## **COMP0078**

# Supervised Learning Coursework 1

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University College London

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## 1 Part 1

### 1.1 Linear Regression

- 1. Fitting polynomials of order  $k \in \{1, 2, 3, 4\}$  to 4 data points.
  - (a) The plot for the polynomial bases fit to the four data points is shown in Figure 1:

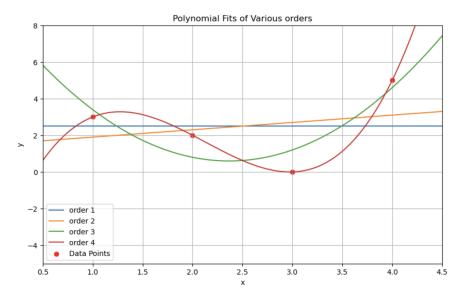


Figure 1: Figure showing the plots of the fitted polynomials with orders  $\in \{1, 2, 3, 4\}$ 

For the rest of Part I and in the code, we use the term "order" to reference the dimensions of the polynomial bases. Figure 1 is similar to the one given in the question as expected.

- (b) The equations corresponding to the curves fitted for k = 1, 2, 3 are given in Table 1:
- (c) The Mean Square Error (MSE) for each fitted curved is also given in Table 1. We see that the MSE decreases as the order increases.

Polynomial Order	Equation	MSE
1	$y = 2.50x^0$	$3.25 \times 10^{0}$
2	$y = 1.50x^0 + 0.40x^1$	$3.05 \times 10^{0}$
3	$y = 9.00x^0 - 7.10x^1 + 1.50x^2$	$8.00 \times 10^{-1}$
4	$y = -5.00x^0 + 15.17x^1 - 8.50x^2 + 1.33x^3$	$5.82 \times 10^{-24}$

Table 1: Table showing the polynomial equations and their MSE values

- 2. Illustrating the phenomena of overfitting.
  - (a) Generating data and fitting polynomial bases
    - i. The plot the function  $sin^2(2\pi x)$  in the range  $0 \le x \le 1$  with the points of the above data set superimposed is shown in Figure 2:

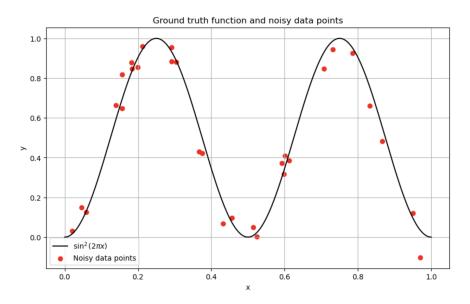


Figure 2: Figure showing the function plotted on top of the generated data

Figure 2 resembles the provided plot as expected.

ii. The plot showing the fit of the data set with polynomial bases of dimension k=2,5,10,14,18 is given in Figure 3:

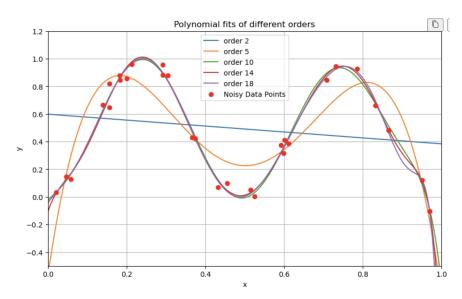


Figure 3: Figure showing the fit of the data set with the different polynomials

(b) The plot the natural log of the training error versus the polynomial dimension is given in Figure 4

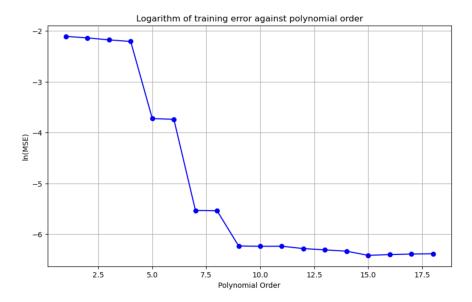


Figure 4: Figure showing the plot the natural log of the training error versus the polynomial dimension

This is a decreasing function, as required.

(c) The plot the natural log of the test error versus the polynomial dimension is shown in Figure 5:

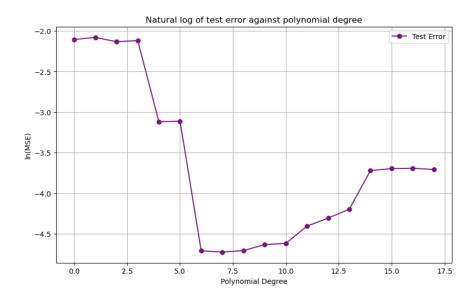


Figure 5: Figure showing the plot the natural log of the test error versus the polynomial dimension

In the figure above, we can see the overfitting in the increase of test error starting at k = 6.

(d) The plot showing the average result for the training and test errors over 100 runs is given in Figure 6:

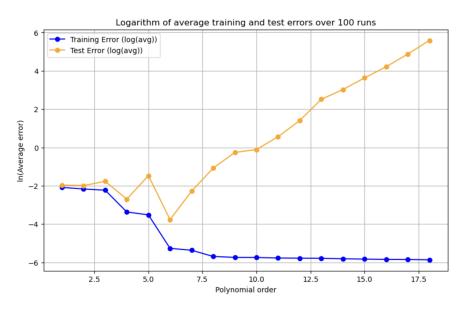


Figure 6: Figure showing the plot showing the average result for the training and test errors over 100 runs

3. In this question, we repeating questions 2b to 2d using a sine basis instead of a polynomial one. The plot of the training error against the order of the sine basis is shown in Figure 7, the test error against the order of the sine basis in Figure 8 and the average train and test error over 100 runs in Figure 9:

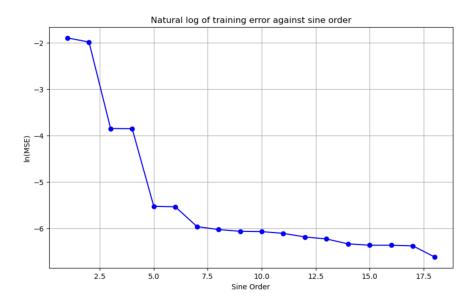


Figure 7: Figure showing the plot showing the training error against the order of the sine basis

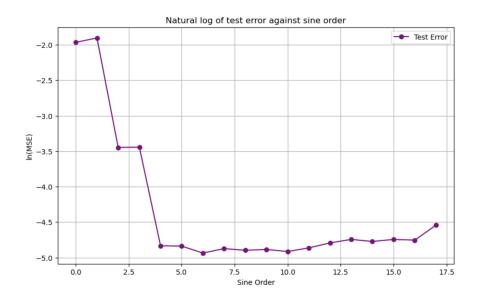


Figure 8: Figure showing the plot showing the test error against the order of the sine basis

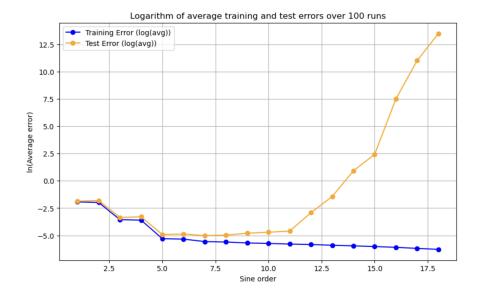


Figure 9: Figure showing the average result for the training and test errors using a sine basis over 100 runs

### 1.2 Filtered Boston housing and kernels

1. Predicting with the mean y-value on the training set. This is the naive regression of fitting the data with a constant function. The performance metrics of this method are shown in Table 2

Metric	Value	
Average Training MSE	$83.4062 \pm 3.5878$	
Average Test MSE	$86.7254 \pm 7.2282$	

Table 2: Naive Regression Performance Metrics

- 2. A simple interpretation of the constant function used in the previous question is that it is the mean of the median house price, the values we are trying to predict.
- 3. Predicting with a single attribute and a bias term. Increasing the complexity from the naive regression, we performed linear regression for each attribute. The resulting training and test Mean Squared Errors are shown in Table 3:

Feature	Training MSE	Test MSE
CRIM	$70.8739 \pm 3.2060$	$74.0706 \pm 6.5122$
ZN	$72.4775 \pm 3.7925$	$75.8473 \pm 7.6186$
INDUS	$63.5788 \pm 3.6801$	$67.3057 \pm 7.4810$
CHAS	$81.3323 \pm 3.6556$	$83.6017 \pm 7.5402$
NOX	$67.7105 \pm 3.6276$	$71.9494 \pm 7.3677$
RM	$43.7150 \pm 3.4237$	$43.6715 \pm 6.8463$
AGE	$70.9769 \pm 3.8339$	$75.8011 \pm 7.7557$
DIS	$77.9363 \pm 3.9469$	$82.0467 \pm 7.9962$
RAD	$71.4678 \pm 3.7423$	$73.8613 \pm 7.6423$
TAX	$65.0696 \pm 3.6075$	$67.9269 \pm 7.3778$
PTRATIO	$62.9703 \pm 3.3148$	$62.4538 \pm 6.6573$
LSTAT	$37.7805 \pm 1.8333$	$40.2146 \pm 3.8145$

Table 3: Single attribute regressions performance metrics

4. Predicting with all the attributes. The training and test MSE after using all the data at once are given in Table 4:

Metric	Value	
Average Training MSE	$22.0224 \pm 1.7731$	
Average Test MSE	$24.2901 \pm 3.7192$	

Table 4: All attributes regression performance metrics

These results outperform the ones from the previous questions as required.

## 1.3 Kernelised ridge regression

- 1. The BostonHousingAnalysis class in the jupyter notebook achieves the implementation of Kernel Ridge Regression using a Gaussian Kernel. As required it: initialises the hyperparameter vectors, performs kernel ridge regression with cross-validation, selects the optimal hyperparameters, retrains and evaluates the model with the MSE of the training and test sets. For the detail of the implementation, please refer to the comments in the code.
- 2. The plot of the cross-validation error as a function of  $\gamma$  and  $\sigma$  is shown in Figure 10:

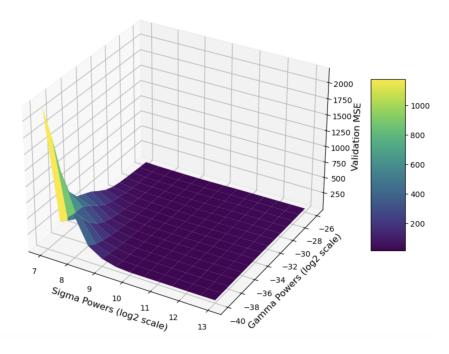


Figure 10: Figure showing the cross-validation error as a function of  $\gamma$  and  $\sigma$ 

3. The Mean Squared Error on the training and test sets for the best  $\gamma$  and  $\sigma$  are:

(a) Training MSE: 8.137205

(b) Test MSE: 14.22324

Note that the results saved in the jupyter notebook aren't the ones that were used in this question. The output of the BostonHousingAnalysis class used in section is given in the appendix.

4. The summary of the results obtained from repeating questions 4a, c and d as well as questions 5 a and c over 20 random (2/3, 1/3) splits of your data are recorded in Table 5:

Method	MSE train	MSE test
Naive Regression	$86.1283 \pm 4.5339$	$81.2697 \pm 8.9661$
Linear Regression (CRIM)	$73.0630 \pm 4.8533$	$70.2882 \pm 10.6816$
Linear Regression (ZN)	$75.0737 \pm 4.2831$	$70.7135 \pm 8.6247$
Linear Regression (INDUS)	$66.5390 \pm 4.3773$	$61.3513 \pm 8.8134$
Linear Regression (CHAS)	$83.1194 \pm 4.2663$	$79.9543 \pm 8.6215$
Linear Regression (NOX)	$70.8872 \pm 4.6983$	$65.6442 \pm 9.3682$
Linear Regression (RM)	$44.9055 \pm 1.9245$	$41.3390 \pm 3.9541$
Linear Regression (AGE)	$74.3430 \pm 4.9046$	$69.0054 \pm 9.8700$
Linear Regression (DIS)	$81.0787 \pm 4.7725$	$75.7129 \pm 9.5114$
Linear Regression (RAD)	$73.8426 \pm 4.8299$	$69.0242 \pm 9.5654$
Linear Regression (TAX)	$67.8265 \pm 4.3736$	$62.3734 \pm 8.6025$
Linear Regression (PTRATIO)	$63.6893 \pm 3.5393$	$60.9643 \pm 7.0877$
Linear Regression (LSTAT)	$39.0384 \pm 2.1745$	$37.7584 \pm 4.2145$
Linear Regression (all attributes)	$22.6646 \pm 1.1973$	$23.3374 \pm 2.5949$
Kernel Ridge Regression	$8.1372 \pm 1.5090$	$14.2232 \pm 8.0884$

Table 5: Table showing the mean squared error for various regression methods

## 2 Part 2

## 2.1 k-Nearest Neighbors

## 2.1.1 Generating the data

Here is the obtained h function, and the associated decision regions (in blue and in red on the figure). You'll find in the attached code the used to obtain this result.

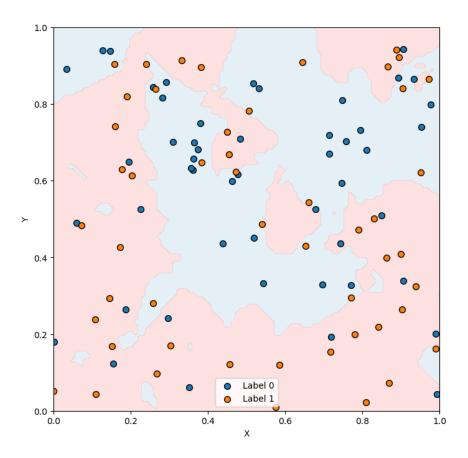


Figure 11: Visualization of a hypothesis  $h_{100.3}$ 

#### 2.1.2 Estimated generalization error of k-NN as a function of k

We used the attached code, and obtained the following plot. We updated the previous algorithms to work as much as possible with matrices to minimize the computation time.

For k in 1,2,3,4, 5, 6, the generalization error is very important, which is logical as we do not inspect a sufficient amount of data to estimate correctly the label of our new data point: we are here subject to overfitting and are capturing the noise in our training dataset (we notice that for k=1,2, our generalization error is close to 0.2, which is the proportion of the noise in our data). Then, for k between 7 and 15, our average generalization error is minimal: we inspect enough training points to avoid overfitting, and sufficiently few training points to stay close to the point we want to evaluate and capture the local pattern. For k>15, the generalization error increases: we are looking at data points situated too far away from the one we are trying to evaluate, and end up misclassifying it.

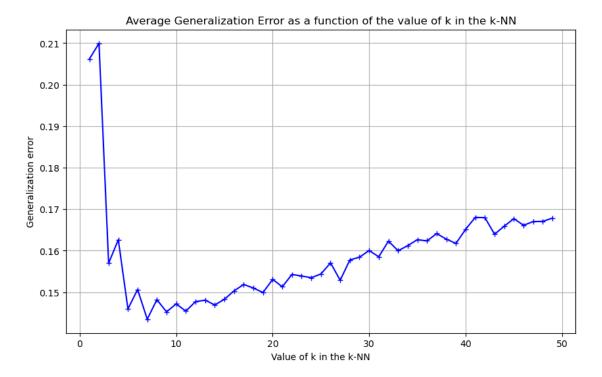


Figure 12: Average Generalization Error as a function of the value of k in the k-NN

# 2.1.3 Determine the optimal k as a function of the number of training points (m)

We used the attached code, and obtained the following plot. We changed the previous algorithms to work as much as possible with matrices to minimize the computation time.

We notice that the more samples we have, the bigger our optimal k is. This result seems logical: the more training samples we have, the more noisy data (in absolute number) we have. We therefore need to look at more neighbours to estimate our label correctly. In other words, the more training samples we have, the more complex/dense our decision space is and the more difficult our decision is to make: the consequence is that we need to look at more neighbours to make an accurate decision. We can also notice that this curve tends to flatten for  $k \geq 1500$ , which is explained by the fact that when we already inspect a large number of neighbours, the additional value of having more is relatively low: we already manage to capture the local pattern with the neighbours that we are inspecting.

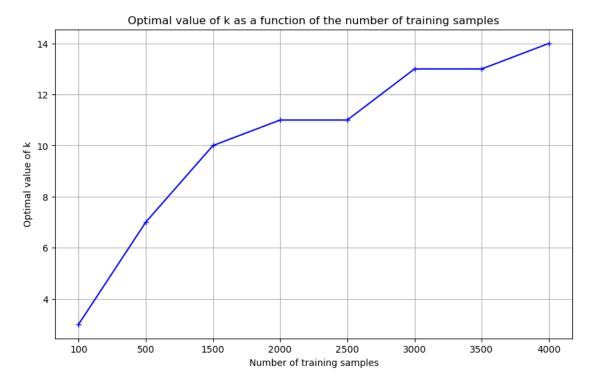


Figure 13: Optimal value of k as a function of the number of training samples

## 3 Part 3

#### 1. Question 9

(a) Let's fix  $\{x_1, ..., x_n\}$  a family of vectors of  $R^n$ .  $\forall i \in [1, n]$  we have  $x_i = [x_{i1}, x_{i2}, ..., x_{in}]^T$ Let's write K, the Kernel matrix associated with this family. We have:

$$K = \begin{bmatrix} c + \sum_{i=1}^{n} x_{1i}^{T} x_{1i} & \cdots & c + \sum_{i=1}^{n} x_{ni}^{T} x_{1i} \\ \vdots & \ddots & \vdots \\ c + \sum_{i=1}^{n} x_{1i}^{T} x_{ni} & \cdots & c + \sum_{i=1}^{n} x_{ni}^{T} x_{ni} \end{bmatrix}$$

$$\implies K = c \begin{bmatrix} 1 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{bmatrix} + \begin{bmatrix} \sum_{i=1}^{n} x_{1i}^{T} x_{1i} & \cdots & \sum_{i=1}^{n} x_{ni}^{T} x_{1i} \\ \vdots & \ddots & \vdots \\ \sum_{i=1}^{n} x_{1i}^{T} x_{ni} & \cdots & \sum_{i=1}^{n} x_{ni}^{T} x_{ni} \end{bmatrix}$$

 $\forall (x,z) \in (R^n)^2, K_c(x,z)$  is a kernel if and only if K is Positive Semi Definite :  $K_c(x,z)$  is a kernel if and only if  $\forall z \in R^n, z^T K z \geq 0$ . Let's fix  $z \in R^n$ .

$$z^{T}Kz = cz^{T} \begin{bmatrix} 1 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{bmatrix} z + z^{T} \begin{bmatrix} \sum_{i=1}^{n} x_{1i}^{T} x_{1i} & \cdots & \sum_{i=1}^{n} x_{ni}^{T} x_{1i} \\ \vdots & \ddots & \vdots \\ \sum_{i=1}^{n} x_{1i}^{T} x_{ni} & \cdots & \sum_{i=1}^{n} x_{ni}^{T} x_{ni} \end{bmatrix} z$$

$$\implies z^T K z = c[\sum_{i=1}^n z_i, \cdots, \sum_{i=1}^n z_i] z + [\sum_{l=1}^n z_l \sum_{i=1}^n x_{1i}^T x_{li}, \cdots, \sum_{l=1}^n z_l \sum_{i=1}^n x_{ni}^T x_{li}] z$$

$$\implies z^T K z = c \sum_{i=1}^n z_i \sum_{l=1}^n z_l + \sum_{j=1}^n z_j \sum_{l=1}^n z_l \sum_{i=1}^n x_{ji}^T x_{li}$$

$$\implies z^T K z = c \left(\sum_{i=1}^n z_i\right)^2 + \sum_{j=1}^n \sum_{l=1}^n \sum_{i=1}^n z_j x_{ji}^T z_l x_{li}$$

We have finally:

$$z^T K z \ge 0 \implies c \left(\sum_{i=1}^n z_i\right)^2 + \sum_{j=1}^n \sum_{l=1}^n \sum_{i=1}^n z_j x_{ji}^T z_l x_{li} \ge 0$$

$$\implies c \ge \frac{-\sum_{j=1}^{n} \sum_{l=1}^{n} \sum_{i=1}^{n} z_{j} x_{ji}^{T} z_{l} x_{li}}{\left(\sum_{i=1}^{n} z_{i}\right)^{2}}$$

- (b) c is a regularizer, it allow to take into consideration rather equally all the training datapoints when making a new prediction, instead of only using training datapoints that are similar to the points we want to classify.
  - The kernel can be rewritten:  $K_c(x, z) = c + \langle \mathbf{x}, \mathbf{z} \rangle$ . Therefore, if x and z point in the same direction, the value of  $K_c(x, z)$  is greater, and x have a more important weight in the value predicted for z. We remark that if x and z are orthogonal, x

will have a null weight and will therefore have no impact in the value predicted for z. Those phenomenons result in the fact that we only use a subset of our training points (the ones that are similar to the data we want to classify) to classify our new data, which could lead to misclassifications.

If c is very big, the impact of this phenomenon is reduced: an important value of c allows to reduce the contribution of the scalar product in the weight given to a training datapoint. Hence, all datapoints participate rather uniformly in the classification of the new points.

#### 2. Question 10:

We can write our prediction function as follows:

$$f(t) = \sum_{i=1}^{m} \alpha_i K_{\beta}(x_i, t)$$

We know that  $\alpha = K^{-1}y$  with y the labels of our target, and K the following matrix :

$$K = \begin{bmatrix} e^{-\beta \|x_1 - x_1\|} & \dots & e^{-\beta \|x_1 - x_m\|} \\ \dots & \dots & \dots \\ e^{-\beta \|x_1 - x_m\|} & \dots & e^{-\beta \|x_m - x_m\|} \end{bmatrix} = \begin{bmatrix} 1 & \dots & e^{-\beta \|x_1 - x_m\|} \\ \dots & 1 & \dots \\ e^{-\beta \|x_1 - x_m\|} & \dots & 1 \end{bmatrix}$$

We notice that if  $\beta >> 0$ ,  $K=I=K^{-1}.$  We have therefore the following prediction function :

$$f(t) = \sum_{i=1}^{m} \alpha_i K_{\beta}(x_i, t) = \sum_{i=1}^{m} sign(y_i) K_{\beta}(x_i, t)$$

If we assume, for simplicity, that our nearest neighbor is the first one (i=1), we can rewrite our prediction function:

$$f(t) = sign(y_1)K_{\beta}(x_1, t) + \sum_{i=2}^{m} sign(y_i)K_{\beta}(x_i, t)$$

If  $sign(y_1) > 0$ , we need to have sign(f(t)) > 0, which implies :

$$sign(y_1)K_{\beta}(x_1,t) + \sum_{i=2}^{m} sign(y_i)K_{\beta}(x_i,t) > 0 \implies e^{-\beta \|x_1 - t\|^2} > -\sum_{i=2}^{m} sign(y_i)e^{-\beta \|x_i - t\|^2}$$

Similarly, if  $sign(y_1) < 0$ , we need to have sign(f(t)) < 0, which implies :

$$sign(y_1)K_{\beta}(x_1, t) + \sum_{i=2}^{m} sign(y_i)K_{\beta}(x_i, t) < 0 \implies -e^{-\beta \|x_1 - t\|^2} < -\sum_{i=2}^{m} sign(y_i)e^{-\beta \|x_i - t\|^2}$$

$$\implies e^{-\beta \|x_1 - t\|^2} > \sum_{i=2}^{m} sign(y_i)e^{-\beta \|x_i - t\|^2}$$

Then, we have this inequality:

$$e^{-\beta \|x_1 - t\|^2} > |\sum_{i=2}^m sign(y_i)e^{-\beta \|x_i - t\|^2}|$$

Finally, if we write  $\epsilon_i = e^{-\beta ||x_i - t||^2}$ , we obtain this equation on beta :

$$e^{-\beta \|x_1 - t\|^2} > |\sum_{i=2}^m sign(y_i)\epsilon_i|$$

To conclude, if  $\beta$  satisfies the previous inequality, our classifier can be assimilated to a 1-Nearest Neighbor.

#### 3. Question 11

(a) 
$$\mathcal{E}_{\rho_i}(f_i) = \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{f_i(x) \neq y\}} d\rho_i(x, y)$$
$$\implies \mathcal{E}_{\rho_i}(f_i) = \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{f_i(x) \neq y\}} \rho_i(x, y) dx dy = \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{f_i(x) \neq y\}} \mathbb{1}_{\{f_i(x) = y\}} \frac{1}{2n} dx dy$$

We remark that  $\mathbb{1}_{\{f_i(x)\neq y\}}\mathbb{1}_{\{f_i(x)=y\}}=0$ , and deduce that  $\mathcal{E}_{\rho_i}(f_i)=0$ 

Since the misclassification excess risk is always positive, we have:

$$0 = \mathcal{E}_{\rho_i}(f_i) \ge \inf_{f: \mathcal{X} \to \mathcal{Y}} \mathcal{E}_{\rho_i}(f) \ge 0 \implies \mathcal{E}_{\rho_i}(f_i) = \inf_{f: \mathcal{X} \to \mathcal{Y}} \mathcal{E}_{\rho_i}(f) = 0$$

(b) Let's first show that  $E_{S \sim \rho_i^n}(\mathcal{E}_{\rho}(A(S))) = \frac{1}{k} \sum_{i=1}^T \mathcal{E}_{\rho_i}(A(S_j^i))$ , for any  $i \in \{1, ..., T\}$ , we can write:

$$\mathcal{E}_{\rho_i}(A(S)) = \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S)(x) \neq y\}} d\rho_i(x, y) = \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S)(x) \neq y\}} \mathbb{1}_{\{f_i(x) = y\}} \frac{1}{2n} dx dy$$

We notice that  $\mathbb{1}_{\{A(S)(x)\neq y\}}\mathbb{1}_{\{f_i(x)=y\}}=0$  for  $(x,y)\notin (S_j^i)_{j\in\{1,k\}}$ , which means that we are constrained in the values that S can take as inputs.

Our previous equation can be rewritten:

$$\mathcal{E}_{\rho_i}(A(S)) = \int_{(x,y)\in(S_j^i)_{j\in\{1,k\}}} \mathbb{1}_{\{A(S_j^i)(x)\neq y\}} \mathbb{1}_{\{f_i(x)=y\}} dx dy$$

$$\implies \mathcal{E}_{\rho_i}(A(S)) = \mathcal{E}_{\rho_i}(A(S)_{|(x,y)\in(S_j^i)_{j\in\{1,k\}}}) = \mathcal{E}_{\rho_i}((S_j^i)_{j\in\{1,k\}})$$

We have an equal probability of sampling each one of the k sets, which gives:

$$E_{S \sim \rho_i^n} \mathcal{E}_{\rho_i}(A(S)) = \mathcal{E}_{\rho_i}((S_j^i)_{j \in \{1, k\}}) = \frac{1}{k} \sum_{j=1}^k \mathcal{E}_{\rho_i}(A(S_j^i))$$

We use the fact that  $\max_{m} \alpha_{m} \geq \frac{1}{m} \sum_{\ell=1}^{m} \alpha_{m}$  to deduce that, one one hand we have:

$$\max_{\{i=1,\dots,T\}} E_{S \sim \rho_i^n} \mathcal{E}_{\rho_i}(A(S)) \ge \frac{1}{T} \sum_{i=1}^T E_{S \sim \rho_i^n} \mathcal{E}_{\rho_i}(A(S)) = \frac{1}{T} \sum_{i=1}^T \frac{1}{k} \sum_{j=1}^k \mathcal{E}_{\rho_i}(A(S_j^i))$$

We then use the fact that  $\frac{1}{m} \sum_{\ell=1}^{m} \alpha_m \ge \min_m \alpha_m$  to deduce that on the other hand we have :

$$\frac{1}{T} \sum_{i=1}^{T} \frac{1}{k} \sum_{j=1}^{k} \mathcal{E}_{\rho_i}(A(S_j^i)) = \frac{1}{k} \sum_{j=1}^{k} \frac{1}{T} \sum_{i=1}^{T} \mathcal{E}_{\rho_i}(A(S_j^i)) \ge \min_{\{j=1,\dots,k\}} \frac{1}{T} \sum_{i=1}^{T} \mathcal{E}_{\rho_i}(A(S_j^i))$$

If we unite our inequalities together, we obtain the demanded result:

$$\max_{\{i=1,\dots,T\}} E_{S \sim \rho_i^n} \mathcal{E}_{\rho_i}(A(S)) \ge \frac{1}{T} \sum_{i=1}^T \frac{1}{k} \sum_{j=1}^k \mathcal{E}_{\rho_i}(A(S_j^i)) \ge \min_{\{j=1,\dots,k\}} \frac{1}{T} \sum_{i=1}^T \mathcal{E}_{\rho_i}(A(S_j^i))$$

$$\implies \max_{\{i=1,...,T\}} E_{S \sim \rho_i^n} \mathcal{E}_{\rho_i}(A(S)) \ge \min_{\{j=1,...,k\}} \frac{1}{T} \sum_{i=1}^T \mathcal{E}_{\rho_i}(A(S_j^i))$$

(c) We have:

$$\frac{1}{T} \sum_{i=1}^{T} \mathcal{E}_{\rho_{i}}(A(S_{j}^{i})) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq y\}} d\rho_{i}(x, y) = \frac{1}$$

$$\implies \frac{1}{T} \sum_{i=1}^{T} \mathcal{E}_{\rho_i}(A(S_j^i)) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \mathbb{1}_{\{A(S_i^j)(x) \neq y\}} \mathbb{1}_{\{f_i(x) = y\}} \frac{1}{2p} dx dy$$

We notice that  $\mathbb{1}_{\{A(S_i^j)(x)\neq y\}}\mathbb{1}_{\{f_i(x)=y\}} = \mathbb{1}_{\{A(S_i^j)(x)\neq f_i(x)\}}$ 

We can rewrite our previous expression:

$$\frac{1}{T} \sum_{i=1}^{T} \mathcal{E}_{\rho_i}(A(S_j^i)) = \frac{1}{T} \sum_{i=1}^{T} \int_{\mathcal{X}, \mathcal{Y}} \frac{1}{2p} \mathbb{1}_{\{A(S_i^j)(x) \neq f_i(x)\}} dx dy$$

We then notice that for  $x \in S_j^i$ ,  $\mathbb{1}_{\{A(S_i^j)(x) \neq f_i(x)\}} = 0$ . Our integral can therefore be rewritten:

$$\frac{1}{T} \sum_{i=1}^{T} \mathcal{E}_{\rho_{i}}(A(S_{j}^{i})) = \frac{1}{T} \sum_{i=1}^{T} \int_{R_{j}} \frac{1}{2p} \mathbb{1}_{\{A(S_{i}^{j})(x) \neq f_{i}(x)\}} dx = \frac{1}{T} \sum_{i=1}^{T} \sum_{v \in R_{i}} \frac{1}{2p} \mathbb{1}_{\{A(S_{i}^{j})(v) \neq f_{i}(v)\}}$$

We then use the fact that  $\frac{1}{m} \sum_{l=1}^{m} \alpha_m \ge \min_{l=1,\dots,m} \alpha_m$  to obtain :

$$\frac{1}{T} \sum_{i=1}^{T} \mathcal{E}_{\rho_i}(A(S_j^i)) = \frac{1}{2} \frac{1}{p} \sum_{v \in R_j} \frac{1}{T} \sum_{i=1}^{T} \mathbb{1}_{\{A(S_i^j)(v) \neq f_i(v)\}} \ge \frac{1}{2} \min_{v \in \mathcal{R}_l} \sum_{i=1}^{T} \mathbb{1}_{\{A(S_i^j)(v) \neq f_i(v)\}}$$

The previous inequality gives the final result:

$$\frac{1}{T} \sum_{i=1}^{T} \mathcal{E}_{\rho_i}(A(S_j^i)) \ge \frac{1}{2} \min_{v \in \mathcal{R}_i} \sum_{i=1}^{T} \mathbb{1}_{\{A(S_i^j)(v) \ne f_i(v)\}}$$

(d) First, we will prove that for any  $v \in R_j$  we can partition  $\mathcal{Y}^{\mathcal{C}}$  into  $\frac{T}{2}$  pairs  $(f_i, f_{i'})$  such that  $f_i(x) \neq f_{i'}(x)$  if and only if x = v. To prove this, we will prove that : for any  $v \in R_j$  we can partition  $\mathcal{Y}^{\mathcal{C}}$  into  $\frac{T}{2}$  pairs  $(f_i, f_{i'})$  such that  $f_i(x) = f_{i'}(x)$  if and only if  $x \neq v$ .

First, for a fixed  $x \in \mathcal{C}$ , we assume that there exist  $(fi', fi'') \in (\mathcal{Y}^C)^2$  so that x=v if and only if  $f_i(x) = f_{i'}(x) = f_{i''}(x)$ , Therefore, if  $x \neq v$ , we have  $f_i(x) \neq f_{i'}(x)$  and  $f_i(x) \neq f_{i''}(x)$ . Those three functions take their values in  $\{-1, 1\}$ , which

implies that if we have  $f_i(x) \neq f_{i'}(x)$  and  $f_i(x) \neq f_{i''}(x)$  at the same time, we automatically have  $\forall i \in C, f_{i''}(x) = f_{i'}(x) \Leftrightarrow f_{i''} = f_{i'}$ .

Hence, there is one only one  $i' \in [1, T]$  so that  $x \neq v$  if and only if  $f_i(x) = f_{i'}(x)$ .

We proved that for any  $v \in R_j$  we can partition  $\mathcal{Y}^{\mathcal{C}}$  into  $\frac{T}{2}$  pairs  $(f_i, f_{i'})$  such that  $f_i(x) \neq f_{i'}(x)$  if and only if x = v.

Now, let's consider one par  $(f_i, f_{i'})$ , and  $v \in R_j$ . Let's also consider  $\mathbb{1}_{\{A(S_j^i)(v) \neq f_i(v)\}} + \mathbb{1}_{\{A(S_j^i)(v) \neq f_{i'}(v)\}}$ . Since  $A(S_j^i)(v) = A(S_j^{i'})(v)$  and  $f_i(v) \neq f_{i'}(v)$  one of the the terms will be 0, and the other will be 1. We have in any cases:  $\mathbb{1}_{\{A(S_j^i)(v) \neq f_{i'}(v)\}} + \mathbb{1}_{\{A(S_j^i)(v) \neq f_{i'}(v)\}} = 1$ 

Finally, we obtain the formula :

$$2\sum_{i=1}^T \mathbb{1}_{\{A(S^i_j)(v) \neq f_i(v)\}} = \sum_{i=1}^T \mathbb{1}_{\{A(S^i_j)(v) \neq f_i(v)\}} + \sum_{i'=1}^T \mathbb{1}_{\{A(S^{i'}_j)(v) \neq f_{i'}(v)\}} = T$$

$$\implies \frac{2}{T} \sum_{i=1}^{T} \mathbb{1}_{\{A(S_j^i)(v) \neq f_i(v)\}} = \frac{1}{T} \Big( \sum_{i=1}^{T} \mathbb{1}_{\{A(S_j^i)(v) \neq f_i(v)\}} + \sum_{i'=1}^{T} \mathbb{1}_{\{A(S_j^{i'})(v) \neq f_{i'}(v)\}} \Big) = 1$$

$$\implies \frac{1}{T} \sum_{i=1}^{T} \mathbb{1}_{\{A(S_j^i)(v) \neq f_i(v)\}} = \frac{1}{2}$$

(e) For any random variable Z and a  $\in \mathcal{R}_+^*$ , Markov's inequality is the following :  $P(Z \ge a) \le \frac{E(A)}{a}$ .

Let's apply this inequality to the positive random variable defined by  $A = -\frac{Z-1}{b}$ , with Z being random variable with values in [0, 1],  $b \in ]0, 1]$  and a = 1. We have:

$$P(A \ge 1) \le \frac{E(A)}{1} \implies P(-\frac{Z-1}{b} \ge 1) \le -E(\frac{Z-1}{b})$$

$$\implies P(Z - 1 \le -b) \le -E\left(\frac{Z - 1}{b}\right) \implies 1 - P(Z - 1 > -b) \le -E\left(\frac{Z - 1}{b}\right)$$

$$\implies 1 - P(Z > 1 - b) \le -\frac{\mu - 1}{b} \implies P(Z > 1 - b) \ge \frac{\mu - 1}{b} + 1$$

$$\implies P(Z > 1 - b) \ge \frac{\mu - (1 - b)}{b}$$

(f) We know that  $\mathcal{E}_{\rho}(A(S))$  is a random variable taking values in [0,1]. For  $i \in [1, T]$ , let's apply the inequality found in 11.e) to  $Z = \mathcal{E}_{\rho_i}(A(S))$  and  $a = \frac{7}{8}$ :

$$P_{S \sim \rho_i^n}(\mathcal{E}_{\rho_i}(A(S)) > 1 - \frac{7}{8}) \ge \frac{E_{S \sim \rho_i^n}(\mathcal{E}_{\rho_i}(A(S))) - (1 - \frac{7}{8})}{\frac{7}{8}}$$

$$\Leftrightarrow P_{S \sim \rho_i^n}(\mathcal{E}_{\rho_i}(A(S)) > \frac{1}{8}) \ge \frac{8E_{S \sim \rho_i^n}(\mathcal{E}_{\rho_i}(A(S))) - 1}{7}$$

This inequality is true for all values of i, and in particular for  $i' = arg \max_{\{i=1,\dots,T\}} E_{S \sim \rho_i^n} \mathcal{E}_{\rho_i}(A(S))$ We obtain for this case :

$$P_{S \sim \rho_i^n}(\mathcal{E}_{\rho_i}(A(S)) > \frac{1}{8}) \ge \frac{8E_{S \sim \rho_{i'}^n}(\mathcal{E}_{\rho_{i'}}(A(S))) - 1}{7} = \frac{8 \max_{\{i=1,\dots,T\}} E_{S \sim \rho_i^n}(\mathcal{E}_{\rho_i}(A(S))) - 1}{7}$$

Next, we know from question 11.b that:

$$\max_{\{i=1,\dots,T\}} E_{S \sim \rho_i^n} \mathcal{E}_{\rho_i}(A(S)) \ge \min_{\{j=1,\dots,k\}} \frac{1}{T} \sum_{i=1}^T \mathcal{E}_{\rho_i}(A(S_j^i))$$

And from question 11.c that:

$$\frac{1}{T} \sum_{i=1}^{T} \mathcal{E}_{\rho_i} \left( A(S_j^i) \right) \ge \frac{1}{2} \min_{v \in R_j} \frac{1}{T} \sum_{i=1}^{T} \mathbb{1}_{\{A(S_j^i)(v) \neq f_i(v)\}}$$

Hence, we have:

$$\max_{\{i=1,\dots,T\}} E_{S \sim \rho_i^n} \mathcal{E}_{\rho_i}(A(S)) \ge \min_{\{j=1,\dots,k\}} \frac{1}{T} \sum_{i=1}^T \mathcal{E}_{\rho_i}(A(S_j^i)) \ge \min_{\{j=1,\dots,k\}} \frac{1}{2} \min_{v \in R_j} \frac{1}{T} \sum_{i=1}^T \mathbb{1}_{\{A(S_j^i)(v) \neq f_i(v)\}}$$

Finally, we learned in question 11.d that:

$$\frac{1}{T} \sum_{i=1}^{T} \mathbb{1}_{\{A(S_j^i)(v) \neq f_i(v)\}} = \frac{1}{2}$$

The previous equality gives us that:

$$\max_{\{i=1,\dots,T\}} E_{S \sim \rho_i^n} \mathcal{E}_{\rho_i}(A(S)) \ge \min_{\{j=1,\dots,k\}} \frac{1}{2} \min_{v \in R_j} \frac{1}{T} \sum_{i=1}^T \mathbb{1}_{\{A(S_j^i)(v) \ne f_i(v)\}} = \frac{1}{2} \frac{1}{2} = \frac{1}{4}$$

Finally, we obtain the inequality:

$$P_{S \sim \rho_i^n}(\mathcal{E}_{\rho_i}(A(S)) > \frac{1}{8}) \ge \frac{8 \max_{\{i=1,\dots,T\}} E_{S \sim \rho_i^n}(\mathcal{E}_{\rho_i}(A(S))) - 1}{7} \ge \frac{8\frac{1}{4} - 1}{7} = \frac{1}{7}$$

The previous inequality being true for all values of i, we obtain the demanded relation:

$$P_{S \sim \rho^n}(\mathcal{E}_{\rho}(A(S) > \frac{1}{8}) > \frac{1}{7}$$

(g) i. We first demonstrated that :  $\inf_{f:\mathcal{X}\to\mathcal{Y}} \mathcal{E}_{\rho}(f) = 0$ . This result shows that, for each distribution  $\rho$ , there exists at least one function that minimizes the misclassification excess risk relative to that distribution. In other words, for any given machine learning problem defined by a distribution  $\rho$ , there is an ideal function or solution that can achieve minimal error.

We then demonstrated that  $P_{S\sim\rho^n}(\mathcal{E}_{\rho}(A(S)) > \frac{1}{8}) \geq \frac{1}{7}$ . This means that, given a dataset sampled from the distribution  $\rho$ , the probability that the

misclassification excess risk of any algorithm A will exceed  $\frac{1}{8}$  is at least  $\frac{1}{7}$ . In other words, there is no universal algorithm that can guarantee low error across all possible datasets. Each algorithm's performance depends on the specific distribution of the data, showing that no single algorithm can fit perfectly across all problems.

The No Free Lunch theorem can therefore be expressed as follows: There exists an optimal solution function for each machine learning problem, but the solutions for two distinct problems are generally distinct. Consequently, there is no single algorithm that performs best on all possible problems; rather, different problems require different solutions.

ii. This theorem means that a space of functions is learnable if  $P(\mathcal{E}_{\rho}(A(S)) \to \inf_{f \in \mathcal{H}} \mathcal{E}_{\rho}(f)) \to 1$ . In other words, a function space is learnable if the probability that: (there exists an algorithm whose misclassification excess risk relative to the distribution  $\rho$  converges towards the misclassification excess risk of the function space) converges towards 1. Said differently, a function space is learnable if all the functions it contains can be approximated perfectly by one algorithm.

The NFL theorem states that there exists an optimal solution function for each machine learning problem, but that there is no single algorithm that performs best on all possible problems. Therefore, if  $\mathcal{Y}^{\mathcal{X}}$  was learnable, this would mean that every function of  $\mathcal{Y}^{\mathcal{X}}$  could be approximated perfectly using the same algorithm A, which is precisely what the NFL theorem rejects.

The mathematical demonstration is the following:

Let's assume that  $\mathcal{Y}^{\mathcal{X}}$  is learnable. Let's fix A, the algorithm associated with  $\delta = \frac{1}{14}$ ,  $\epsilon = \frac{1}{8}$  and  $\rho$ , a distribution over  $\mathcal{X} \times \mathcal{Y}$ . Since  $\mathcal{Y}^{\mathcal{X}}$  is learnable, there exists an integer  $\bar{n}$  such that for any  $n \geq \bar{n}$ ,  $\mathbb{P}_{S \sim \rho^n} \left( \mathcal{E}_{\rho}(A(S)) - \inf_{f \in \mathcal{Y}^{\mathcal{X}}} \mathcal{E}_{\rho}(f) \leq \epsilon \right) \geq 1 - \delta$ .

The NFL theorem gives us that :  $\inf_{f \in \mathcal{Y}^{\mathcal{X}}} \mathcal{E}_{\rho}(f) = 0$ .

For 
$$n \geq \bar{n}$$
, we have :  $\mathbb{P}_{S \sim \rho^n} \left( \mathcal{E}_{\rho}(A(S)) \leq \frac{1}{8} \right) \geq 1 - \frac{1}{14} = \frac{13}{14}$ .

We then write that :  $1 = P_{S \sim \rho_i^n}(\mathcal{E}_{\rho}(A(S)) > \frac{1}{8}) + P_{S \sim \rho_i^n}(\mathcal{E}_{\rho}(A(S)) \leq \frac{1}{8}).$ 

We demonstrated earlier that :  $P_{S \sim \rho_i^n}(\mathcal{E}_{\rho}(A(S)) > \frac{1}{8}) \geq \frac{1}{7}$ .

It gives us that :  $1 = P_{S \sim \rho_i^n}(\mathcal{E}_{\rho}(A(S)) > \frac{1}{8}) + P_{S \sim \rho_i^n}(\mathcal{E}_{\rho}(A(S)) \le \frac{1}{8}) \ge \frac{1}{7} + \frac{13}{14} = \frac{15}{14}$ .

This conclusion is absurd.

Therefore,  $\mathcal{Y}^{\mathcal{X}}$  is not learnable.

iii. The NFL theorem implies that the design of a machine learning algorithm is dependent on the problem we want to solve, because there is no "perfect universal algorithm". Hence, every specific problem has its own specific solution. It means that we will always need an external (human?) intervention to adapt the algorithm we use to the problem we face: we need a certain domain knowledge and information on our data to try to find the "best algorithm for our problem".

## **Appendix**

#### Output of the BostonHousingAnalysis class used for KRR

```
=== Run 1 ===
Training Naive Regression...
Training Linear Regression (Single Attributes)...
Training Linear Regression (All Attributes)...
Training Kernel Ridge Regression...
Tuning hyperparameters for Kernel Ridge Regression...
Best Gamma: 2^-32 = 2.3283064365386963e-10
Best Sigma: 2^9.5 = 724.0773439350247
Minimum Validation MSE: 11.931392970644907

Training Kernel Ridge Regression with best hyperparameters...
Kernel Ridge Regression - Train MSE: 8.0057, Test MSE: 48.5310
Run 1 completed.
=== Run 2 ===
```

Training Linear Regression (Single Attributes)... Training Linear Regression (All Attributes)... Training Kernel Ridge Regression... Tuning hyperparameters for Kernel Ridge Regression... Best Gamma:  $2^{-37} = 7.275957614183426e-12$ Best Sigma:  $2^9.5 = 724.0773439350247$ Minimum Validation MSE: 11.860204322434146 Training Kernel Ridge Regression with best hyperparameters... Kernel Ridge Regression - Train MSE: 5.4721, Test MSE: 16.2048 Run 2 completed. === Run 3 === Training Naive Regression... Training Linear Regression (Single Attributes)... Training Linear Regression (All Attributes)... Training Kernel Ridge Regression... Tuning hyperparameters for Kernel Ridge Regression... Best Gamma:  $2^-28 = 3.725290298461914e-09$ Best Sigma: 2^8.5 = 362.03867196751236 Minimum Validation MSE: 12.588952057066566 Training Kernel Ridge Regression with best hyperparameters... Kernel Ridge Regression - Train MSE: 7.4034, Test MSE: 11.4026 Run 3 completed. === Run 4 === Training Naive Regression... Training Linear Regression (Single Attributes)... Training Linear Regression (All Attributes)... Training Kernel Ridge Regression... Tuning hyperparameters for Kernel Ridge Regression... Best Gamma:  $2^-29 = 1.862645149230957e-09$ Best Sigma: 2^9.5 = 724.0773439350247 Minimum Validation MSE: 12.80301410938443

Training Naive Regression...

Training Kernel Ridge Regression with best hyperparameters... Kernel Ridge Regression - Train MSE: 8.9253, Test MSE: 12.2664 Run 4 completed. === Run 5 === Training Naive Regression... Training Linear Regression (Single Attributes)... Training Linear Regression (All Attributes)... Training Kernel Ridge Regression... Tuning hyperparameters for Kernel Ridge Regression... Best Gamma:  $2^{-30} = 9.313225746154785e-10$ Best Sigma: 2^9.5 = 724.0773439350247 Minimum Validation MSE: 11.42041665869226 Training Kernel Ridge Regression with best hyperparameters... Kernel Ridge Regression - Train MSE: 8.0103, Test MSE: 13.7130 Run 5 completed. === Run 6 === Training Naive Regression... Training Linear Regression (Single Attributes)... Training Linear Regression (All Attributes)... Training Kernel Ridge Regression... Tuning hyperparameters for Kernel Ridge Regression... Best Gamma:  $2^-26 = 1.4901161193847656e-08$ Best Sigma: 2^8.5 = 362.03867196751236 Minimum Validation MSE: 14.221439436477969 Training Kernel Ridge Regression with best hyperparameters... Kernel Ridge Regression - Train MSE: 8.2566, Test MSE: 14.1950 Run 6 completed. === Run 7 === Training Naive Regression... Training Linear Regression (Single Attributes)... Training Linear Regression (All Attributes)...

Training Kernel Ridge Regression...

Tuning hyperparameters for Kernel Ridge Regression...

Best Gamma:  $2^{-38} = 3.637978807091713e-12$ 

Best Sigma:  $2^11.0 = 2048.0$ 

Minimum Validation MSE: 15.737590612846745

Training Kernel Ridge Regression with best hyperparameters... Kernel Ridge Regression - Train MSE: 8.9220, Test MSE: 9.7406

Run 7 completed.

=== Run 8 ===

Training Naive Regression...

Training Linear Regression (Single Attributes)...

Training Linear Regression (All Attributes)...

Training Kernel Ridge Regression...

Tuning hyperparameters for Kernel Ridge Regression...

Best Gamma:  $2^{-31} = 4.656612873077393e-10$ 

Best Sigma: 2^9.5 = 724.0773439350247

Minimum Validation MSE: 13.028877975647111

Training Kernel Ridge Regression with best hyperparameters... Kernel Ridge Regression - Train MSE: 8.4563, Test MSE: 10.3046

Run 8 completed.

=== Run 9 ===

Training Naive Regression...

Training Linear Regression (Single Attributes)...

Training Linear Regression (All Attributes)...

Training Kernel Ridge Regression...

Tuning hyperparameters for Kernel Ridge Regression...

Best Gamma:  $2^-29 = 1.862645149230957e-09$ 

Best Sigma:  $2^9.5 = 724.0773439350247$ 

Minimum Validation MSE: 12.663426603759158

Training Kernel Ridge Regression with best hyperparameters... Kernel Ridge Regression - Train MSE: 8.3621, Test MSE: 12.7939

# Run 9 completed. === Run 10 === Training Naive Regression... Training Linear Regression (Single Attributes)... Training Linear Regression (All Attributes)... Training Kernel Ridge Regression... Tuning hyperparameters for Kernel Ridge Regression... Best Gamma: $2^{-26} = 1.4901161193847656e-08$ Best Sigma: 2^8.5 = 362.03867196751236 Minimum Validation MSE: 14.569873663595263 Training Kernel Ridge Regression with best hyperparameters... Kernel Ridge Regression - Train MSE: 8.6596, Test MSE: 10.0943 Run 10 completed. === Run 11 === Training Naive Regression... Training Linear Regression (Single Attributes)... Training Linear Regression (All Attributes)... Training Kernel Ridge Regression... Tuning hyperparameters for Kernel Ridge Regression... Best Gamma: $2^-28 = 3.725290298461914e-09$ Best Sigma: $2^9.0 = 512.0$ Minimum Validation MSE: 12.583033383274081 Training Kernel Ridge Regression with best hyperparameters... Kernel Ridge Regression - Train MSE: 8.6044, Test MSE: 11.8639 Run 11 completed. === Run 12 === Training Naive Regression... Training Linear Regression (Single Attributes)... Training Linear Regression (All Attributes)... Training Kernel Ridge Regression... Tuning hyperparameters for Kernel Ridge Regression... Best Gamma: $2^-39 = 1.8189894035458565e-12$

Best Sigma: 2^12.5 = 5792.618751480198

Minimum Validation MSE: 15.754175865449833

Training Kernel Ridge Regression with best hyperparameters... Kernel Ridge Regression - Train MSE: 11.9567, Test MSE: 11.5086

Run 12 completed.

=== Run 13 ===

Training Naive Regression...

Training Linear Regression (Single Attributes)...

Training Linear Regression (All Attributes)...

Training Kernel Ridge Regression...

Tuning hyperparameters for Kernel Ridge Regression...

Best Gamma:  $2^-30 = 9.313225746154785e-10$ 

Best Sigma:  $2^9.5 = 724.0773439350247$ 

Minimum Validation MSE: 10.654494738410884

Training Kernel Ridge Regression with best hyperparameters... Kernel Ridge Regression - Train MSE: 6.9306, Test MSE: 14.6110

Run 13 completed.

=== Run 14 ===

Training Naive Regression...

Training Linear Regression (Single Attributes)...

Training Linear Regression (All Attributes)...

Training Kernel Ridge Regression...

Tuning hyperparameters for Kernel Ridge Regression...

Best Gamma:  $2^-29 = 1.862645149230957e-09$ 

Best Sigma:  $2^9.0 = 512.0$ 

Minimum Validation MSE: 11.424868676237889

Training Kernel Ridge Regression with best hyperparameters... Kernel Ridge Regression - Train MSE: 7.4946, Test MSE: 13.0233

Run 14 completed.

=== Run 15 ===

Training Naive Regression... Training Linear Regression (Single Attributes)... Training Linear Regression (All Attributes)... Training Kernel Ridge Regression... Tuning hyperparameters for Kernel Ridge Regression... Best Gamma:  $2^{-30} = 9.313225746154785e-10$ Best Sigma:  $2^9.0 = 512.0$ Minimum Validation MSE: 12.684412028885935 Training Kernel Ridge Regression with best hyperparameters... Kernel Ridge Regression - Train MSE: 6.9675, Test MSE: 15.0990 Run 15 completed. === Run 16 === Training Naive Regression... Training Linear Regression (Single Attributes)... Training Linear Regression (All Attributes)... Training Kernel Ridge Regression... Tuning hyperparameters for Kernel Ridge Regression... Best Gamma:  $2^-30 = 9.313225746154785e-10$ Best Sigma: 2^9.5 = 724.0773439350247 Minimum Validation MSE: 12.75802376186986 Training Kernel Ridge Regression with best hyperparameters... Kernel Ridge Regression - Train MSE: 8.2031, Test MSE: 13.7010 Run 16 completed. === Run 17 === Training Naive Regression... Training Linear Regression (Single Attributes)... Training Linear Regression (All Attributes)... Training Kernel Ridge Regression... Tuning hyperparameters for Kernel Ridge Regression... Best Gamma:  $2^-40 = 9.094947017729282e-13$ Best Sigma: 2^10.5 = 1448.1546878700494 Minimum Validation MSE: 13.686638047868803

Training Kernel Ridge Regression with best hyperparameters... Kernel Ridge Regression - Train MSE: 7.0184, Test MSE: 11.1920 Run 17 completed. === Run 18 === Training Naive Regression... Training Linear Regression (Single Attributes)... Training Linear Regression (All Attributes)... Training Kernel Ridge Regression... Tuning hyperparameters for Kernel Ridge Regression... Best Gamma:  $2^-33 = 1.1641532182693481e-10$ Best Sigma:  $2^9.0 = 512.0$ Minimum Validation MSE: 12.255561517293717 Training Kernel Ridge Regression with best hyperparameters... Kernel Ridge Regression - Train MSE: 5.3683, Test MSE: 14.1585 Run 18 completed. === Run 19 === Training Naive Regression... Training Linear Regression (Single Attributes)... Training Linear Regression (All Attributes)... Training Kernel Ridge Regression... Tuning hyperparameters for Kernel Ridge Regression... Best Gamma:  $2^-29 = 1.862645149230957e-09$ Best Sigma:  $2^9.0 = 512.0$ Minimum Validation MSE: 14.305506285771116 Training Kernel Ridge Regression with best hyperparameters... Kernel Ridge Regression - Train MSE: 8.5865, Test MSE: 10.7351 Run 19 completed. === Run 20 === Training Naive Regression... Training Linear Regression (Single Attributes)... Training Linear Regression (All Attributes)...

Training Kernel Ridge Regression...

Tuning hyperparameters for Kernel Ridge Regression...

Best Gamma:  $2^{-36} = 1.4551915228366852e-11$ 

Best Sigma: 2^11.5 = 2896.309375740099

Minimum Validation MSE: 16.475565570229378

Training Kernel Ridge Regression with best hyperparameters... Kernel Ridge Regression - Train MSE: 11.1406, Test MSE: 9.3262

Run 20 completed.

=== Model Performance Summary ===

\*\*Naive Regression\*\*

Training MSE:  $86.1283 \pm 4.5339$ Testing MSE:  $81.2697 \pm 8.9661$ 

\*\*Linear Regression (Single Attributes)\*\*

Feature: CRIM

Training MSE:  $73.0630 \pm 4.8533$ Testing MSE:  $70.2882 \pm 10.6816$ 

Feature: ZN

Training MSE:  $75.0737 \pm 4.2831$ Testing MSE:  $70.7135 \pm 8.6247$ 

Feature: INDUS

Training MSE:  $66.5390 \pm 4.3773$ Testing MSE:  $61.3513 \pm 8.8134$ 

Feature: CHAS

Training MSE:  $83.1194 \pm 4.2663$ Testing MSE:  $79.9543 \pm 8.6215$ 

Feature: NOX

Training MSE:  $70.8872 \pm 4.6983$ Testing MSE:  $65.6442 \pm 9.3682$ 

Feature: RM

Training MSE:  $44.9055 \pm 1.9245$ Testing MSE:  $41.3390 \pm 3.9541$ 

Feature: AGE

Training MSE:  $74.3430 \pm 4.9046$ Testing MSE:  $69.0054 \pm 9.8700$ 

Feature: DIS

Training MSE:  $81.0787 \pm 4.7725$ Testing MSE:  $75.7129 \pm 9.5114$ 

Feature: RAD

Training MSE:  $73.8426 \pm 4.8299$ Testing MSE:  $69.0242 \pm 9.5654$ 

Feature: TAX

Training MSE:  $67.8265 \pm 4.3736$ Testing MSE:  $62.3734 \pm 8.6025$ 

Feature: PTRATIO

Training MSE:  $63.6893 \pm 3.5393$ Testing MSE:  $60.9643 \pm 7.0877$ 

Feature: LSTAT

Training MSE:  $39.0384 \pm 2.1745$ Testing MSE:  $37.7584 \pm 4.2145$ 

\*\*Linear Regression (All Attributes)\*\*

Training MSE:  $22.6646 \pm 1.1973$ Testing MSE:  $23.3374 \pm 2.5949$ 

\*\*Kernel Ridge Regression\*\*
Training MSE: 8.1372 ± 1.5090
Testing MSE: 14.2232 ± 8.0884}