# Neural Networks with Functional Response

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## Introduction

In functional data analysis (FDA), the regression of a functional response on a set of predictors can be a challenging task, especially if the relation between those predictors and the response is nonlinear. In this work, we adapt neural networks, a machine learning technique, to solve this problem.

We design a feed-forward neural network (NN) to predict functional curves with scalar inputs, using the following procedure:

1. Transform the functional response to a finite-dimensional vector of coefficients.
2. Construct a NN with those coefficients as outputs and the scalar predictors as inputs.
3. Train the NN with the proposed objective function.
4. Predict the functional response using NN outputs.

## Basic Assumptions

Suppose we have $N$ subjects, and for the $i$-th subject, the input is a set of scalar variables $\boldsymbol{X}_i = \{X_{i1}, X_{i2}, ..., X_{iP}\}$, and the output is a functional variable $Y_i(t), t \in \mathcal{T}$ in the $L^2(t)$ space.
**Note:** In reality, $Y_i(t)$ is usually measured in a discrete manner, i.e., $Y_i(t_{ij})$ at $m_i$ time points or locations $\{t_{ij}\}_{j=1}^{m_i}$, with some observation error.

## Representations of a Function (Dimension Reduction)

### - Mapping to Basis Coefficients -

In FDA, it is common to represent functions using basis expansion. Specifically, the information of $Y_i(t)$ can be summarized into a set of finite-dimensional vector of basis coefficients as:

$$Y_i(t) = \sum_{k=1}^{K} c_{ik}\theta_k(t) = \boldsymbol{\theta}'\boldsymbol{C}_i \quad (1)$$

- $\boldsymbol{\theta}$: vector of the basis functions $\theta_1(t), ..., \theta_K(t)$ from a selected basis system, e.g. Fourier or B-spline.
- $\boldsymbol{C_i}$: vector of the basis coefficients $\{c_{ik}\}_{k=1}^{K}$.
- $K$: a pre-defined truncation integer.

### - Mapping to FPC Scores -

The other popular method for dimension reduction is functional principal component analysis (FPCA). Let $\mu(t)$ and $K(t, t')$ be the mean and covariance functions of $Y(t)$, and accordingly, $K(t,t') = \sum_{k=1}^{\infty} \lambda_k\phi_k(t)\phi_k(t')$, where $\{\lambda_k, k \geq 1\}$ are the eigenvalues and $\phi_k$'s are the corresponding eigenfunctions satisfying $\int \phi_k^2(t)dt = 1$.

Denote $\tilde{Y}_i(t) = Y_i(t) - \mu(t)$ as the centered functional response, following the Karhunen-Loéve expansion, $\tilde{Y}_i$ can be approximated as:

$$\tilde{Y}_i(t) = \sum_{k=1}^{K} \xi_{ik}\phi_k(t) = \boldsymbol{\phi}'\boldsymbol{\xi}_i \quad (2)$$

- $\boldsymbol{\phi}$: vector of the first $K$ functional principal components (FPC).
- $\boldsymbol{\xi}_i$: vector of the FPC scores $\{\xi_{ik}\}_{k=1}^{K}$, where $\xi_{ik} = \int\{Y_i(t) - \mu(t)\}\phi_k(t)dt$.
- K: the truncation integer determined by the desired proportion of variance explained.

## NNBB & NNSS

### - NN for Basis Coefficients (NNBB) -

Given Eq.(1), learning how $\boldsymbol{X}$ regress on $Y(t)$ can be naturally replaced with learning how $\boldsymbol{X}$ regress on the basis coefficients $\{c_k\}_{k=1}^{K}$. Hence, we set $\{c_k\}_{k=1}^{K}$ to be a function of $\boldsymbol{X}$, with a mapping function $F(\cdot)$ from $\mathbb{R}^P$ to $\mathbb{R}^K$, as:

$$\boldsymbol{C}_i = F(\boldsymbol{X}_i) \quad (3)$$

Eq.(3) can be extended to the mapping from $\boldsymbol{X}$ to the functional response $Y(t)$ as $Y_i(t) = \boldsymbol{\theta}'F(\boldsymbol{X}_i)$.

Then we propose to apply a dense feed-forward NN as the mapping function $F(\cdot)$, and the basis coefficients $[c_{i1}, c_{i2}, ..., c_{ik}] \in \mathbb{R}^k$ are the outputs of the NN. The model can be expressed as:

$$\boldsymbol{C}_i = \text{NN}_\eta(\boldsymbol{X}_i) = g_L\left(\cdots g_1\left(\sum_{p=1}^{P} w_{1p}X_{ip} + b_1\right)\right) \quad (4)$$

- $g_1, ..., g_L$: the activation functions at each layer.
- $\eta$: NN parameter set consisting of weights $\{w_{\ell k}\}_{\ell=1}^{L}$ and bias $\{b_\ell\}_{\ell=1}^{L}$ of all hidden layers.

$\text{NN}_\eta(\cdot)$ is optimized by minimizing the objective function:

$$L_{\boldsymbol{C}}(\eta) = \frac{1}{n_{\text{train}}}\sum_{i=1}^{n_{\text{train}}}\sum_{k=1}^{K}(\hat{c}_{ik} - c_{ik})^2 \quad (5)$$

where $n_{\text{train}}$ is the number of observations in the training set, and $c_{ik}$'s are obtained following Eq.(1).

### - NN for FPC Scores (NNSS) -

Similarly, the FPC scores can represent $Y(t)$ and then act as the outputs of the NN, and we obtain:

$$\boldsymbol{\xi}_i = \text{NN}_\eta(\boldsymbol{X}_i) = g_L\left(\cdots g_1\left(\sum_{p=1}^{P} w_{1p}X_{ip} + b_1\right)\right) \quad (6)$$

and $\text{NN}_\eta(\cdot)$ is trained w.r.t. the objective function $L_{\boldsymbol{\xi}}(\eta) = \frac{1}{n_{\text{train}}}\sum_{i=1}^{n_{\text{train}}}\sum_{k=1}^{K}(\hat{\xi}_{ik} - \xi_{ik})^2$.

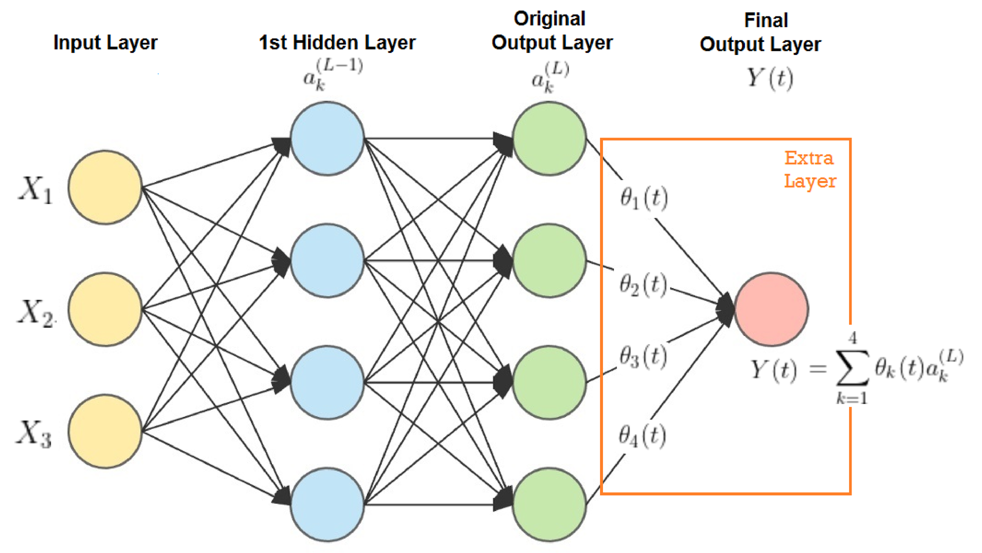
## NNBR & NNSR

We further propose to modify the objective function to directly minimize the prediction error of the response variable:

$$L_{\boldsymbol{Y}}(\eta) = \frac{1}{n_{\text{train}}}\sum_{i=1}^{n_{\text{train}}}\sum_{j=1}^{m_i}(Y_i(t_{ij}) - \hat{Y}_i(t_{ij}))^2 \quad (7)$$

**Note:** Eq.(7) is implementable because the relation between $\hat{Y}_i(t_{ij})$ and $\hat{\boldsymbol{C}}_i$ (or $\hat{\boldsymbol{\xi}}_i$) is linear, thus we can easily compute the derivative of $\hat{Y}_i(t_{ij})$ as well as the gradient of $(Y_i(t_{ij}) - \hat{Y}_i(t_{ij}))^2$ w.r.t. $\hat{\boldsymbol{C}}_i$ (or $\hat{\boldsymbol{\xi}}_i$).

NNBB (or NNSS) trained by minimizing Eq.(7) is named NNBR (or NNSR), and can be treated as a NN with an extra output layer, where the final output is the weighted sum of the original outputs.




A graphical representation of the proposed neural network with an extra output layer ($L = 2, P = 3, K = 4$).

## More Extensions

Eq.(7) can be further modified for different needs:

- **Irregularly-spaced functional data**

$$L_{\boldsymbol{Y}_{\text{irr}}}(\eta) = L_{\boldsymbol{Y}}(\eta) \cdot 1\,(Y_i(t_{ij}) \text{ is observed}) \quad (8)$$

- **Smoothness control for $\hat{Y}(t)$**

$$L_{\boldsymbol{pen}}(\eta) = L_{\boldsymbol{Y}}(\eta) + \lambda\sum_{k=3}^{K}(\Delta c_k)^2 \quad (9)$$

where $\Delta^2 c_k = c_k - 2c_{k-1} + c_{k-2}$ is the difference of a set of consecutive basis coefficients, and $\lambda$ is the smoothing parameter.

## Implementation

### - Data & Models for Comparison -

- **Data**: generated by

$$Y(t_j) = \sum_{k=1}^{10}\zeta_k(\boldsymbol{X})\psi_k(t_j) + \epsilon(t_j), j = 1, ..., 40$$

  - $\boldsymbol{X} = \{X_1, ..., X_{10}\}$: vector of random predictors.
  - $\zeta_k(\cdot)$: nonlinear functions for some $k$.
  - $\psi_k(\cdot)$: B-spline basis functions.
  - $\epsilon(\cdot)$: random noise function.
- **Models**: Function-on-scalar regression model (FoS), NNBB, NNSS, NNBR & NNSR.

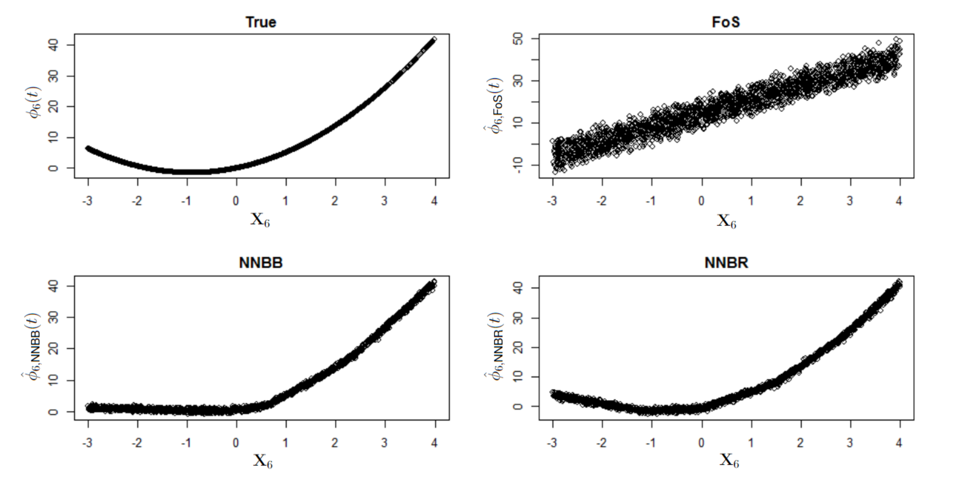
### - Results -

- **Prediction Accuracy**

| Methods | FoS | NNBB | NNSS | NNBR | NNSR |
|---|---|---|---|---|---|
| Mean | 24.5373 | 3.8478 | 5.7422 | 1.1548 | 1.7862 |
| Std. Dev. | 0.7632 | 0.7914 | 0.2055 | 0.0958 | 0.0810 |
| $p$-value | - | <2.2e-16 | <2.2e-16 | <2.2e-16 | <2.2e-16 |

Table of Mean and Standard Deviation of the MSEs between $Y(t_j)$ and $\hat{Y}(t_j)$ in the test sets (20% Obs.) of 20 replications, along with the $p$-value of the two-sided paired $t$-test which compares the MSEs of each NN-based model to those of FoS.

- **Relation Reconstruction**




Visualizations of true $\phi_6(t)$ (top left), $\hat{\phi}_{6,\text{FoS}}(t)$ (top right), $\hat{\phi}_{6,\text{NNBB}}(t)$ (bottom left), and $\hat{\phi}_{6,\text{NNBR}}(t)$ against $\boldsymbol{X}_6$ (bottom right), respectively.

## Summary

### - Highlights-

- Have superior predictive power, especially when the relation between the predictors and the response is non-linear.
- Flexible for both regularly or irregularly spaced functional data.
- Can handle a large number of predictors.

### - Limitations -

- Contain many hyper-parameters and the tuning process could be time-consuming.

### - Potentials -

- Extend to predict a multi-dimensional (mainly two-dimensional) functional response.
- Combine with existing work to construct a NN taking functional inputs and functional outputs.

## References

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