

# Estimation of the Mean Function of Functional Data via Deep Neural Networks

Guanqun Cao



Spring School on Models and Data 2021  
University of South Carolina  
*April 10th, 2021*

## Acknowledgement

- Collaborators
  - ▶ Mr. Shuoyang Wang, Auburn University
  - ▶ Dr. Zuofeng Shang, New Jersey Institute of Technology
- Partially funded by NSF award DMS-1736470
- ENAR Distinguished Student Paper Award 2021

# Outline

1

## 1 Introduction

- Functional regression model
- Deep neural networks

2

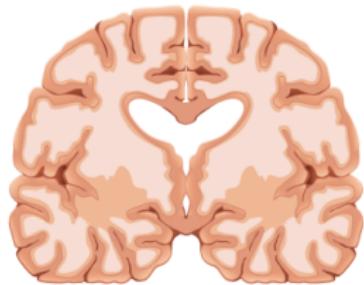
## 2 Methods

- Estimation of mean function via deep neural networks
- Non-asymptotic convergency rate

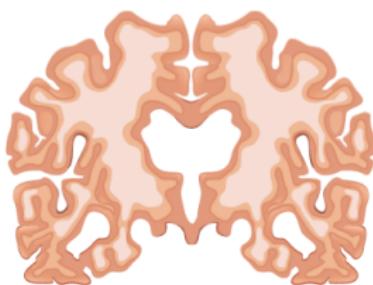
3

## 3 Real data analysis

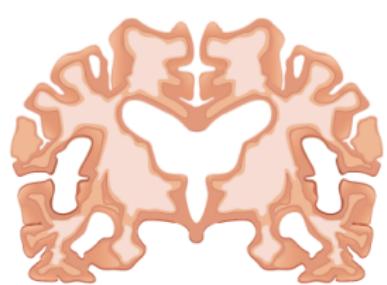
## Progression of Alzheimer's Disease



Healthy Brain



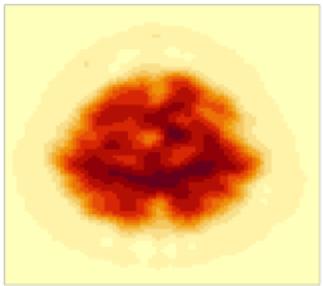
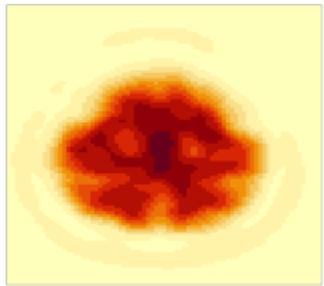
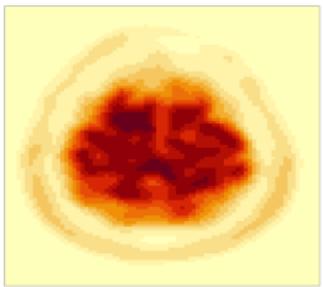
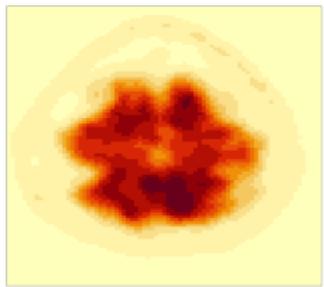
Mild Alzheimer's Disease



Severe Alzheimer's Disease

Source: <https://www.caring.com/caregivers/alzheimers/>

# Positron Emission Tomography (PET) Images



## Functional regression model

$$Y_{ij} = f_0(\mathbf{X}_j) + \eta(\mathbf{X}_j) + \epsilon_i(\mathbf{X}_j), \quad i = 1, 2, \dots, n, j = 1, 2, \dots, N,$$

- $f_0 : \mathbb{R}^d \rightarrow \mathbb{R}$ ,  $E(Y_{ij}) = f_0(\mathbf{X}_j)$ ;  $\mathbf{X}_j \in \mathbb{R}^d$ ;
- $\eta(\cdot)$ : individual curve variations; zero mean Gaussian process;
- $\epsilon_i(\cdot)$  : zero mean measurement error;
- $n$ : sample size;
- $N$ : number of observations for each subject.

How to estimate mean function  $f_0(\cdot)$ ?

# Deep neural networks

## Definition

$$f(\mathbf{x}) = \mathbf{W}_L \sigma(W_{L-1} \dots \sigma(\mathbf{W}_2 \sigma(\mathbf{W}_1 \mathbf{x} + \mathbf{v}_1) + \mathbf{v}_2) \dots + \mathbf{v}_{L-1}),$$

- $d = d_0 \rightarrow d_1 \rightarrow \dots, \dots \rightarrow d_L \rightarrow d_{L+1} = 1$  ;
- $\sigma(x) = \max(x, 0)$ : ReLU activation function;
- $\mathbf{W}_\ell : p_\ell \times p_{\ell+1}$  weight matrix;

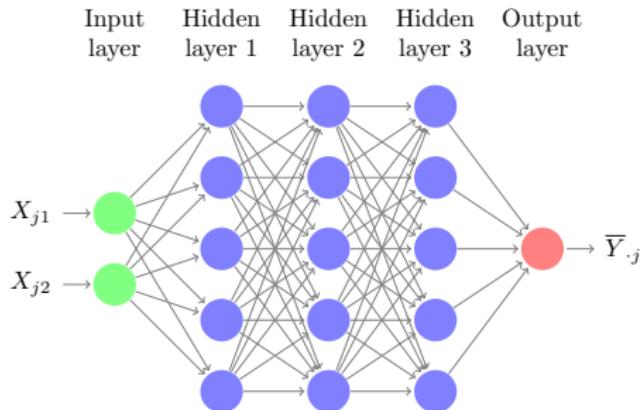
Sparse network space:

$$\mathcal{F}_{DNN}(L, \mathbf{p}, \mathbf{s}) = \left\{ f : \max_{\ell=0, \dots, L} \|\mathbf{W}_\ell\|_\infty + |\mathbf{v}_\ell|_\infty \leq 1, \sum_{\ell=0}^L \|\mathbf{W}_\ell\|_0 + |\mathbf{v}_\ell|_0 \leq \mathbf{s} \right\}$$

## Structured compositions of Hölder Functions

- $g_i : [a_i, b_i]^{d_i} \rightarrow [a_{i+1}, b_{i+1}]^{d_{i+1}}$ ,  $g_i = (g_{ij})_{j=1, \dots, d_{i+1}}^\top$ , ambient
- Each component  $g_{ij}$  is  $\beta_i$ -Hölder function with at most  $t_i$ -variate:  
$$\left\{ g_{ij} \in \mathcal{C}_{t_i}^{\beta_i} \left( [a_i, b_i]^{t_i}, K_i \right), |a_i|, |b_i| \leq K_i \right\}$$
 intrinsic
- True underlying function space:  $\mathcal{G}(q, \{d_i, t_i, \beta_i, K_i\}_{i \in [q]})$  consists of  
 $f = g_q \circ g_{q-1} \circ \dots \circ g_1 \circ g_0$
- Smoothness of  $f_i = g_q \circ g_{q-1} \circ \dots \circ g_i$   
 $\beta_i^* := \beta_i \prod_{k=i+1}^q (\beta_k \wedge 1)$

# Functional regression via Deep neural networks



## Empirical risk minimization

$$\hat{f} = \arg \min_{f \in \mathcal{F}_{DNN}} \frac{1}{N} \sum_{j=1}^N \{\bar{Y}_{\cdot j} - f(\mathbf{X}_j)\}^2,$$

where  $\bar{Y}_{\cdot j} = n^{-1} \sum_{i=1}^n Y_{ij}$ ,  $\mathbf{X}_j = (X_{j1}, \dots, X_{jd})$

## Non-asymptotic convergency rate

### Theorem 1

Under mild assumptions, with probability greater than  $(1 - \frac{2}{nN^\varrho})^{\log(nN^\varrho) + 1} \rightarrow 1$ , we have

$$\|\hat{f} - f_0\|_N^2 \leq c(nN^\varrho)^{-\frac{\theta}{\theta+1}} \log^6(nN^\varrho),$$

where  $\varrho \geq 0$ ,  $\theta = \min_{i=0,\dots,q} \frac{2\beta_i^*}{t_i}$  and  $c$  depend on true function class of  $f_0$ .

- $(nN^\varrho)^{-\frac{\theta}{\theta+1}} = (nN^\varrho)^{-\alpha}$  and  $\alpha = \min_{i=0,\dots,q} \frac{2\beta_i^*}{2\beta_i^* + t_i}$
- If  $\varrho = 0$ ,  $\|\hat{f} - f_0\|_N^2 \leq cn^{-\frac{\theta}{\theta+1}} \log^6(n)$



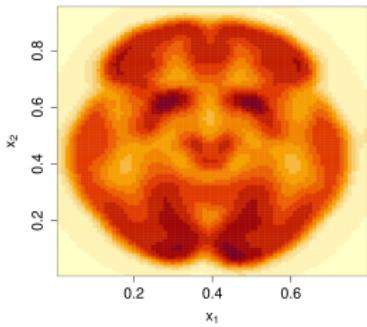
- 79 patients from the AD group.
  - ▶ 33 females
  - ▶ 46 males



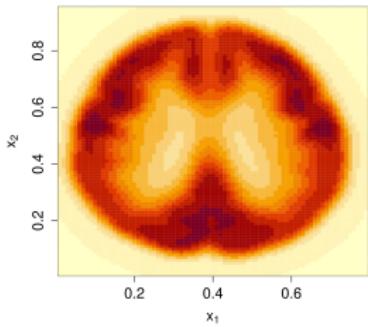
- 79 patients from the AD group.
  - ▶ 33 females
  - ▶ 46 males
- reoriented into  $79 \times 95 \times 69$  voxels.
- each patient has 69 sliced 2D images with  $79 \times 95$ .

## Recovery ( $79 \times 95$ ) from 3D scans

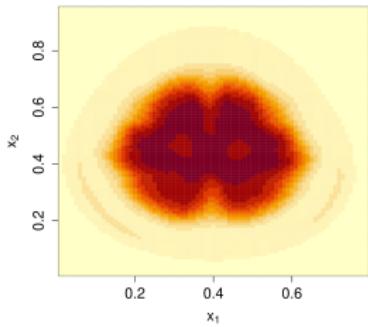
20-th



40-th



60-th





- Wang, S., Cao, G. and Shang, Z. (2020) Estimation of the Mean Function of Functional Data via Deep Neural Networks. *arxiv.org*

## R Package

<https://github.com/FDASTATAUBURN/FDADNN>.

## Assumptions

(A1) The true regression function  $f_0$  has a composition structure.

### Deep and wide neural networks

(A2)  $\hat{f} \in \mathcal{F}(L, \mathbf{p}, s)$ , s.t.

- Depth:  $L \asymp \log(nN^\varrho)$ ,  $\varrho \geq 0$ ;

## Assumptions

(A1) The true regression function  $f_0$  has a composition structure.

### Deep and wide neural networks

(A2)  $\hat{f} \in \mathcal{F}(L, \mathbf{p}, s)$ , s.t.

- Depth:  $L \asymp \log(nN^\varrho)$ ,  $\varrho \geq 0$ ;
- Width:  $\min_{l=1, \dots, L} p_l \asymp (nN^\varrho)^{\frac{1}{\theta+1}}$ , where  $\theta = \min_{i=0, \dots, q} \frac{2\beta_i^*}{t_i}$

## Assumptions

(A1) The true regression function  $f_0$  has a composition structure.

### Deep and wide neural networks

(A2)  $\hat{f} \in \mathcal{F}(L, \mathbf{p}, s)$ , s.t.

- Depth:  $L \asymp \log(nN^\varrho)$ ,  $\varrho \geq 0$ ;
- Width:  $\min_{l=1, \dots, L} p_l \asymp (nN^\varrho)^{\frac{1}{\theta+1}}$ , where  $\theta = \min_{i=0, \dots, q} \frac{2\beta_i^*}{t_i}$
- sparsity:  $s \asymp (nN^\varrho)^{\frac{1}{\theta+1}}$ ;

## Assumptions

(A1) The true regression function  $f_0$  has a composition structure.

### Deep and wide neural networks

(A2)  $\hat{f} \in \mathcal{F}(L, \mathbf{p}, s)$ , s.t.

- Depth:  $L \asymp \log(nN^\varrho)$ ,  $\varrho \geq 0$ ;
- Width:  $\min_{l=1, \dots, L} p_l \asymp (nN^\varrho)^{\frac{1}{\theta+1}}$ , where  $\theta = \min_{i=0, \dots, q} \frac{2\beta_i^*}{t_i}$
- sparsity:  $s \asymp (nN^\varrho)^{\frac{1}{\theta+1}}$ ;

## Assumptions

(A3) The maximal eigenvalue of the kernel matrix is  $O(N^{-\varrho})$  for some constant  $\varrho \geq 0$ .