathcal{I})$ inner product to support a functional response. Furthermore, we use a centered stochastic process $X^C(t) = X(t) - \mu(t)$ instead of $X(t)$:

$$\begin{aligned} Y &= \beta_0 + \left\langle X^C, \beta\right\rangle + \epsilon \\ &= \beta_0 + \int_I X^C(t)\beta(t)dt + \epsilon \end{aligned} \tag{2}$$

where $\beta(t) \in L^2(I)$.

When $X(t)$ and $\beta(t)$ are representatives using an orthonormal basis $\{\phi_i(t)\}_{i=1}^\infty$ then $X(t) = \sum_{i=1}^\infty c_i\phi_i(t)$, $\beta(t) = \sum_{i=1}^\infty b_i\phi_i(t)$, and equation 2 is equivalent to:

$$Y = \beta_0 + \sum_{i=1}^{\infty} c_i b_i + \epsilon \tag{3}$$

In practice, the sum is truncated to the first K terms:

$$Y \approx \beta_0 + \sum_{i=1}^{K} c_i b_i + \epsilon \tag{4}$$

This estimation is equivalent to a lineal multivariate regression model using normal regression equations [42].

C. ADDITIVE REGRESSION MODEL

In this paper, we use the classic additive regression model [45], but with functional covariates [46], since it allows the use of non-linear relationships between the data. Let us suppose that $X = (X_1, \ldots, X_p)$ is a p-dimensional functional random variable in $L^2(\mathcal{I}_1) \times L^2(\mathcal{I}_2) \times \cdots \times L^2(\mathcal{I}_p)$ space, where $\mathcal{I}_k$ denote X_k domain, and Y is a random response variable. The relationship between the variables X and Y in a spectral additive regression model (*GSAM*) is:

$$E(Y|X) = \beta_0 + \sum_{k=1}^{p} f_k(X_k) \tag{5}$$

where each f_k is a smooth function and $E(f_k(X_k)) = 0$ for all $k \in \{1, \ldots, p\}$.

Every functional variable X_k (with $k = 1, \ldots, p$) can be expressed as follows using Karhunen-Loeve theorem:

$$X_k(t) = \mu(t) + \sum_{j=1}^{\infty} c_{kj}\phi_{kj}(t) \tag{6}$$

where $\phi_{kj}(t)$ is the j-th eigenfunction for the k-th functional variable and c_{kj} is a score term. Thus, equation (5) can be approximated as follows:

$$E(Y|X) \approx \beta_0 + \sum_{k=1}^{p}\sum_{m=1}^{r_k} f_k(c_{km}) \tag{7}$$

where c_{mk} is the m-th principal component score of the k-th functional covariate and r_k is the number of principal components considered for the k-th functional covariate.

TABLE 3. Participant characteristics.

	196 Men				
	Min	**Max**	$\overline{x}$	$\widetilde{x}$	**RMSE**
Age	10.00	46.00	18.46	17.00	5.85
Weight (kg)	35.20	132.00	72.56	70.45	17.37
Height (cm)	108.00	194.00	174.77	176.00	9.90
MHR (b·min^{-1})	175.00	215.00	195.88	196.50	8.20
	164 Women				
	Min	**Max**	$\overline{x}$	$\widetilde{x}$	**RMSE**
Age	13.00	44.00	16.53	16.00	3.75
Weight (kg)	40.40	77.10	58.08	58.45	6.54
Height (cm)	151.50	179.00	164.84	164.00	6.01
MHR (b·min^{-1})	178.00	218.00	196.84	197.00	7.92

$\overline{x}$ = mean; $\widetilde{x}$ = median; RMSE = root mean square error.

The estimation of the smooth functions is carried out using the technique known as principal component analysis with conditional expectation (PACE). This method selects automatically the number of eigenfunctions to be chosen for every functional covariate by means of the AIC criterion [46].

IV. RESULTS

A. EXPERIMENTAL APPROACH TO THE PROBLEM

A maximal, incremental treadmill test designed to elicit VO_2 max was used to elicit MHR. MHR was recorded at the end of the test and predicted using a number of traditional uni and multivariate approaches. In addition, FDA was applied to the HR data captured every 5 seconds for the first 6-minutes of the incremental test to predict MHR. The predicted MHR values from the different approaches were compared to the actual MHR at the termination of the incremental test to establish the magnitude of predictive error.

B. SUBJECTS

Three hundred and sixty participants (164 women and 196 men), aged between 10 and 46 of age, participated in this study. All the participants were competitive athletes from different sports including: athletics, badminton, handball, basketball, cycling, football, judo, wrestling, canoeing, rowing, squash, taekwondo, triathlon and sailing (see Table 3). The data were obtained from a continuous, incremental treadmill protocol, and collected from the High Performance Center of Pontevedra (Spain) between the years 2010-2015. Prior to the study, informed consent was obtained from all individual participants included in the study, where they were under 18 years of age parental assent was given. The study received institutional ethical approval and conformed to the Helsinki declaration.

C. PROCEDURES

Prior to the treadmill test, stature and mass were recorded. All participants then completed a maximal incremental treadmill test. The treadmill test began at 6 $km \cdot h^{-1}$ increasing by 0.25 $km \cdot h^{-1}$ every 15 seconds until exhaustion. Every 5 seconds throughout the test, HR and breath by breath expired gases were recorded on a Jaegger CPX master screen gas analyser, which was calibrated according to the manufacturer's instructions before each test.

The accuracy of the proposed new method for estimating MHR was based on comparing the MHR at the end of the test (the point of exhaustion), with the MHR predicted from data collected during the first 6-minutes of the test analysed using FDA. For example, a similar approach has been successfully applied to predict maximum oxygen uptake in athletes [47].

The HR data collected every 5 seconds were plotted against time and then analysed using FDA. During the first 6 minutes of the test participants reached approximately 70% of the treadmill speed attained at the point of exhaustion.

D. STATISTICAL ANALYSIS

The analysis consisted, firstly, of adjusting linear regressions for age. We then added more explanatory variables, such as height, weight and sex as categorical variables. The choice of predictive variables was carried out using a stepwise forward selection. A significance test with a post-selection inference [48] was applied to the variables of the regression model. In a second step, a functional additive model with functional covariates was adjusted using information from the HR in the first six minutes of the exercise test. Finally, we selected the additive model [46] (see [49] for more information about additive models), since it achieved the best results.

In all the cases, the r^2 and the standard deviation of the residuals were calculated. All statistical analyses were performed with the statistical software R. Stepwise regressions were implemented with the *selectiveInference* package [50], while the regression models with functional covariates have been fitted with the *fda.usc* package [51].

V. RESULTS

Firstly, a linear regression model was adjusted, and found sex, weight, and height to be statistically non-significant. The best model from our data was (a) $MHR = 209.9 - 0.77 \cdot \text{age}$. This highlights that MHR is predicted, to a large extent, by age alone and is independent of sex, height, and weight.

TABLE 4. Goodness-of-fit of a linear and functional regressions for the dataset considered in this study.

Regression type	Model (MHR=)	r^2	RMSE
Linear regression	$209.9 - 0.77 \cdot A$	0.238	7.044
Functional regression	$s(HR_{[0,6]}) + s(dHR_{[0,6]}) + s(HR^{max}_{[0,6]}) + s(A)$	0.737	4.143

r^2 = r-squared; RMSE = root mean square error; MHR = maximum heart rate; A = age.

Finally, a model containing functional and scalar covariates was fitted: (b) $MHR = s(HR_{[0,6]}) + s(dHR_{[0,6]}) + s(\text{age})$ where $HR_{[0,6]}$ and $dHR_{[0,6]}$ are the HR and the derivative of HR in the first six minutes of the treadmill test, respectively. The function $s(\cdot)$ denotes an additive effect over the variable. Other covariates, such as the second derivative of HR, were also considered during the experimentation. However, these variables were not statistically significant, and the fitted regression model did not improve the predictive capacity.

Table 4 shows the goodness-of-fit of the former three models. The r^2 and the standard deviation of the residuals are used as measurement error. The new model reduces the prediction error compared to the traditional regression models, as reflected by the substantial r^2 increase and the reduction in the standard deviation of the residuals. The increase in precision is clearly visible in Figure 1, where errors of the functional and linear models are represented as HR residual plots, respectively. The error of traditional models reaches 20 $b \cdot min^{-1}$ while the functional model does not exceed 10 $b \cdot min^{-1}$ (50-80% of the observations have an error below 3 $b \cdot min^{-1}$).

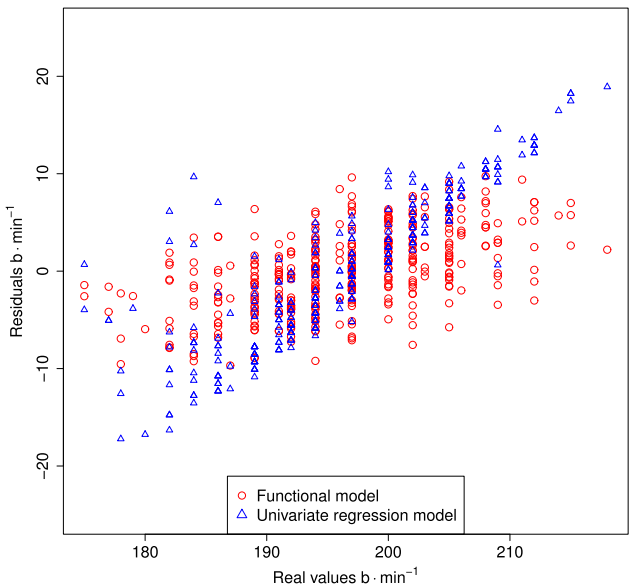

FIGURE 1. Comparison of residual produced by the functional model and the linear regression model.

A. COMPARISON WITH OTHER REGRESSION MODELS

Table 5 compares the performance of our solution with three other regression methods: Support Vector Machines (SVM), Multilayer Perceptron (MLP) and Random Forest (RF).

TABLE 5. Comparison of the goodness-of-fit between different regression methods for a 10-fold cross validation.

Regression type	r^2	RMSE
Functional regression	0.62	4.50
MLP	0.35	5.77
RF	0.46	5.34
SVM	0.48	5.33

r^2 = r-squared; RMSE = root mean square error.

These methods were selected because they are universal function approximators (UFA), and thus are able to approximate any continuous function from a sufficiently large amount of data. In addition, all methods are among the five best regressor families [52]. We limited the experimentation to the former three methods since the objective of this study was not a thorough comparison, but to show that our approach is able to fit models with a similar predictive capacity as some of the best machine learning regressors.

We used the implementations of SVM, MLP, and RF available in the *e1071* [53], *neuralnet* [54], and *randomForest* [55] R packages, respectively. Data were split in two datasets for training and test, containing 80% and 20% of the data, respectively. We used the *Caret* package [56] to optimize the hyper-parameters of the former statistical methods during the training phase, using a grid search over parameter ranges, in a 10-fold cross-validation.

SVM regression was configured with a radial basis function (RBF) kernel, $k(x, y) = \exp(-\gamma \cdot \|\text{x-y}\|^2)$, which is a universal kernel [57], a necessary condition to ensure UFA property. The γ parameter was configured to range between 2^{-5} and 2^5. The value of γ in the best model was 2^{-4}.

The MLP was set up with three hidden layers, up to 15 neurons per hidden layer. We decided not to experiment with more neurons per hidden layer to avoid over-fitting. The backpropagation algorithm was set as supervised learning technique for training. We experimented with three small learning rates (0.1, 0.01, and 0.001) to avoid an unstable training process and learning a sub-optimal set of weights too fast. The number of neurons in the hidden layers for the optimal model was 5, 5, and 10.

Finally, we used the default values for the number of trees to grow (500) and for the minimum size of terminal nodes (5 for regression) in RF. The number of variables available for splitting at each tree node (*mtry* parameter) was set to range between 2^0 and 2^3. The value of *mtry* in the best model was 2^2, which coincides with the recommended value for regressions (the number of variables divided by three, rounded down) [58].

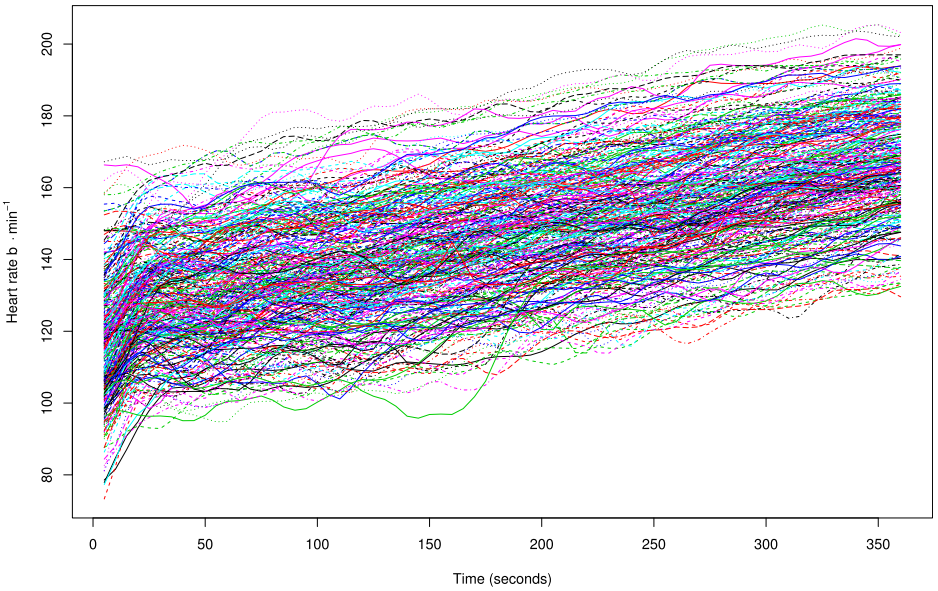

FIGURE 2. Heart rate in the first 6-minutes of the stress test.

In the experiment, we used the same variables as those of the functional model but with the difference that a PCA is carried out previously, selecting 7 components combining 98.4% of explained variance. As listed in Table 5, functional regression predictions are slightly better. Certainly, the high dimensionality and structure of the data have a greater impact on the other regressors. This is particularly apparent for the MLP which obtains the worst results, despite using three hidden layers and small learning rates. In the case of SVM, the low γ value of the best model is an indication of a Gaussian function with a large variance. Thus, two points can be considered similar even if they are far from each other, similarly as in a linear regression. Finally, RF obtains similar results as SVM, although 18% worse than the functional regression.

B. INTERPRETABILITY AND SIGNIFICANCE OF RESULTS

Figure 2 shows the evolution of the HR over time. Each curve represents the submaximal test of a participant. As can be seen, the relationship between these two variables is not linear. Moreover, the variations are smooth and progressive.

Figure 3 depicts the HR derivative over the 6-minutes. In this case, the evolution of the derivative is heterogeneous and individualized. Despite this fact, this derivative is an important element in the prediction.

Table 6 shows the significance of the functional variables *HR* and *dHR*. Specifically, it shows the p-value associated with the coefficient $c_{k,j}$ of Eq. 6 for each one of the k-dimensions of the FPCA. As we can see, the p-value of $s(HR_{[0,6]})$ is lower than 0.05 for all scores but the first one, which means that the dimension with more variance is the less significant. The same happens for variable *dHR*.

TABLE 6. P-value of functional variables.

Variable	Score	p-value
$s(HR_{[0,6]})$	1	0.897
$s(HR_{[0,6]})$	2	0.021
$s(HR_{[0,6]})$	3	$8.29e-06$
$s(HR_{[0,6]})$	4	$2.27e-05$
$s(HR_{[0,6]})$	5	$7.75e-04$
$s(dHR_{[0,6]})$	1	0.087
$s(dHR_{[0,6]})$	2	$5.24e-11$
$s(dHR_{[0,6]})$	3	0.001
$s(dHR_{[0,6]})$	4	$4.70e-04$
$s(dHR_{[0,6]})$	5	$9.78e-04$

TABLE 7. Estimate value and p-value of non-functional variables.

Variable	Estimate	p-value
(Intercept)	201.83057	$< 2e-16$
age	-0.31374	$5.85e-07$

Table 7 shows the significance of non-functional variables. Results show that *HR* decreases 0.31374 per year.

VI. DISCUSSION

The primary finding of the present study are that traditional uni and multivariate methods of predicting MHR based on age contain large predictive errors. This study is the first to use FDA to predict MHR, finding that it significantly increased the accuracy of MHR prediction compared to traditional models. The margin of error from FDA was low, with a mean predictive error 4.1 $b \cdot min^{-1}$ and a maximum error of 10 $b \cdot min^{-1}$. This compared to a mean error of 7.0 and a maximum error of almost 20 $b \cdot min^{-1}$ when using the univariate and multivariate approaches. Furthermore, we found

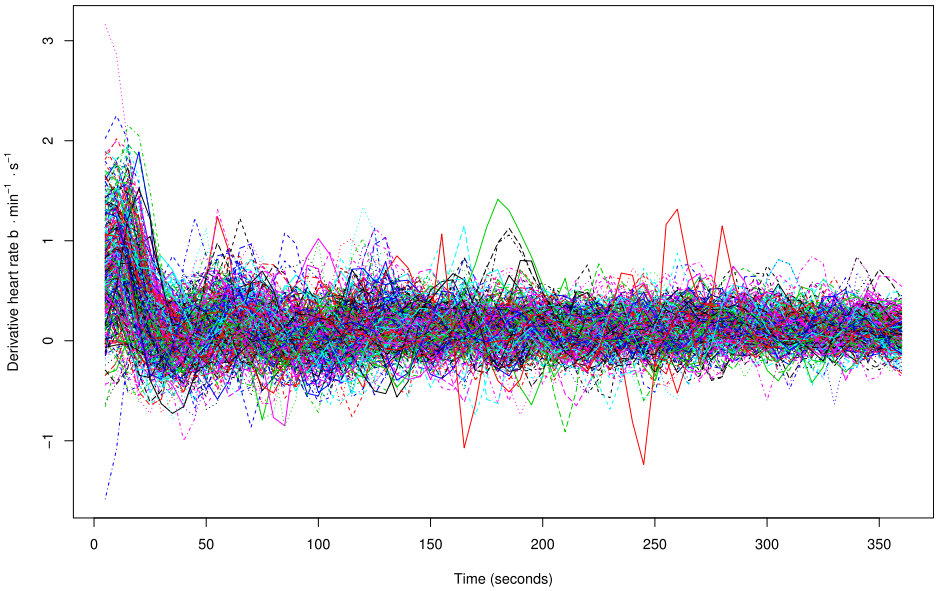

FIGURE 3. Derivative of the heart rate in the first 6-minutes of the stress test.

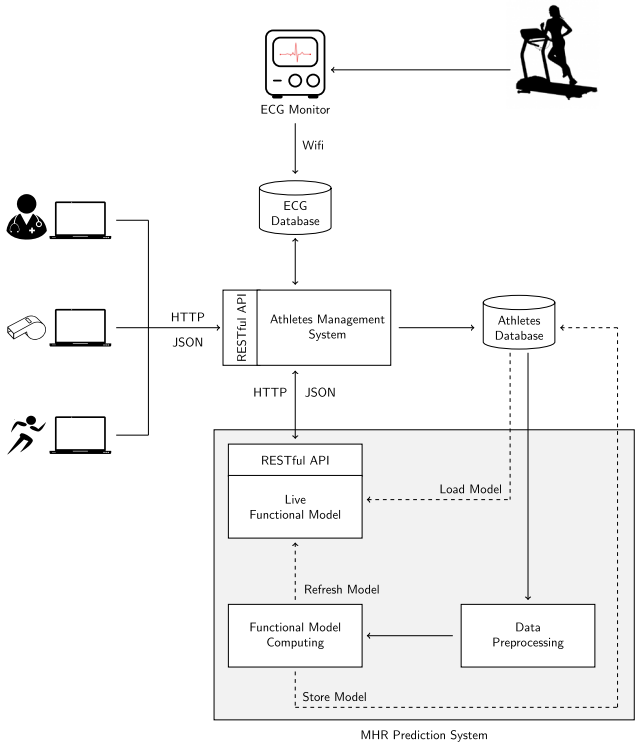

FIGURE 4. System architecture.

that MHR prediction to be independent of sex, height, and weight.

Reducing predictive error through the use of FDA could have benefits for both practitioners and exercise prescription. The importance of this cannot be understated considering the implications of an incorrect MHR value when interpreting treadmill test data, in both clinical and exercise settings, and also for exercise prescription. In the context of cardiovascular fitness assessment, a stress test is usually terminated when participants reach a stipulated percentage of predicted MHR (e.g., 85% MHR) [59]. Errors in excess of $10-20\ b \cdot min^{-1}$, higher or lower, could result in a premature test termination, overexertion or inaccurate predictions of VO_2 max. For exercise prescription, HR training zones are often determined based on percentages MHR. Prediction errors could therefore lead to inaccurate training intensities resulting in the loss of the desired effects of the training plan, or overtraining. Reduced predictive error, together with its relative simplicity, make FDA a valuable tool for use in situations where a maximal stress test cannot be utilised.

Using a univariate approach Tanaka and colleagues Tanaka et al. [13] derived the formulae of $208-(0.7\cdot$ age) and $209-(0.7\cdot$ age) from a meta-analysis and experimental data respectively. This is very similar to our univariate formula of $209-(0.77\cdot$ age), however we did observe a large discrepancy in r^2 values. This could be explained by the different populations. Our participants were all from sporting backgrounds and aged between 10 and 46, whereas Tanaka et al's [13] participants were aged between 18 and 81, with a wide variation in habitual physical activity levels. In a similar age range to this study, a subset of participants aged between 10 to 33 was used but a high predictive error was found [25]. Arena et al. [41] derived the formulae $209.2-(0.72\cdot$ age) which has the lowest RMSE ($7.053\ b \cdot min^{-1}$) of all traditional univariate approaches, although their participant's average age was approximately 20 years older. This predictive error is close to the RMSE ($7.044\ b \cdot min^{-1}$) of the formulae adjusted by our linear regression, but still 41% worse than the predictive error of FDA model. Using a multivariate approach, we saw no improvement in predictive power. The best equations in the previously literature

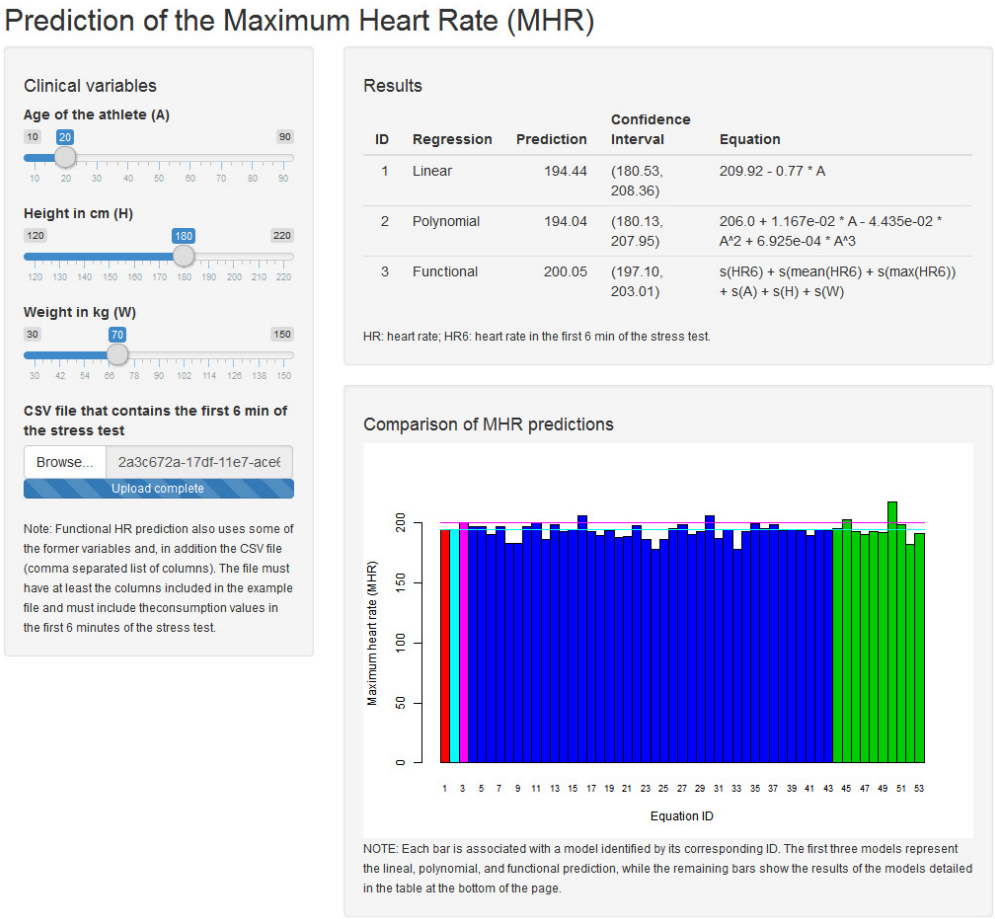

FIGURE 5. Screenshot of the MHR prediction web application.

Londeree and Moeschberger [14] obtained a good fit, with a RMSE of 7.077 $b \cdot min^{-1}$, similar to our linear regression. Some formulae listed in Appendix were not tested since some variables could not be calculated from the information available in our dataset.

While the novel application of FDA has resulted in a much reduced predictive error, it does require the use of a 6-minutes treadmill test during which time HR must be collected every 5 seconds. The treadmill test is sub-maximal, with participants only reaching an average of 70% of the running speed during the maximal test, therefore it is relatively easy to perform for athletic populations, even in children as young as 10. Further research is required to see the extent to which this method would need to be modified for clinical, older or sedentary populations. This study utilised a ramp protocol, whether the same results can be achieved with square wave increments or different modes of exercise is unknown. In this new era of personalized diagnostics and treatments [60] in which the models should be adjusted individually from the enormous amount of the data collected on each patient, often in real time, the functional data analysis is a valuable tool. Although in this paper our approach is based on dense functional data, as data are regularly spaced and captured at high frequency, other functional approaches can be better suited depending on the data structure. For instance, a sparse functional data is better aligned to deal with irregularly spaced longitudinal data [61], where the number of repeated measurements available per subject is small. Moreover, situations in which only partial information on the variables of interest is available also require a censored data approach [62].

From a methodological point of view, FDA is able to take advantage of all the information recorded by the ECG to build reproducible models, as demonstrated by the variables significance. In addition to the model robustness, FDA obtains better results than other universal function approximators such as SVM and MLP. Moreover, SVM and MLP can have behave far from the ideal in contexts of collinearity with finite samples. FDA has also the advantage that statistical inference can be directly applied to the model, contrary to SVM and MLP that are black boxes.

VII. SYSTEM IMPLEMENTATION

The system architecture developed for the High Performance Center of Pontevedra (Spain) is depicted in Figure 4. The core of the infrastructure is the Athletes Management System (AMS), which manages all the information generated for

and by sportsmen and sportswomen. AMS provides several web interfaces, where each one is targeted to a specific profile such as medical staff, coaches, or sportsmen and sportswomen. In this paper, AMS was extended with new functionalities to improve training planning using the predicted MHR.

As aforementioned, HR is measured by electrodes on the chest of athletes running on the treadmill. However, we plan to use HR bands in the future to reduce the cost but also to facilitate the measurement of cardiac stress outside medical facilities. It is also intended to create various predictive models based on HR variability to detect future episodes of overtraining [63].

Although electrocardiogram data are stored in a proprietary software, we developed a module to extract these data and to integrate them in the AMS database. After each new sub-maximal stress test, a trigger invokes the prediction service to estimate the MHR. The patient profile is then updated to adjust training loads taking this new MHR prediction or other physiological measurement into account. Furthermore, stress test data are accessible by the medical staff and by the athlete, as well as MHR predictions. The web interface also shows a comparative study between the last tests.

Finally, we also developed a public web interface using the *Shiny* [64] R package to access the MHR predictor.[1] In this application (Figure 5) the user can input the age, mass, stature, and the HR from the initial 6-minutes of the stress test in a CSV file. This application calculates the prediction and its confidence interval. In addition, it also provides a histogram in which the prediction is compared with all the multivariate and univariate equations described in tables 1 and 2.

VIII. CONCLUSION

This is the first paper to utilise functional data analysis (FDA) in the prediction of maximal HR. In this paper we recorded HR every 5 seconds during the first 6-minutes of a sub-maximal incremental treadmill test. By applying FDA to the data of a heterogeneous sample, we were able to predict MHR with far lower predictive than the traditional approaches currently available. The new approach proposed has important benefits for clinicians and practitioners when using MHR to evaluate fitness or prescribe exercise.

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