**Abstract**

Neural networks have excelled at regression and classification problems when the input space consists of scalar variables. As a result of this proficiency, several popular packages have been developed that allow users to easily fit these kinds of models. However, the methodology has excluded the use of functional covariates and to date, there exists no software that allows users to build deep learning models with this generalized input space. To the best of our knowledge, the functional neural network (FuncNN) library is the first such package in any programming language; the library has been developed for R and is built on top of the keras architecture. Throughout this paper, several functions are introduced that provide users an avenue to easily build models, generate predictions, and run cross-validations. A summary of the underlying methodology is also presented. The ultimate contribution is a package that provides a set of general modelling and diagnostic tools for data problems in which there exist both functional and scalar covariates.

**Keywords**: functional inputs, deep learning, R, keras.

1. **Introduction**

In recent years, deep learning methodologies have become the standard approach for prediction problems. For example, He, Zhang, Ren, and Sun (2016) broke previous benchmarks by developing deep neural networks with over a hundred hidden layers; this was made possible by an innovation brought upon by a simple adjustment of the algorithm – adding the output of a previous layer back into the layers following it. Another set of examples can be found in any one of the annual ImageNet Large-Scale Visual Recognition Challenges (Krizhevsky, Sutskever, and Hinton 2012; Russakovsky, Deng, Su, Krause, Satheesh, Ma, Huang, Karpathy, Khosla, Bernstein et al. 2015) where neural networks are consistently on the podium. These innovations naturally sparked the development of software that supplied users with an arsenal of tools to apply these methods.

There is a wide array of software available in multiple programming languages that implements a variety of methods in deep learning and neural networks. For example, R packages nnet (Venables and Ripley 2002) and neuralnet (Fritsch, Guenther, and Wright 2019) are standard sets of tools in the training of and prediction from neural networks using the Broyden-Fletcher-
Goldfarb-Shanno (BFGS) algorithm and backpropagation, respectively. Both of these allow for some flexibility in terms of user selected activation functions and error measurements, but vastly more broad selections of tools are available within the RSNNS (Bergmeir and Benítez 2012) and keras (Allaire and Chollet 2020) application programming interfaces (API), which may be used in both R and Python. Both of these make detailed user customization possible and are intended to facilitate the development of deep learning models and methodologies.

Central to this paper is functional data analysis (FDA), an area of modern applied statistics that has witnessed swift development due to its ability to deal with a large and distinct class of statistical problems. In particular, it is often the case that data is collected at high resolution at many points in space or time, resembling and being treated as a smooth function - this is known as functional data. FDA is used instead of the standard approach of analysing single points when we are interested in framing an analysis of a set of points as if they are samples from a specific curve.

Presently, the primary software for FDA in any programming language is the fda package (Ramsay, Graves, and Hooker 2020) in R, designed to accompany the textbooks of Ramsay and Silverman (2005) and Ramsay, Hooker, and Graves (2009). The main functionality within the package revolves around functional regression, allowing users to fit regression models where one or several of the response and explanatory variables are functions instead of scalar valued. Several packages in R build upon this base by extending standard statistical methods to functional data. For example, funHDDC (Schmutz and Bouveyron 2019) and funFEM (Bouveyron 2015) handle functional clustering, FDbost (Brockhaus and Ruegamer 2018) applies gradient boosting in functional regression and GPFDA (Shi and Cheng 2014) incorporates functional regression as the mean response in Gaussian processes, among other packages. Another library, fda.usc (Febrero-Bande and Oviedo de la Fuente 2012), streamlines the fitting process of many common functional modelling approaches such as non-parametric functional regression (Ferraty and Vieu 2006) and functional partial least squares methods (Aneiros-Pérez and Vieu 2006). Additionally, the BFDA package (Yang and Ren 2019) in MATLAB provides a library for Bayesian FDA.

To the best of our knowledge, the applications of these packages do not extend to include deep learning models. For this reason, this paper introduces the FuncNN package, which allows users to include functions as input variables in neural networks and implements the theoretical discussion in Thind, Multani, and Cao (2020) and Rossi and Conan-Guez (2005). This methodology has been shown to outperform many other functional and multivariate methods in a number of real world and simulated examples as seen in Thind et al. (2020).

The FuncNN package introduces several functions. The primary function fnn.fit(), grants users the ability to effortlessly generate models for their data; they also gain access to several customization options in the form of hyperparameters. The output of this function can be acted upon by several other functions within the package such as fnn.predict() and fnn.fnc() which serve to be predictive and visualization functions. Moreover, we introduce tuning and cross-validation functions aptly named fnn.tune() and fnn.cv(), respectively. The package is readily available on CRAN can be installed as follows:

R> install.packages("FuncNN")

Or through GitHub using the devtools (Wickham, Hester, and Chang 2020) package:

R> devtools::install_github("b-thi/FuncNN")
The rest of the article is organized as follows: Section 2 explores some of the theoretical background associated with the package. In Section 3, the bulk of the functions are presented, including the model building and prediction functions; some visualization tools are also showcased with accompanying examples. In Section 4, helper functions such as those for cross-validation and tuning are detailed. Lastly, Section 5 includes concluding thoughts and scheduled updates for the package.

2. Functional neural networks (FNN)

The conventional neural network is a contiguous combination of hidden layers, each of which contains some number of neurons. Let \( n_u \) denote the number of neurons in the \( u \)-th hidden layer. We can define the first hidden layer (denoted by the superscript) as: \( \mathbf{v}^{(1)} = g \left( \mathbf{W}^{(1)} \mathbf{x} + \mathbf{b}^{(1)} \right) \), where \( \mathbf{x} \) is a vector of \( J \) covariates, \( \mathbf{W}^{(1)} \) is an \( n_1 \times J \) weight matrix, \( \mathbf{b}^{(1)} \) is the bias (or the intercept), and \( g : \mathbb{R}^{n_1} \rightarrow \mathbb{R}^{n_1} \) is some activation function that transforms the resulting linear combination (Tibshirani, Hastie, and Friedman 2009). The vector \( \mathbf{v}^{(1)} \) is \( n_1 \)-dimensional and becomes the input to the next layer i.e., it takes the place of the \( \mathbf{x} \) in the proceeding layer.

Observe that the classic neural network framework only permits the vectors (of the \( n_1 \) observations) \( \{\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N\} \) to contain elements that are finite scalar values. We now consider the case when \( \mathbf{x}_\ell : \ell \in \{1, ..., N\} \) can be a combination of functional and scalar inputs. In this scenario, the input space takes the following form:

\[
\text{input}_\ell = \{x_1(t), x_2(t), ..., x_K(t), z_1, z_2, ..., z_J\},
\]

where \( K \) and \( J \) are the number of functional and scalar covariates, respectively. This set is unique for each of the \( N \) observations. With this generalization, the \( i \)-th neuron of the first hidden layer corresponding to each of the \( \ell \) observations takes the form (Thind et al. 2020):

\[
v^{(1)}_i = g \left( \sum_{k=1}^{K} \int_{T_k} \beta_{ik}(t) x_k(t) dt + \sum_{j=1}^{J} w_{ij}^{(1)} z_j + b_i^{(1)} \right),
\]

where \( \beta(t) \) is the weight on the functional covariate; this is of a functional form because each of the \( k \) functional inputs must be weighted at every point along their domains, \( T_k \). In order to estimate \( \beta(t) \), it is rewritten as a linear combination of basis functions:

\[
v^{(1)}_i = g \left( \sum_{k=1}^{K} \int_{T_k} \sum_{m=1}^{M_k} c_{ikm} \phi_{ikm}(t) x_k(t) dt + \sum_{j=1}^{J} w_{ij}^{(1)} z_j + b_i^{(1)} \right),
\]

(1)

\[
= g \left( \sum_{k=1}^{K} \sum_{m=1}^{M_k} c_{ikm} \int_{T_k} \phi_{ikm}(t) x_k(t) dt + \sum_{j=1}^{J} w_{ij}^{(1)} z_j + b_i^{(1)} \right),
\]

(2)

In Equation (1), \( \beta_{ik}(t) \) is approximated by \( \sum_{m=1}^{M_k} c_{ikm} \phi_{ikm}(t) \) where \( \phi_{ik}(t) \) is the set of basis functions and \( c_{ik} \) is the set of basis coefficients to be estimated by the functional neural network; in Equation (2), the integral and sum are swapped and the term \( \int_{T_k} \phi_{ikm}(t) x_k(t) dt \) can be approximated using any of the usual approximation methods such as Simpson’s rule (Sājlī and Mayers 2003). Note that \( x_k(t) \) is defined by its own set of basis functions.
A by-product of this method is the set of functional weights, \( \beta(t) \), as represented by their basis expansions. These weights differ in comparison to the usual weights (found in conventional neural networks) in that they can be easily visualized over the corresponding continuum. This visualization illuminates the underlying relationship between the functional covariate and the scalar response. Moreover, passing in information in this functional form preserves the autocorrelation structure associated with the data. Due to the random initializations in the conventional neural network, these properties of the data become difficult to maintain if passed in discretely. In the canonical cases where we have more than one neuron, the average of the functional weights \( \hat{\beta}_k(t) = \frac{\sum_{i=1}^{n_1} \hat{\beta}_{ik}(t)}{n_1} \), is used as the output.

This formulation of the neural network was shown (Thind et al. 2020) to be a universal approximator just as conventional neural networks are (Cybenko 1989). While the details are omitted, the gist of the proof was to show that this form of the neuron, once simplified, held the same properties as the usual neural network.

3. Fitting, prediction, and visualization

3.1. Data description

Throughout this paper, we will focus on three main data sets: the tecator data set, the gasoline data set and the gait data set. The classic tecator data from the fda.usc package provides measurements of the near infrared absorbance spectrum and the moisture (water), fat and protein contents of 215 meat samples. Samples composed of different fat, water and protein contents may behave inconsistently in incident radiation absorption, which can be measured by absorbance spectroscopy. The data were recorded on a tecator infratec food and feed analyzer with wavelength range from 850 nm to 1050 nm using the near infrared transmission (NIT) principle. This data set consists of a list named \texttt{absorp.fdata} and a simple data frame labelled with \texttt{y}. The list \texttt{absorp.fdata} includes the matrix \texttt{data} summarizing a 100 channel spectrum of absorbance of each meat sample, where absorbance is \(-\log_{10}\) of the transmittance determined by the spectrometer, and the vector \texttt{argvals} which contains the value of the 100 discretized channels from 850 nm to 1050 nm. The data frame \texttt{y} lays out the contents of the fat, water and protein of the 215 meat samples that are determined by analytic chemistry and measured in percent. This data has been applied with the goal of classifying the fat content levels of the meat samples with the functional covariate of the near infrared absorbance spectrum and the scalar covariate of the water content.

Secondly, we consider the gasoline data set sourced from the refund package (Goldsmith, Scheipl, Huang, Wrobel, Di, Gellar, Harezlak, McLean, Swihart, Xiao, Crainiceanu, and Reiss 2019). This data set contains the near infrared reflectance (NIR) spectra and the specified octane numbers of 60 gasoline samples. For each gasoline sample, 401 NIR spectra were measured at different wavelengths, from 900 nm to 1700 nm in 2-nm intervals, and recorded using diffuse reflectance as \( \log(1/\text{reflectance}) \). As a simple data frame, the gasoline data consists of a vector containing the octane levels for each of the 60 collected samples, and a \( 60 \times 401 \) matrix regarding the details of NIR measurements. This data set has been used in examples with the aim of determining the octane number, a scalar value, of gasoline based on the functional predictor of the NIR measurements. Studies in past years (Kelly, Barlow, Jinguji, and Callis 1989; Æzdemir 2005) have supported the concept that a relationship
exists between the chemical structure and the fuel-performance property of octane, while NIR spectroscopy is a popular method for simultaneous chemical analysis. Therefore, it has been implied that the properties of gasoline with different octane levels can be reflected by different NIR spectral features.

Finally, the examples given in this paper also make use of the gait data set obtained from the fda package. This data catalogs the hip and knee angles measured in degree through a twenty-point gait cycle for 39 boys. It is in the form of an array of dimension $20 \times 39 \times 2$, indicating the 20 evenly-spaced standardized gait times (from 0.025 to 0.975), the 39 subjects of observation, and the two gait variables Hip Angle and Knee Angle, respectively. It is unsurprisingly apparent that hip rotation has a regular association with knee movement in a normal walk. Therefore, in our example, we consider using hip movement as a functional covariate to make a prediction for the functional response knee angle.

3.2. Pre-processing

The FuncNN package allows two types of inputs of data; data can be passed in raw or pre-processed. As with most functional data analysis coding, pre-processing is required to approximate the raw data $x(t)$, using basis expansions. However, this can be tedious and ultimately, a barrier for anyone who is not familiar with the required procedures. The FuncNN package provides a remedy by letting novice users input their data without the heavy lifting of converting it into its functional form while also granting the opportunity for further customization for users who require a more specific or specialized pre-processing. In the case where the data is passed in raw, the FuncNN package will do a simple pre-processing using a Fourier basis expansion with 31 terms. While this is an average-case compromise that minimizes initial effort, the alternative approach of pre-processing allows for greater flexibility in the development of $x(t)$.

Since the functional observations can be passed in two different ways, they can be one of two object types. In the raw case, the functional covariates are passed in as a $K$-dimensional list where each element of the list is an $N \times p$ data.frame() containing $p$ measurements over the domain for each of the $N$ subjects.

```r
R> func_cov_list = list(func_cov_1, func_cov_2, ..., func_cov_K)
```

The scalar covariates can be passed in similar to most predictive functions i.e., as an $N \times J$ matrix containing information on the $J$ scalar variables for each of the $N$ observations.

If pre-processing is done beforehand, then the object being passed in must be a tensor. In R, the tensor-type object exists as an array(). The dimensionality of the tensor will be $M_k \times N \times K$ where each row corresponds to the estimated coefficient when the basis expansion was made, each column is an individual observation, and each “slice” corresponds to one of the $K$ functional covariates. Note that scaling is handled internally by the fnn.fit() function. The response can be passed in as a vector of length $N$.

While the focus here is on scalar responses, the FuncNN package can handle a version of functional responses; this version entails a basis expansion of the response curves from which the basis coefficients are extracted and passed in as a matrix into the model function. The model will then attempt to predict these coefficients. More details are provided later in the article.
3.3. Classification

In this example, we will focus on the *tecator* data set. The response will be the classification of the fat content of the meat samples as “high” or “low”, denoted by 1 and 0, respectively. The threshold is 25 percent i.e., if the fat content of a sample is greater than 25, then we designate the response associated with that sample as 1:

```r
R> tecator_resp = as.factor(ifelse(tecator$y$Fat > 25, 1, 0))
```

We use the water content of the meat samples as a scalar covariate; as alluded to earlier, this will be stored in a `data.frame()` object.

```r
R> tecator_scalar = data.frame(water = tecator$y$Water)
```

Since this is a prediction problem, we split the data into a training and test set; a random sample of 75% of the data will be used to build the model and evaluation is performed on the rest. We will let the modelling function handle the pre-processing for this example and therefore, the object type to be passed in must be a list which can be generated as follows:

```r
R> func_covs_train = list(train_x)
R> func_covs_test = list(test_x)
```

where `func_covs_train` and `func_covs_test` are the functional covariate matrices for the training and test sets, respectively (in this example, there is just one functional covariate). Finally, we can fit the model:

```r
R> fit_class = fnn.fit(resp = train_y,
+                   func_cov = func_covs_train,
+                   scalar_cov = scalar_train,
+                   domain_range = list(c(850, 1050)),
+                   raw_data = T)
```

```
[1] "Evaluating Integrals:"
[++]|++++++++++++++++++++++++++++++++++++++++++++++++++| 100% elapsed=06s
```

The first item printed refers to the integral approximations that take place as shown in Section 2; a progress bar is printed indicating the proportion of work completed in this phase. The training error plot for this model is in Figure 1 – note that this output is a `ggplot()`.
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(Wickham 2016) object; this is the same type of object you would extract from the keras package. As with any Keras model, you can observe the total number of parameters of the model in the display (in this case, 4886); this printing of information can be muted by setting print_info to FALSE. There are a number of hyperparameters that will be discussed later in the article; in this simple example, we stick to the defaults. The only additional specifications required in the model are to indicate that raw data is being passed in (the default is set to FALSE) and the range of the domain. This simple syntax removes the steep learning curve that comes with functional methods in some of the other packages discussed earlier. The output contains a Keras model object as well the generated functional observations (if the raw data was passed in), parameter information, and error rates over the training iterations. Additional information about the output object can be found in the R documentation for the FuncNN package. We now have a fitted model to make predictions with. As with most predictive functions, when one uses fnn.predict(), the fitted model is passed in along with the “new data” e.g., the func_covs_test object from before (along with the scalar counterpart).

R> predict_class = fnn.predict(fit_class,
+ func_cov = func_covs_test,
+ scalar_cov = scalar_test,
+ domain_range = list(c(850, 1050)),
+ raw_data = T)

The syntax is similar again. The function will automatically recognize that this is a classification problem and output class probabilities (the sum of each row will be 1). We can round these probabilities to get classifications and plot the confusion matrix (using the caret package (Kuhn 2020)); this is showcased in the following code chunk:

R> caret::confusionMatrix(as.factor(rounded_preds), as.factor(test_y))

Confusion Matrix and Statistics

Reference
The **FuncNN** Package

| Prediction | 0 1 |
|------------|-----|
|            | 0 40 0 |
|            | 1 1 13 |

**Accuracy :** 0.9815  
95% CI : (0.9011, 0.9995)  
**No Information Rate :** 0.7593  
P-Value [Acc > NIR] : 6.299e-06

**Kappa :** 0.9506

**Mcnemar’s Test P-Value :** 1

**Sensitivity :** 0.9756  
**Specificity :** 1.0000  
**Pos Pred Value :** 1.0000  
**Neg Pred Value :** 0.9286

We can also visualize the relationship between the functional covariates and the scalar response by way of the functional weights using the **fnn.fnc()** function. The syntax is fairly straight-forward:

```R
R> fnc_tec = fnn.fnc(fit_class, domain_range = list(c(850, 1050)))
```

As a point of interest, the **fnc** part of the **fnn.fnc()** function stands for functional neural coefficient; this is legacy code naming convention but as a reference, anytime this is mentioned, it refers to the functional weights of the model. For this function, we only need to pass in the model along with the domain. The output will be the effect of the functional weight on the response over the continuum as estimated by the functional neural network; these can be made sense of at times, however, contextual information is required. We do hazard that because of the plethora of other parameters in the network, it can be difficult to interpret these parameters – these interpretations should be considered carefully on a case-by-case basis. In this example, we observe that there seems to be two primary spikes over the continuum. The resulting functional weight from this model is given in Figure 2.

### 3.4. Regression

We now consider an example of a regression problem; we will investigate the relationship between the near-infrared reflectance spectra (functional covariate) and and octane values (scalar response) of 60 gasoline observations in the **gasoline** data set. In this example, we will process the raw data beforehand and then pass it into **fnn.fit()**; we will also use multiple functional covariates by taking the derivatives of the functional data estimated using the raw data. In order to generate the functional observations, we use 9 Fourier basis functions. The **Data2fd()** function from the **fda.usc** package will allow us to create these functions with the following code:

```R
R> nbasis = 9  
R> spline_basis = create.fourier.basis(c(900, 1700), nbasis)
```
Figure 2: The functional weight estimated through the functional neural network for the tecator data set. We observe two spikes. We also note that the magnitude of the effect depends on the scale of both the functional data and the functional weight.

```r
R> gasoline_fd = Data2fd(timepts, t(gasoline[,,-1]), spline_basis)
R> gasoline_deriv1 = deriv.fd(gasoline_fd)
R> gasoline_deriv2 = deriv.fd(gasoline_deriv1)
```

where `gasoline_fd` is the functional data object converted from the functional predictor. As alluded to earlier, when the data is pre-processed manually out of the function, we have to pass it in as a tensor object i.e., `arrays` in R. We can develop the array with the following code:

```r
R> gasoline_data = array(dim = c(nbasis, 60, 3))
R> gasoline_data[,1] = gasoline_fd$coefs
R> gasoline_data[,2] = gasoline_deriv1$coefs
R> gasoline_data[,3] = gasoline_deriv2$coefs
```

We now fit the model using a functional weight defined with five basis functions. In this initial release, we allow users to use Fourier and B-spline basis functions for the functional weights. Note that we specified the learning rate and the number of epochs in this model as well, along with the number of layers – these are just some of the numerous hyperparameters that can be adjusted in this function.

```r
R> gasoline_example <- fnn.fit(resp = train_y,
+ func_cov = gasoline_data_train,
+ scalar_cov = NULL,
+ basis_choice = c("bspline"),
+ num_basis = c(5),
+ hidden_layers = 2,
+ neurons_per_layer = c(64, 64),
+ activations_in_layers = c("relu", "linear"),
+ domain_range = list(c(900, 1700)),
+ epochs = 300,
+ learn_rate = 0.0001,
+ early_stopping = T)
```
Observe the warning present in the output – the *FuncNN* package has many stop checks built to provide clear information to the user regarding errors and warnings. In this case, we had 3 functional covariates but only specified information for one functional weight - i.e., we specified the functional weight to be a B-spline expansion of five terms. To make up for the lack of information, `fnn.fit()` will just repeat this same setup for all of the inputted functional covariates.

Again, we provide the Keras model information. We observe that there were 5249 parameters being trained during the model building process. The error plot is given in Figure 3 – observe that the *early_stopping* parameter was triggered in this case so the plot does not extend to the specified 300 epochs. More information on this parameter is provided later in the article. Predictions are handled using the same function, `fnn.predict()`: again, the only difference

**Figure 3**: The iterative error plot over the training process as measured by mean squared error for the *gasoline* data set.

will be that the output will be a vector of values as opposed to a matrix containing class probabilities.
3.5. Functional responses

To demonstrate functional responses, we will predict knee movement using hip movement with the information presented in the gait data set. While we present a straightforward approach to functional response prediction, we will update the package with a more refined and sophisticated approach as we continue to develop such methodology. The approach used in the following example boils down to predicting the coefficients of the functional data object corresponding to the response. To begin, we read in the data and generate our functional observations:

\[
R> \text{hipbasis13 = create.fourier.basis}(c(0,1), 13) \\
R> \text{kneebasis11 = create.fourier.basis}(c(0,1), 11) \\
R> \text{timepts = as.numeric(rownames(gait))} \\
R> \text{hip_fd = Data2fd(timepts, gait[,1], hipbasis13)} \\
R> \text{knee_fd = Data2fd(timepts, gait[,2], kneebasis11)}
\]

In this example, we use 13 and 11 basis functions to generate the hip and knee observations, respectively. The pre-processing is done in a manner similar to that of the regression case above. A notable point is that the response will now be a \(N \times M_{\text{resp}}\) matrix object where \(N\) is the number of functional observations and \(M_{\text{resp}}\) is the number of basis functions used to define these observations – the values in the matrix correspond to the estimated basis coefficients (in this example, we have 11 per observation).

We now fit the model using four layers containing 64 neurons each with relu (Hahnloser, Sarpeshkar, Mahowald, Douglas, and Seung 2000) activation function. The learning rate was selected after a small grid search.

\[
R> \text{gait_fit <- fnn.fit}(\text{resp = resp_train,} \\
+ \quad \text{func_cov = data_train,} \\
+ \quad \text{hidden_layers = 3,} \\
+ \quad \text{activations_in_layers = c("relu", "relu", "relu"),} \\
+ \quad \text{neurons_per_layer = c(128, 128, 32),} \\
+ \quad \text{epochs = 300,} \\
+ \quad \text{learn_rate = 0.0007})
\]

The error plot corresponding to this model is given in Figure 4. This model was, thus far, the most parameter heavy of the examples with a total of 22,027. Predictions are made in a
similar manner as before; the output object will be a matrix with a number of columns equal to that of $M_{\text{resp}}$ and a row dimensionality the same as the number of functional observations in the test set.

```r
R> predictions = fnn.predict(model = gait_fit, 
+ func_cov = data_test)
```

To visualize the results, the `fnn.plot()` function can be used which will output the evaluations of the functional response prediction over the domain. The syntax consists of specifying the prediction object, the domain, a step size which determines how finely evaluations are made, and the type of basis function to be used for the plot.

```r
R> gait_func_pred = fnn.plot(predictions, 
+ domain_range = c(0, 1), 
+ step_size = 0.05, 
+ Basis_Type = "fourier")
```

Using these predictions, we can compare our predicted curve to the true functional response; Figure 5 shows one such comparison.

4. Model improvement tools

4.1. Hyperparameters

Thus far, we have generated models largely using the default settings of the FuncNN package; however, there is ample opportunity to adjust these models so that they are best suited for a particular context. These adjustments come by way of toying with the hyperparameter options available to us in the modelling process.
Figure 5: A comparison of a knee angle prediction $\hat{y}(t)$ over a 1 second interval (functional response) with the observed movement, $y(t)$.

| Parameter       | Type       | Details                                                                 |
|-----------------|------------|-------------------------------------------------------------------------|
| $\beta(t)$      | Estimated  | Coefficient function found by the FNN.                                  |
| $w$             | Estimated  | The scalar covariate weights.                                           |
| $b$             | Estimated  | The intercept in each neuron.                                           |
| Number of layers | Hyperparameter | The depth of the FNN.                                         |
| Neurons per layer | Hyperparameter | Number of neurons in each layer of the FNN.                      |
| Learn rate      | Hyperparameter | The learning rate of the FNN.                                       |
| Decay rate      | Hyperparameter | A weight on the learning process across training iterations for the FNN. |
| Validation split | Hyperparameter | The split of training set during learning process.                    |
| Functional weight basis | Hyperparameter | The size of $M$ for the estimation of $\beta(t)$.              |
| Training iterations | Hyperparameter | The number of learning iterations.                                   |
| Batch size      | Hyperparameter | Subset of data per pass of the FNN.                                   |
| Activations     | Hyperparameter | The choice of $g(\cdot)$ for each layer.                             |
| Early stopping  | Hyperparameter | Stops the model building process if no improvement in error.           |
| Dropout         | Hyperparameter | Randomly drops some specified percentage of neurons from one layer to the next. |

Table 1: A list of the parameters in the network.

Some parameters, such as the ones seen explicitly in Equation 1, are estimated through gradient descent - i.e., the "learning" process of the model results in the final values. Others, such as the number of hidden layers and the neurons within each of these layers, are adjusted for by the user. For example, as demonstrated earlier in the article, the `early_stopping` option halts the learning process when significant decreases in error have not been observed for some number of training iterations – this number, known as the patience parameter, is also a hyperparameter. Another example is that of the learning rate, $\gamma$, and the decay rate, which both govern how quickly we move in the direction of the gradient. The complete list of hyperparameters along with descriptions is provided in Table 1.

4.2. Cross-validation

A first step in choosing parameter values in any modelling process is to find a reliable measuring stick to assess how a model performs. One approach to solving this problem is cross-validation. The general definition for a k-fold cross-validation error is
MSPE = \sum_{k=1}^{K} \sum_{l \in S_k} \left( \hat{y}_l^{(-k)} - y_l \right)^2 / (|S_k|K)

where \{S_k\}_{k=1}^{K} is a partition of the data set, |S_k| denotes cardinality, and \( \hat{y}_l^{(-k)} \), \( l \in S_k \), is the predicted value for \( y_l \) obtained by training the functional neural network using data points with indices not contained in \( S_k \). Choosing to measure error in this way ensures that our measurement is computed using data that was not used to train the model, reducing the bias relative to other estimations of test error.

This paradigm is at the core of \texttt{fnn.cv()}, the package’s cross-validation function. Much of the syntax overlaps with the \texttt{fnn.fit()} function. We demonstrate the cross-validation function using the \texttt{gasoline} data set. Instead of splitting the data into test and training sets, we can pass in the entire data set – the cross-validation function will take care of this internally. The \texttt{nfolds} option determines the number of subsets in our partition of the full data set – this is the only syntax difference between the \texttt{fnn.fit()} and \texttt{fnn.cv()} functions.

```r
R> gasoline_cv <- fnn.cv(nfolds = 10,
+   resp = octane,
+   func_cov = gasoline_data,
+   scalar_cov = NULL,
+   basis_choice = c("bspline", "bspline", "bspline"),
+   num_basis = c(5, 5, 5),
+   hidden_layers = 2,
+   neurons_per_layer = c(64, 64),
+   activations_in_layers = c("relu", "linear"),
+   domain_range = list(c(900, 1700),
+                      c(900, 1700),
+                      c(900, 1700)),
+   epochs = 300,
+   learn_rate = 0.0001,
+   early_stopping = T)
```

While the function is running, the number of completed folds will be displayed and updated, for example:

```
[1] "Folds Done: 1"
[1] "Folds Done: 2"
...```

The output will contain the overall cross-validated error as well as the errors corresponding to each fold. The indices for each fold split will also be available for users if they choose to reproduce the function results manually. In this example, a 10-fold cross-validation was done and the MSPE was 0.0735. We look to improve on this in the next section.

4.3. Tuning

Having honed in on a more robust measure of error, we can begin to outline the tuning approach, which consists of a classic grid search to develop testable combinations of hyper-parameters. Algorithm 1 below details the tuning process used in \textbf{FuncNN}.
Algorithm 1: Tuning (Hyperparameter optimization)

**Input:** A subset of all possible values for each of the hyperparameters of interest, including: number of hidden layers, number of neurons, number of training iterations, percentage of split, patience, learning rate, number of basis functions, and activation function.

**Output:** The optimal set of hyperparameters ($\eta$) over all combinations of the elements in Input

1. Input the grid, along with the functional and scalar observations, and set the non-tuning hyperparameters, e.g., type of basis functions, number of folds ($k$) for cross-validation, rate of decay, etc.
2. Generate all possible combinations of hyperparameters, denoted $\eta_1, \eta_2, ..., \eta_n$, where $n$ is the total number of combinations.
3. For each hyperparameter combination $\eta_i$, $i = 1, ..., n$
4. Construct the functional neural network with $\eta_i$
5. Train the designed functional neural network
6. Calculate the $k$-fold cross-validation error $\text{MSPE}(\eta_i)$

End

Return $\eta = \{\eta_k : \text{MSPE}(\eta_k) \leq \text{MSPE}(\eta_i) \text{ for all } i\}$

The **FuncNN** package makes this intuitive and easy. There is no automated pre-processing for the tuning function, **fnn_tune()**; this decision was made due to efficiency concerns but will be remedied for in the future. The syntax is as follows:

```r
defn_tune(tune_list, 
             resp, 
             func_cov, 
             scalar_cov = NULL, 
             basis_choice, 
             domain_range, 
             batch_size = 32, 
             decay_rate = 0, 
             nfolds = 5, 
             cores = 4, 
             raw_data = F)
```

Some of these have already been presented before. The ones to note are the `tune_list` and `cores` parameters. The latter is an efficiency parameter that allows for parallelization. This is handled internally by the dependency **future** (Bengtsson 2020). The former must be a list object that contains the grid of combinations to be tested. An example of what this list might look like is:

```r
R> tune_list_gasoline = list(num_hidden_layers = c(2), 
                          +     neurons = c(32, 64), 
```

This object is not processed as obviously as it may seem. We assign each of the hidden layer choices (in this case, just the one choice of 2 hidden layers) all combinations of neurons and activation functions. This is exemplified below:

```
L1_Act L2_Act FW_1 FW_2 FW_3 L1_N L2_N Epochs ValSplit Patience LearnRate
1 relu relu 5 5 5 32 32 250 0.2 15 0.000100
2 relu relu 5 5 7 32 64 250 0.2 15 0.000550
3 relu relu 5 5 5 32 64 250 0.2 15 0.000550
4 relu relu 5 5 5 32 64 250 0.2 15 0.001000
5 relu relu 5 5 5 32 64 250 0.2 15 0.000100
6 relu relu 5 5 7 32 32 250 0.2 15 0.000325
7 relu relu 5 5 5 32 32 250 0.2 15 0.000325
8 relu relu 5 5 5 64 32 250 0.2 15 0.001000
9 relu relu 5 5 5 32 32 250 0.2 15 0.000775
10 relu relu 5 5 5 64 32 250 0.2 15 0.000100
11 relu relu 5 5 9 32 32 250 0.2 15 0.000550
12 relu relu 5 5 7 32 32 250 0.2 15 0.000550
13 relu relu 5 5 5 32 32 250 0.2 15 0.000550
14 relu relu 5 5 5 32 32 250 0.2 15 0.001000
15 relu relu 5 5 5 64 32 250 0.2 15 0.000325
```

Observe that we are cycling through all of the possible combinations of neuron numbers, activation functions, and functional weight basis counts from the list. We did not need to specify the number of neurons for each layer separately. While this is less obvious of an approach than allowing the user to set the grid for each layer, it is much more efficient when one considers that they may want to be tuning over many layers. For example, tuning over 10 hidden layers in the traditional approach would require a list object that contains over 30 elements, whereas in this case, the length of the list remains the same no matter how many layers you are attempting to tune for.

Having set up the tuning list, we can now consider the code required to run the tuning function:

```
R> gasoline_tuned = fnn.tune(tune_list = tune_list_gasoline,
+   resp = octane,
+   func_cov = gasoline_data,
+   basis_choice = c("fourier", "fourier",
+                     "fourier"),
+   domain_range = list(c(900, 1700),
+                       c(900, 1700),
+                       c(900, 1700)))
```
With respect to `nftolds`, we see that the tuning comparisons will be done with a 2-fold cross-validated error. Increasing this number, as expected, will increase the computational time of this function. You may tune for a multiple number of layers at once. In that case, the grid above is reproduced for each hidden layer. The output will be a list object containing the final grid (as seen above), the cross-validated MSPE values for every combination, the best from each choice of layers, and the overall best across all layers (along with the corresponding parameters).

While the functions runs, we took advantage of the `pbapply` package (Solymos and Zawadzki 2019) to provide users with a progress bar.

```
|++++++++++++++++++++++++++++++++++++++++++++++++ | 94% ~3m 49s
```

This progress bar displays the approximate amount of time remaining until the tuning is finished; this information offers some obvious benefits to a user’s quality of experience.

Our goal for this tuning (applied to the `gasoline` data set) was to significantly outperform the cross-validated error from the default settings presented before. After running the tuning function, the optimal parameters over the pre-defined grid were:

```
R> gasoline_tuned$Parameters

$MSPE
[1] 0.002492664

$num_basis
[1] 7 9 9

$hidden_layers
[1] 2

$neurons_per_layer
[1] 32 32

$activations_in_layers
[1] "sigmoid" "relu"

$epochs
[1] 250

$val_split
[1] 0.2

$patience_param
[1] 15
```
$\text{learn\_rate}$
[1] 0.001

Using these parameter choices, we can run the cross-validation function again (with ten folds for the purposes of comparison under equivalent circumstances):

```r
R> gasoline_tuned_cv <- fnn.cv(nfolds = 10,
+   resp = octane,
+   func_cov = gasoline_data,
+   scalar_cov = NULL,
+   basis_choice = c("bspline", "bspline",
+                   "bspline"),
+   num_basis = c(7, 9, 9),
+   hidden_layers = 2,
+   neurons_per_layer = c(32, 32),
+   activations_in_layers = c("sigmoid", "relu"),
+   domain_range = list(c(900, 1700),
+                       c(900, 1700),
+                       c(900, 1700)),
+   epochs = 250,
+   learn\_rate = 0.001,
+   early\_stopping = T)
```

And the resulting cross-validated MSPE was 0.0043. The results are summarized in Table 2:

| Model   | CV MSPE | Standard error |
|---------|---------|----------------|
| Default | 0.0735  | 0.0534         |
| Tuned   | 0.0043  | 0.00275        |

Table 2: Tuning vs. default model results.

We observe a much smaller standard error on our tuned model, indicating a greater level of consistency with respect to the predictions. The high variance in the default model suggests that there is some propensity for that particular model to overfit the data; it seems that behaviour is largely contained in the tuned model.

5. Conclusion and future work

Functional data analysis is an emerging field where new and exciting research is being conducted through a different data paradigm than the usual multivariate lens; this paper has illustrated how the functions introduced in the FuncNN take advantage of this paradigm and allow users to generate useful models which apply deep learning to functional data. Since FuncNN package is built on top of the Keras architecture, many of the numerous parameters available to users implementing Keras models are also available for the software introduced here.
Throughout the article, we presented a number of functions. This includes core functions such as those for model fitting (\texttt{fnn.fit()}) and predicting (\texttt{fnn.predict()}) but also additional convenience functions for easier validation of analysis (e.g., \texttt{fnn.cv()}, \texttt{fnn.tune()}). These functions were highlighted with the use of examples including those in the context of regression, classification, and functional responses.

A number of updates to the package have been scheduled including the introduction of more core Keras options. We also are working on a better parallelization of the underlying processes to help with efficiency. Lastly, while we presented one way of handling functional responses in this article, there is a novel extension that is being worked on – this approach will also be available in future versions of \texttt{FuncNN}.

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## A. Computational times for all models

| Section                      | Method      | Run time |
|------------------------------|-------------|----------|
| 3.3 - Classification         | fnn.fit()   | 13.0s    |
| 3.3 - Classification         | fnn.predict() | 2.22s   |
| 3.3 - Classification         | fnn.fnc()   | 0.170s   |
| 3.4 - Regression             | fnn.fit()   | 4.22s    |
| 3.4 - Regression             | fnn.predict() | 2.45s   |
| 3.4 - Regression             | fnn.fnc()   | 0.410s   |
| 3.5 - Functional responses   | fnn.fit()   | 5.61s    |
| 3.5 - Functional responses   | fnn.predict() | 0.410s |
| 3.3 - Functional responses   | fnn.plot()  | 0.230s   |
| 3.5 - Functional responses   | fnn.fnc()   | 0.270s   |
| 4.2 - Cross-validation       | fnn.cv()    | 1m12s    |
| 4.3 - Tuning                 | fnn.tune()  | 8h24m    |

Table 3: Computational run times for every function used in this article from the **FuncNN** package.
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