FYS-STK3155/4155 Applied Data Analysis and Machine Learning - Project 2: Classification and Regression

Lotsberg, Bernhard Nornes
Nguyen, Anh-Nguyet Lise

https://github.com/liseanh/FYS-STK4155-project2/

October - November 2019

Abstract

blip blop opnion wrong

1 Introduction

Classification in statistical analysis is a useful tool, e.g. for predicting outcomes of various situations or classifying and sorting large amounts of data.

The aim of this project is to study classification and regression problems through our own implementation of logistic regression and a multilayer perceptron (MLP) in Python. The particular data set we will be studying for classification has been used in a prior research paper by Yeh, I. C. and Che-hui Lien about data mining techniques [7], which we will compare some of our results with. The full data set can be downloaded from the UCI Machine Learning Repository [6]. The data set contains certain features of credit card clients' default payment from a Taiwanese bank. For the regression problem we will use the MLP to approximate Franke's function and compare with results from a prior project where we used ordinary least squares, ridge and lasso regression to approximate it. [4].

2 Data

2.1 Classification - Credit card client data

For the classification part of this project, we are using credit card payment data from a Taiwanese bank downloaded from the UCI Machine Learning Repository. The response variable is a binary variable of default payment with Yes = 1, No = 0. The original data set consists of 30 000 observations, with 6636 amount of observations with default payments. There are 23 features, cited from the original paper they are described as [7]:

- $X1$: Amount of the given credit (NT dollar): it includes both the individual consumer credit and his/her family (supplementary) credit.
- $X2$: Gender (1 = male; 2 = female).
- $X3$: Education (1 = graduate school; 2 = university; 3 = high school; 4 = others).
- $X4$: Marital status (1 = married; 2 = single; 3 = others).
- $X5$: Age (year).
- $X6$ - $X11$: History of past payment. We tracked the past monthly payment records (from April to September, 2005) as follows:

$X6$ = the repayment status in September, 2005; $X7$ = the repayment status in August, 2005; . . .;$X11$ = the repayment status in April, 2005. The measurement scale for the repayment status is: -1 = pay duly; 1 = payment delay for one month; 2 = payment delay for two months; . . .; 8 = payment delay for eight months; 9 = payment delay for nine months and above.

- $X12 - X17$: Amount of bill statement (NT dollar). $X12$ = amount of bill statement in September, 2005; $X13$ = amount of bill statement in August, 2005; . . .; $X17$ = amount of bill statement in April, 2005.
- $X18 - X23$: Amount of previous payment (NT dollar). $X18$ = amount paid in September, 2005; $X19$ = amount paid in August, 2005; . . .; $X23$ = amount paid in April, 2005.

2.2 Regression - Franke's function

For the regression part part of this project we will be performing regression analysis on Franke's function $g(x, y)$ with added Gaussian noise $\varepsilon \sim N(0,\ \sigma^2)$. Franke's function is given by

$$\begin{aligned} g(x,y) = &\frac{3}{4}\exp\left(-\frac{(9x-2)^2}{4} - \frac{(9y-2)^2}{4}\right) \\ &+ \frac{3}{4}\exp\left(-\frac{(9x+1)^2}{49} - \frac{(9y+1)}{10}\right) \\ &+ \frac{1}{2}\exp\left(-\frac{(9x-7)^2}{4} - \frac{(9y-3)^2}{4}\right) \\ &- \frac{1}{5}\exp\left(-(9x-4)^2 - (9y-7)^2\right) \end{aligned} \quad (1)$$

and is defined on $x,\ y \in [0, 1]$. The data we are fitting is given by

$$G(\boldsymbol{x}, \boldsymbol{y}) = g(\boldsymbol{x}, \boldsymbol{y}) + \varepsilon,$$

where $\boldsymbol{x},\ \boldsymbol{y}$ are vectors of uniformly spaced values from 0 and 1 of length n_x and n_y respectively. To directly compare with our previous project, *Project 1: Regression analysis and resampling methods* [4], we choose to generate and analyze the data sets `franke0`, `franke1`, `franke2` as configured in Table 1. To generate the points, we grid over n_x points in x-direction and n_y points in y-direction. In the previous project we used a 4th order two-dimensional polynomial function to model Franke's function. To get an understanding of the performance of our regression model using a neural network compared to a more simple regression method, we will compare the R^2 scores of our neural network results with the best model obtained in our prior work, which was found using the ordinary least squares (OLS) method for a 4th order two-dimensional polynomial. The R^2 scores from the linear regression can be found in Table 4 along with our neural network results. From the previous project we however only had results from data sets corresponding to `franke0` and franke1. For a more detailed explanation of how the OLS model was obtained, please refer to our previous project *Project 1: Regression analysis and resampling methods* [4].

Table 1: Table of the configurations for our generated data sets using Franke's function given in Equation (1) with added noise $\varepsilon \sim N(0,\ \sigma^2)$. n_x and n_y indicate the number of points used to produce the grid in their respective directions.

Data set	Data points	n_x	n_y	σ
`franke0`	400	20	20	1.0
`franke1`	400	20	20	0.10
`franke2`	40 000	200	200	0.10

2.3 Preprocessing

As the Franke data set is simulated, it does not require as much preprocessing as the real-life credit card data set does. Additionally, the credit card data set contains both categorical and continuous variables, whereas the Franke data set only contains continuous variables. Due to this, we will start by discussing the inital steps in the preprocessing of the credit card data.

We first removed feature outliers in the credit data set by looking at the supposed discrete values of $X2 - X4$ and $X6 - X11$. However, though in the original paper they stated that $X6 - X11 \in \{-1, 1, 2, 3, \ldots, 9\}$, the majority of the samples contained the values 0 and 2, which were undefined. Removing these would have reduced the data set down to only approximately four thousand data points, so we have opted to keep them in our analysis as unexplained variables and ended up with a data set of 29603 points, 6606 of which were default payments.

To ensure that the categorical variables $X2$-$X4$ in the credit card set were considered equal by the classifiers, we incorporated the use of dummy variables and one-hot encoded the variables.

We use `Scikit-learn's`[2] library to split both data sets into test and training sets, and to scale and center the data. For both data sets we used 1/3rd of the total data as testing data and the remaining 2/3rds as training. To center the data, the means of the continuous variables in the training set were subtracted from both the training and the test sets. Each continuous variable in the training and test sets was scaled with respect to its standard deviation in the training set.

Before scaling the credit card data set, we first opted to upsample the number of default payment samples in the training set by using `imblearn.over_sampling.RandomOverSampler` from the library `imbalanced-learn`, which randomly duplicates the default payment samples, until there was an equal amount of default payment samples as non-default samples. This was done to improve the model prediction. Note that we did not upsample the amount of defaults in the test set.

3 Learning methods

3.1 Logistic Regression (LR)

Logistic regression (LR) is a statistical model that can be used to predict a binary dependent variable, which in our project will be one of the methods used for binary classification of the credit card default/non-default payments. LR outputs the probability of a sample to be in either 1 (default) or non-default (0), with the probability being given by the logit (Sigmoid) function, such that

$$p(y = 1|\boldsymbol{X}, \boldsymbol{\beta}) = \frac{1}{1 + e^{-\boldsymbol{X}\boldsymbol{\beta}}} = \frac{e^{\boldsymbol{X}\boldsymbol{\beta}}}{e^{\boldsymbol{X}\boldsymbol{\beta}} + 1}, \quad (2)$$

$$p(y \neq 1|\boldsymbol{X}, \boldsymbol{\beta}) = 1 - p(y = 1|\boldsymbol{X}, \boldsymbol{\beta}) \; . \quad (3)$$

Here $\boldsymbol{X}$ is the feature matrix, and $\boldsymbol{\beta}$ is a vector containing the weights assigned to each feature in $\boldsymbol{X}$. The cost function most commonly used in this case is called the cross entropy, which is the negative log-likelihood of a prediction being in the dataset and is given by

$$\mathcal{C}_{\mathrm{LR}}(\boldsymbol{\beta}) = -\sum_{i=0}^{n-1} [\, y_i \log p(y_i|x_i, \boldsymbol{\beta}) + (1 - y_i) \log(1 - p(y_i|x_i, \boldsymbol{\beta})] \quad (4)$$

To optimize the cost function, we find the optimal weights $\boldsymbol{\beta}$ by solving $\mathrm{argmin}_{\boldsymbol{\beta}}$. Similarly to for LASSO regression, which we used in our previous project, this has no analytical solution and must be estimated using numerical methods, e.g. gradient descent [4]. This along with its stochastic sibling is described in section 3.4.

When using the model for prediction, $\hat{y} = p(X) \in [0, 1]$, where we say that outcome 0 is predicted if $\hat{y} < 0.5$ and outcome 1 else.

In this project we will use LR on the Taiwanese credit card data to try to predict default ($y = 1$) or non-default ($y = 0$) payment and evaluate the model's predictive accuracy in this particular classification problem.

3.2 Neural Networks (NN)

An artificial neural network (NN) is a computational model consisting of interconnected nodes. The interconnected nodes aim to emulate a simplified biological neural network and neuronal firing in a brain, and are therefore also commonly referred to as neurons. The node performs a weighted sum of its inputs that is subsequently passed through a mathematical function to determine its output. This mathematical function is called an activation function $f(z)$, and should emulate neuronal firing.

There is a wide variety of different neural networks. Commonly, they consist of layers of nodes separated into the input layer and output layer, and may also contain one or more in-between layers called hidden layers. One such NN is the multilayer perceptron (MLP), which is what we will be using in this project for both classification and regression.

3.3 Multilayer perceptron (MLP)

3.3.1 Feed-forward

The multilayer perceptron is a feed-forward neural network (FFNN), which means that the information flows forward only, starting from the input layer and to the output layer. Additionally, if each of the nodes in a layer are connected to all of the nodes in the succeeding layer, the network is fully connected. The inputs of the node are the weighted outputs of the nodes from the preceding layer, in addition to a bias term that can control whether or not the neuron fires if all the inputs are zero [5]. The weighted sum of the inputs of each node is called the activation.

Mathematical algorithm

Input layer
Starting with the input layer, which is the first layer in the MLP, the activation is calculated using the input coordinates x_j,

$$z_i^1 = \sum_{j=1}^{M_1} w_{ij}^1 x_j + b_i^1, \tag{5}$$

where the superscript 1 indicates the first layer, M_1 is the number of inputs to the ith node in the first layer, b_i is the bias and w_{ij} represents the weights.

The output of the nodes in the input layer is determined by the activation function $f(z)$,

$$f(z_i^1) = f\left(\sum_{j=1}^{M_1} w_{ij}^1 x_j + b_i^1\right) \tag{6}$$

Hidden layers and output layer
Similarly for the subsequent layers; the hidden layers and the output layer, the activation of the jth neuron of layer l is defined as

$$z_j^l = \sum_{i=1}^{M_{l-1}} w_{ij}^l a_j^{l-1} + b_j^l, \tag{7}$$

where b_j^l and w_{ij}^l are the biases and weights at layer l, M_{l-1} is the number of nodes at layer $l-1$ and $a_j^{l-1} = f(z_j^{l-1})$. The output of each node is then decided by passing the activation through the activation function,

$$f(z_j^l) = f\left(\sum_{i=1}^{M_{l-1}} w_{ij}^l a_j^{l-1} + b_j^l\right) \tag{8}$$

This is nearly identical to the method for the input layer, except that the inputs of these layers are the outputs from the previous layer.

3.3.2 Backpropagation

In order for the NN to learn, the weights and biases are initialized with values that we will discuss shortly. The weights and biases are then optimalized to minimize the cost function through a process called backpropagation, where we iterate backwards from the last layer to the first hidden layer. Another feed-forward process is initiated from the input layer to the output layer with the new biases and weights. If the cost function is not yet sufficiently minimized, then backpropagation is performed again. This process is repeated until the cost function is optimalized.

Mathematical algorithm
To calculate the optimal biases and weights for the problem, we initialize the gradients of the cost function $\mathcal{C}$ with respect to the weights W and biases b at the output layer $l = L$ and the output error δ_L as

$$\frac{\partial \mathcal{C}}{\partial w_{jk}^L} = \delta_j^L a_k^{L-1}, \tag{9}$$

$$\frac{\partial \mathcal{C}}{\partial b_j^L} = \delta_j^L, \tag{10}$$

$$\delta_j^L = f'(z_j^L)\frac{\partial \mathcal{C}}{\partial a_j^L}, \tag{11}$$

before propagating backwards through the hidden layers using the general equations

$$\frac{\partial \mathcal{C}}{\partial w_{jk}^l} = \delta_j^l a_k^{l-1}, \tag{12}$$

$$\frac{\partial \mathcal{C}}{\partial b_j^l} = \delta_j^l, \tag{13}$$

$$\delta_j^l = \sum_k \delta_k^{l+1} w_{kj}^{l+1} f'(z_j^l). \tag{14}$$

The full derivation of these equations can be found in *Neural networks, from the simple perceptron to deep learning* by Morthen Hjorth-Jensen [3].

3.3.3 Choosing activation function

There are certain properties that an activation function $f(z)$ should possess [5]:

1. $f(z)$ should be differentiable (continuous).
2. $f(z)$ should be non-constant and reach saturation at both ends of the range.
3. $f(z)$ should change quickly between the saturation values at the middle of the range.

It is clear from Equation (14) in the backpropagation algorithm that the activation function $f(z)$ should be differentiable, while the remaining properties are mainly related to the emulation of firing of neurons in a brain.

There are several functions that meet these requirements. Historically, the sigmoid function has been a popular choice of activation function until recently. To compare our results with the original paper from 2009 by I-Cheng Yeh and Che-hui Lien [7], we have chosen to use the sigmoid function in our implementation of the MLP, as it is likely the same function they used. The function is given by

$$f(z) = \frac{1}{1+e^{-z}} \,. \tag{15}$$

Its gradient is given by

$$\frac{\partial f}{\partial z} = \frac{e^{-z}}{(1+e^{-z})^2}. \tag{16}$$

However, there are cases where we do not want a sigmoidal output activation function, such as for regression problems where the outputs should be from a continuous range instead of binary. Instead of a sigmoidal activation function for the regression case at output layer $l = L$, we implement a linear activation function, such that

$$f(z_j^L) = z_j^L = \sum_{i=1}^{M_{L-1}} w_{ij}^L a_j^{L-1} + b_j^L. \tag{17}$$

For our binary classification case, we keep the sigmoid function as the output activation function.

3.3.4 Choosing cost function

Looking at the equations for backpropagation, it is clear that the chosen cost function $\mathcal{C}$ should be differentiable as well. Additionally, the cost function should be chosen with the desired functionality in mind, i.e. the cost functions for regression and classification should be different.

For the classification part of this project we have chosen to use the logistic loss as cost function, which is the negative log-likelihood,

$$\mathcal{C}_{\text{NN}}^{\text{C}}(\boldsymbol{W},\boldsymbol{b}) = -\sum_{i=0}^{n-1}\Big[\, a_i^l \log p\left(a_i^l|z_i^l,\ \boldsymbol{W},\ \boldsymbol{b}\right) \tag{18}$$

$$+(1-a_i^l)\log\left(1-p(a_i^l|z_i^l,\ \boldsymbol{W},\ \boldsymbol{b})\right)\Big]\,,$$

with $a_i^l = f(z_i^l)$ as before. The gradient at the last layer is

$$\frac{\partial \mathcal{C}_{\text{NN}}^{\text{C}}}{\partial a_i^L} = a_i^L - t_i, \tag{19}$$

where t_i is the target.

For the regression part we will use the cost function

$$\mathcal{C}_{\text{NN}}^{\text{R}} = \frac{1}{2}\sum_{i=0}^{n-1}(t_i - a_i^l)^2. \tag{20}$$

The gradient in the last layer is given by

$$\frac{\partial \mathcal{C}_{\text{NN}}^{\text{R}}}{\partial a_i^L} = t_i - a_i^L\ . \tag{21}$$

The gradients in Equation (19) and (21) can then be inserted into Equation (14) in the backpropagation algorithm.

3.3.5 Initialising the weights and biases

The biases can be initialized to zero, but we have chosen an initial value of 0.01 to ensure that all of the neurons have some initial output. Initializing the weights to zero, however, will result in all neurons outputting the same value. Instead, the weights are initialized with values drawn from a uniform distribution such that $w_{kj} \in (-1/\sqrt{n},\ 1/\sqrt{n})$, where n is the amount of nodes in the input layer, to ensure uniform learning [5].

3.3.6 Regularization

As neural networks often have large amounts of parameters, they are considered very high variance low bias estimators. This means they are very prone to overfitting. To counteract this, we introduce regularization using the L_2 penalty on the weights similarily to Ridge regression. Mathematically, this means adding the regularized cost function becomes

$$\mathcal{C}_{\text{Regularized}} = \mathcal{C}_{\text{NN}}^{C/R} + \lambda||\boldsymbol{W}||_2^2 \tag{22}$$

and its derivative becomes

$$\frac{\partial \mathcal{C}}{\partial \boldsymbol{W}}_{\text{Regularized}} = \frac{\partial \mathcal{C}_{\text{NN}}^{\text{C/R}}}{\partial \boldsymbol{W}} + \lambda \boldsymbol{W}. \tag{23}$$

Here λ is a hyperparameter we need to tune.

3.4 Stochastic Gradient Descent (SGD)

It is clear that in order to find the best possible fit, we need to optimize the cost function $\mathcal{C}$ by finding its minimum. A common method to achieve this is the gradient descent (GD) method, in which the parameters θ are iteratively adjusted in the direction of the largest negative value of the gradient for a given number of epochs or until it reaches a given tolerance. Mathematically, this is expressed as

$$\theta_{i+1} = \theta_i - \eta\nabla\mathcal{C}(\theta_i), \tag{24}$$

where η is the learning rate, which is a hyperparameter that controls the step length and by extension the convergence time. For smaller values of η, the method will take longer to converge or might not converge at all within the maximum number of epochs. For larger values of η, the method might be unstable or pass the minimum altogether and diverge. The parameter θ is β in the LR case, and the weights W and biases b in the MLP case. Our definition of convergence is when the cost function does not change by more than a factor 0.01 for ten epochs.

However, calculating the gradient on the entire data set can be computationally expensive and inefficient for large amounts of data. Additionally, there is a high possibility of a local minimum being misinterpreted as a global minimum by the algorithm. To alleviate these problems, we can use stochastic gradient descent (SGD) with minibatches. A minibatch is a subset of the data, on which we can perform GD. By using stochasticity to perform gradient descent on randomly chosen minibatches of size M, we have a more efficient way to approximate the gradient of the total data set as it might not need to use the entire set. Additionally, the stochasticity reduces the possibility of getting stuck in a local minimum.

3.5 Tuning hyperparameters

Hyperparameters are not estimated when fitting a model, and must instead be found by other means. A naive approach when you have few hyperparameters could be to find them manually by trial and error. A slightly better approach is to grid over your hyperparameter space. However, this can be very computationally expensive. Studies indicate that a random search is preferable, as it is less systematic than a grid search, and thus more statistically likely to find better hyperparameters [1]. For each trial parameter, one evaluates the model on the training data, preferably either splitting some of the training data into validation data or using cross validation to avoid overfitting. The final best model is then evaluated using the test data.

For non-penalized logistic regression with stochastic gradient descent, the two hyperparameters are learning rate and batch size. We have chosen to use a batch size of 200, inspired by the default value of Scikit-Learn. If we had more time or more powerful hardware, we would ideally also try different batch sizes. The learning rate is found using a randomized search with cross validation.

Neural networks contain many hyperparameters. The amount of layers, nodes in each layer, batch size, learning rate and penalization should all ideally be tested. As with LR, we have chosen to use a constant batch size of 200. For the layers and nodes, we have chosen to limit ourself to two hidden layers with many nodes. A neural network with a single hidden layer with a large amount of nodes is already sufficient enough to be considered a universal approximator. With two hidden layers, the amount of nodes needed is reduced [5], making a two hidden layer neural network sufficient for most cases. For both datasets analyzed, our first hidden layer has 100 nodes, the second has 50. This leaves the learning rate and the regularization parameter which are found using randomized search.

To perform the parameter search we use the `RandomizedSearchCV` class provided by `Scikit-Learn` [2] on 100 samples of hyperparameters, with 5-fold cross validation to evaluate each sample. The maximum number of epochs is set to 300 for all models. Our evaluation methods are explained in the next section.

4 Model evaluation

4.1 Regression

To evaluate the performance of our regression model, we consider the R^2 score, given by

$$R^2(\boldsymbol{y}, \hat{\boldsymbol{y}}) = 1 - \frac{\sum_{i=0}^{n-1}(y_i - \hat{y}_i)^2}{\sum_{i=0}^{n-1}(y_i - \bar{y})^2}, \tag{25}$$

where $\boldsymbol{y}$ is the given data, $\hat{\boldsymbol{y}}$ is the model and $\bar{y}$ is the mean value of $\boldsymbol{y}$. The R^2 score evaluates how well your model $\hat{\boldsymbol{y}}$ fits the true values $\hat{y}$, with a value of 1 indicating a perfect fit. An R^2 score of 0 indicates that the model is as good of an estimator as the mean value $\bar{y}$, and a lower value means that the mean value is a better estimator than the model.

4.2 Classification

To evaluate the performance of our classification model, we consider the accuracy score, given by

$$\text{accuracy} = \frac{\sum_{i=1}^{n} I(t_i = y_i)}{n}, \tag{26}$$

where t_i is the target, y_i is the model output, n is the number of samples and I is the indicator function,

$$I = \begin{cases} 1, & t_i = y_i \\ 0, & t_i \neq y_i \end{cases}.$$

The error rate used in the original article [7] is then defined as

$$\text{error} = 1 - \text{accuracy}. \tag{27}$$

For the data used in this project, this is not a very good metric however. This is because even a model that predicts 0 for all cases would get an accuracy score of nearly 0.8 due to the large ratio of non-default payments to default payments in the credit card data set. The need for a better model evaluation is clear, and we employ the same technique as in the original article by I-Cheng Yeh and Che-hui Lien, which was the area ratio [7] between the baseline and our model in a cumulative gains plot divided by the area between the theoretically best model and the baseline. To generate cumulative gains plots, we used the Python library `Scikit-Plot`'s function `plot_cumulative_gain`. An area ratio of 1 would simply be the theoretically most optimal fit, whereas lower ratios indicate lower predictive ability of the model.

5 Results

Figure 1 shows the accuracy score for LR on the credit card training and validation data set for 100 different values of the learning rate η found using randomized search. Looking at the figure, we observe that the accuracy score drops significantly for learning rates at the higher and lower values of the range. The learning rate value that maximizes the accuracy score is considered the best value and is shown in Table 2.

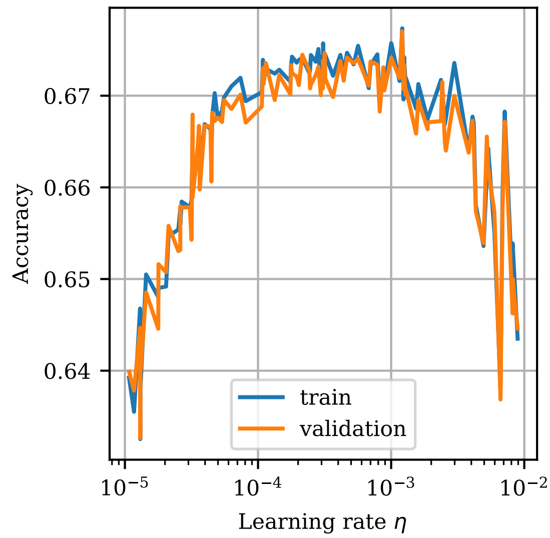


Figure 1: Accuracy score of validation set of the credit data using logistic regression for various values of the shrinkage parameter chosen using randomized search.

Similarly, Figure 2 shows the accuracy score for the MLP classifier used on the credit card data set for 100 different combinations of values for the learning rate η and the shrinkage parameter λ configured using random search. The figure shows that most of the combinations of our learning and shrinkage parameters in our chosen range give an accuracy score between approximately 0.65-0.70, with the exception of a few outliers. Generally, it seems like accuracy scores improve with smaller learning rates within our chosen range. The effect of the choice of shrinkage parameter is not as conclusive, although it seems like the score is lower when the shrinkage parameter is of orders larger than 10^{-2}. The combination of learning rate and shrinkage parameter that gives the highest accuracy score is considered the most optimal of our combinations, and is also shown in Table 2.

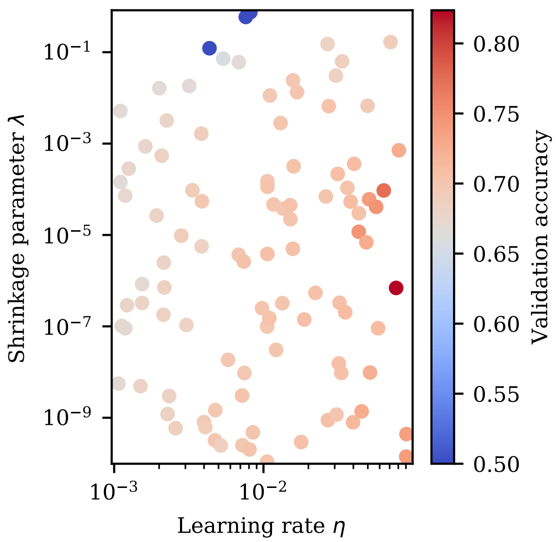


Figure 2: Accuracy score of validation set of the credit card data using the multilayer perceptron classifier on the credit card data for various shrinkage parameters and learning rates chosen using randomized search.

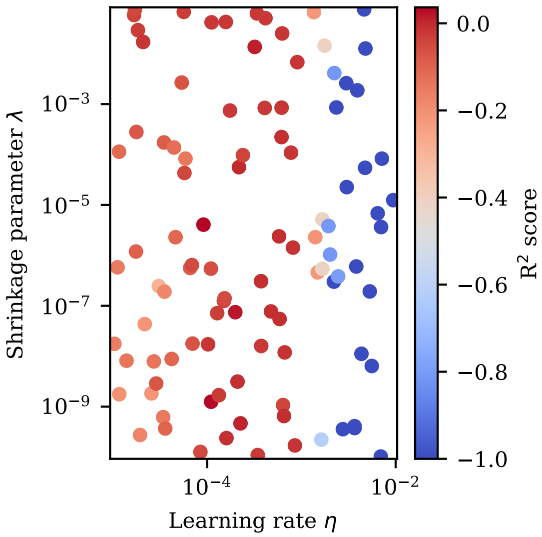
Figure 3, 4 and 5 show the validation R^2 scores for the MLP regressor on the `franke0`, `franke1` and `franke2` data sets, respectively. For a reminder of the differences between these data sets, please refer to Table 1. As for the classification methods, the models were evaluated for 100 different combinations of learning rate and shrinkage parameter values.

For `franke0` in Figure 3, the R^2 score is the lowest for the higher values of the learning rate in the chosen range at around order $10^{-3} - 10^{-2}$ and the highest between approximately $10^{-4} - 10^{-3}$. The shrinkage parameter values in our range do not seem to have a large effect on the R^2 score of the model.

For `franke1` in Figure 4, the learning rates of order around 10^{-2} seem to result in the lowest R^2 scores, as well as a small amount of outliers at learning rates of order 10^{-5}, whereas the highest R^2 scores seem to be at around learning rates of order 10^{-4}. Shrinkage parameters of order 10^{-2} and higher result in a lower R^2 score.

For `franke2` in Figure 5, there is not a large difference in R^2 scores between learning rates of order $10^{-5} - 10^{-3}$, where they are the highest. They are lowest for larger values of learning rates. Additionally, the shrinkage parameters of order 10^{-3} or larger drastically reduce the R^2 scores, while smaller values seem to result in better scores.

The most optimal models for the regression case were the ones that maximized the R^2 scores. The corresponding shrinkage parameter and learning rate values can be found in Table 2.



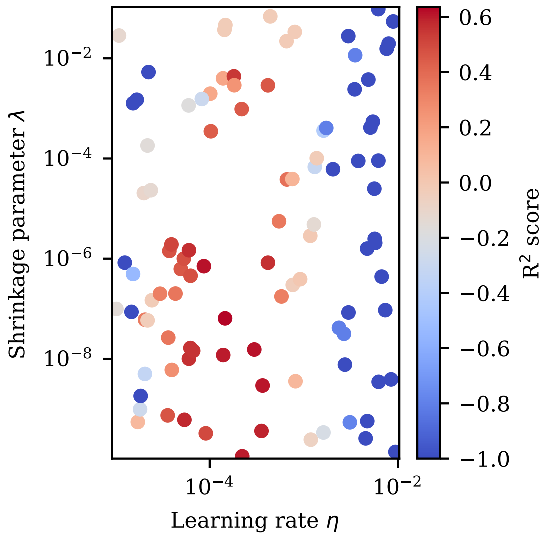


Figure 3: R^2 score of validation set on the `franke0` data set using the multilayer perceptron regressor for various shrinkage parameters and learning rates chosen using randomized search.

Figure 4: R^2 score of validation set on the `franke1` data set using the multilayer perceptron regressor for various shrinkage parameters and learning rates chosen using randomized search.

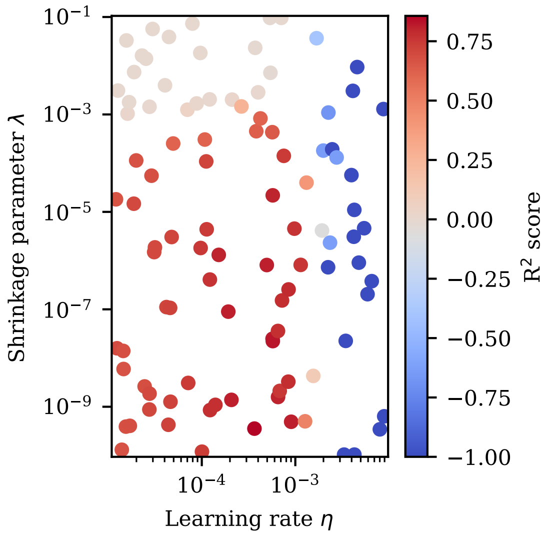


Figure 5: R^2 score of validation set on the `franke2` data set using the multilayer perceptron regressor for various shrinkage parameters and learning rates chosen using randomized search.

Table 2: Table of the best hyperparameters values for shrinkage λ and learning rate η for the logistic regression (LR) and neural network (NN) models. The parameters were found using 5-fold cross validation. The minibatch size was kept constant at $M = 200$. All the results have been modelled using these values.

Model	Shrinkage λ	Learning rate η
LR credit data	N/A	$4.4 \cdot 10^{-4}$
NN credit data	$6.9 \cdot 10^{-7}$	$7.7 \cdot 10^{-2}$
NN `franke0`	$4.1 \cdot 10^{-6}$	$9.1 \cdot 10^{-5}$
NN `franke1`	$6.4 \cdot 10^{-8}$	$1.5 \cdot 10^{-4}$
NN `franke2`	$3.6 \cdot 10^{-10}$	$3.7 \cdot 10^{-4}$

5.1 Classification

Figure 6 shows the cumulative gains plot for the LR. From the figure, we can see that our LR model performs worse when predicting non-default outcomes than default. Both area ratios can be found in Table 3.

Figure 7 shows the cumulative gains plot for the MLP classifier. From the figure, we can see that similarly to for the LR model, the MLP classifier model's predictive abilities are better for default outcomes than for non-default. Both area ratios can be found in 3.

From Table 3 containing the area ratios for LR and MLP, we see that the MLP network has a lower error rate than LR, in addition to having higher area ratios for both default and non-default outcomes.

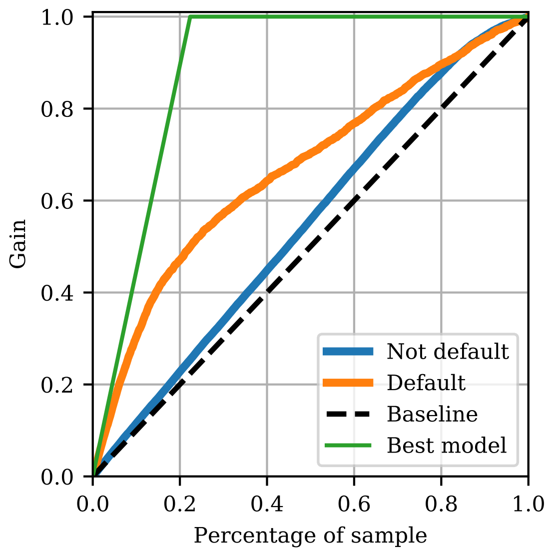


Figure 6: Cumulative gains plot for the logistic regression model fit on the credit card data.

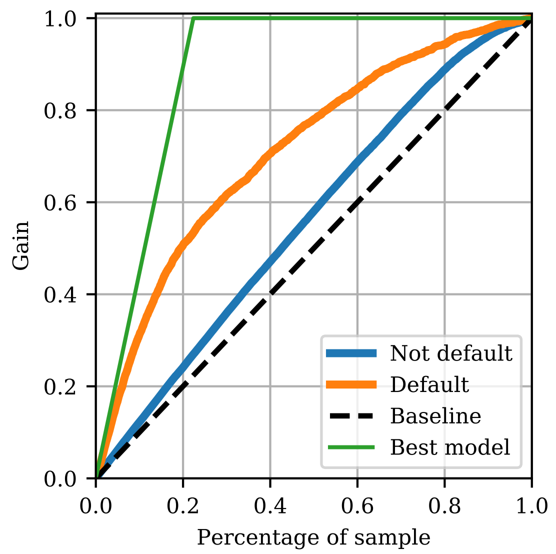


Figure 7: Cumulative gains plot for the multilayer perceptron model fit on the credit card data.

Table 3: Table of error rates and area ratios for classification of the credit card data using logistic regression (LR) and the multilayer perceptron (MLP) neural network (NN).

Method	Error rate	Area ratio default	Area ratio non-default
LR	0.31	0.43	0.12
NN	0.22	0.55	0.16

5.2 Regression

Table 4 shows the R^2 scores for the `franke0`, `franke1` and `franke2` data sets using the MLP regressor in addition to the scores found using the OLS model. For the `franke0` set, the MLP and OLS seem to perform similarly, with scores lying in a small interval around zero. For `franke1` the score for OLS is significantly higher, while the OLS model for `franke1` and the MLP model for `franke2` show similar performances. The consistency of the R^2 score across training and test sets is better for the MLP model in the cases of `franke1` and `franke2`.

Figure 8, 9 and 5 show the MLP models for the `franke0`, `franke1` and `franke2` data sets plotted with the true values.

Table 4: Table of R2 scores for our neural network (NN) regression models on the three Franke data sets and the ordinary least squares (OLS) model from our previous study [4].

	R^2	`franke0`	`franke1`	`franke2`
NN	Train	0.0052	0.59	0.84
	Test	- 0.057	0.59	0.83
OLS	Train	0.024	0.87	N/A
	Test	- 0.040	0.82	N/A

6 Discussion

Hyperparameters: * different learning rate nn logreg same data * low penalties because no overfit, maybe more relevant with a better optimizer than sgd, ADAM? * Unsure because only 100 samples * maybe different results with vary epochs(?), rtol(?), layers, nodes and batch size * activation function impact

6.1 Classification

From Table 2, we see that the learning rate η for LR and MLP in the classification case differ by two orders of magnitude. This

The area ratios in Table 3 along with Figure 6 and 7 align closely with the results from the original paper [7], with the neural network being noticeably better at predicting the default of a credit card user. While both models can predict the positive outcome with modest success, they are not suited for predicting the negative outcome within any kind of satisfactory margin. This is not all bad, though, as it is more important for a lender to avoid false negatives than false positives. As we

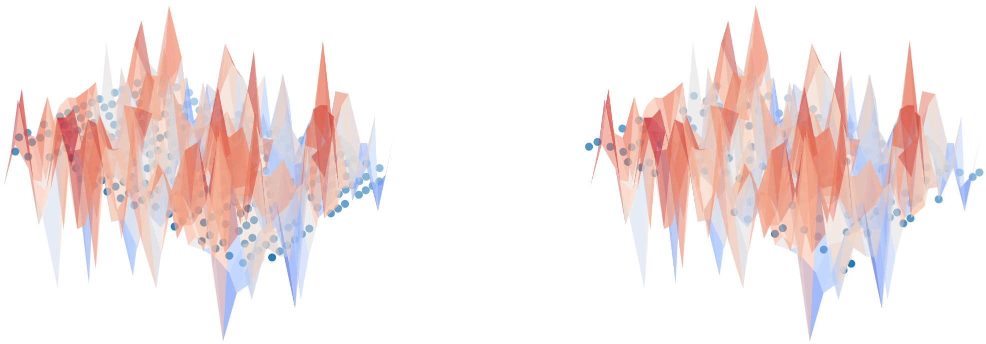


Figure 8: 3D plot of the Franke function with added noise $\sim \mathcal{N}(0, \sigma^2)$ with $\sigma = 1.0$. The dotted markers represent the regression model found using MLP. The left plot shows the model fitted on the training set, the right shows the model fitted on the test set. The total data set consist of 400 points, using two thirds ($2/3$) as the training set and the remaining points ($1/3$) as the test set.

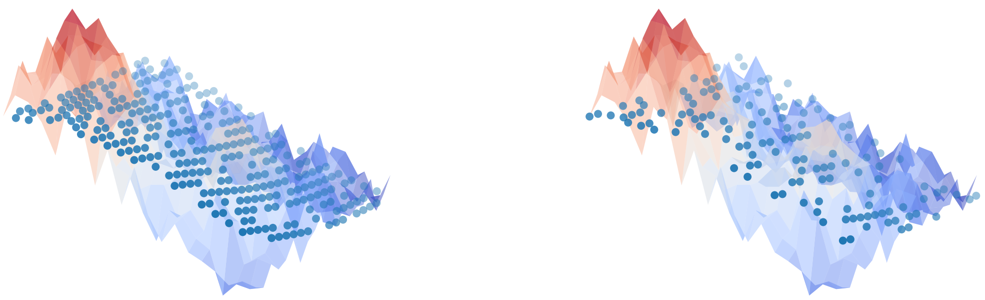


Figure 9: 3D plot of the Franke function with added noise $\sim \mathcal{N}(0, \sigma^2)$ with $\sigma = 0.1$. The dotted markers represent the regression model found using MLP. The left plot shows the model fitted on the training set, the right shows the model fitted on the test set. The total data set consist of 400 points, using two thirds ($2/3$) as the training set and the remaining points ($1/3$) as the test set.

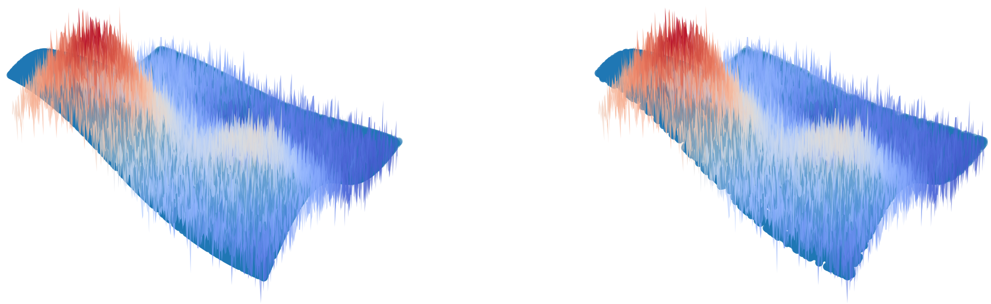


Figure 10: 3D plot of the Franke function with added noise $\sim \mathcal{N}(0, \sigma^2)$ with $\sigma = 0.1$. The dotted markers represent the regression model found using MLP. The left shows the model fitted on the training set, the right shows the model fitted on the test set. The total data set consist of 40 000 points, using two thirds ($2/3$) as the training set and the remaining points ($1/3$) as the test set.

see no clear signs of overfitting, we may also be able find better fit by for instance running a significantly higher amount of hyperparameter samples in the randomized search, or by also searching for the best batch size, which we have neglected completely because of computational cost, as our program runs very slowly for small batch sizes.

6.2 Regression

Looking at the shrinkage parameters for the regression models in Table 2, the shrinkage parameter seems to decrease as the signal to noise ratio increases. For `franke0`, the data set is quite noisy with the standard deviation of the added noise at $\sigma = 1.0$ and a shrinkage parameter of $\lambda = 4.1 \cdot 10^{-6}$. However, taking Figure 3 into consideration, it is quite clear that the shrinkage parameter does not seem to have a significant effect on the result as opposed to the learning rate η, and the choice of shrinkage parameter may have been irrelevant as it arbitrarily coincided with the optimal learning rate. This is due to the very low signal to noise ratio, as can be seen in the plot of the model and true values in Figure 8. It is impossible to identify the original shape of the Franke function, and the model seems to have approximated the mean value of the `franke0` set. This is also reflected in the R^2 scores in Table 4, where the scores for both training and test set are close to zero. Due to the noise, the choice of shrinkage parameter does not matter, as Figure 3 the MLP models yield an R^2 score of around 0 for learning rates of order $10^{-4} - 10^{-3}$ regardless of shrinkage. Nevertheless, the mean seems like a decent approximation in this case, as tuning the other hyperparameters such as number of hidden layers and nodes could possibly result in a severe overfit. Comparing with the scores for the corresponding OLS model, the MLP seems to perform on par with the OLS, but at significantly higher computational cost.

For the `franke1` set, the shrinkage parameter does seem to impact the performance of our MLP model. From Figure 4, it appears that higher shrinkage has a negative effect on the model performance when the standard deviation of the noise is only at $\sigma = 0.1$. The optimal shrinkage parameter is at $\lambda = 6.4 \cdot 10^{-8]}$, which is higher than for the `franke0` set. Again, this is likely due to the higher signal to noise ratio in the data set, as we from Figure 9 are able to discern the rough shape of the original Franke function and the model is able to approximate the slope of the function. The R^2 scores from Table 4 show that the MLP model performs far better in this case with a test score of 0.59. Regardless, the OLS model outperforms the MLP in this case as well, and still at a significantly lower computational cost. It is probably still possible for the MLP to approximate a better model by increasing the model complexity. By tuning the other hyperparameters in combination with the learning rate and shrinkage parameter, we would likely be able to achieve a better fit, as the consistency of the R^2 scores we achieved for both test and training sets of `franke1` indicate that we have yet to overfit the data. However, this would again be quite costly and excessive compared to the simplicity of the OLS.

The optimal shrinkage parameter for `franke2` is the smallest of the three at $\lambda = 3.6 \cdot 10^{-10}$, and is likely because the amount of data points in this set is 100 times larger than for `franke0` and `franke1`. It is interesting to note that the shrinkage parameter is smaller than for `franke1` when the added noise is still of the same order, but the number of available data points is much higher. Due to the larger amount of data, the MLP is less likely to overfit and requires a smaller shrinkage. Looking at Figure 10 of the model and data plot, it does appear that the MLP is able to model a relatively good fit. The corresponding R^2 scores in Table 4 are quite satisfactory and consistent in comparison to the OLS model for `franke1`. However, the OLS would likely perform as well or possibly better at 40 000 available data points instead of only 400. The MLP regressor proves to be quite costly and excessive in this case compared to the OLS, as it in this case needs a hundred times more data points and tuning of several hyperparameters to perform on par with the OLS.

In summary, there seems to be very few benefits of using neural networks for regression of simple, well behaved functions, especially considering the amount of hyperparameters to tune using NN instead of a simple linear regression model. One benefit of neural networks versus linear regression is the simplicity of the feature matrix. To implement the OLS in this case, we needed to create a large feature matrix to encompass the fourth order two-dimensional polynomial fit, which can for large datasets be memory costly. Regardless, in the case of the Franke function this was insignificant, as the extra amount of data and hyperparameter tuning needed for the MLP to perform equally to OLS far surpasses the cost of implementing the OLS.

For all three cases, the choice of learning rates had a more significant impact on model performance than the shrinkage parameter. This implies that we could likely increase the MLP model complexity to achieve more optimal fits, although as argued above this would be computationally expensive compared to the OLS.

7 Conclusion

Better model each case: Credit card: NN, as prediction power very important because serious topic

Franke: OLS, only one hyperparameter (poly degree), no fuzz, more memory usage, but still better

Conclusion: Powerful models are better at predicting, but are much harder to implement. Should carefully consider what to use as to not waste resources.

References

[1] James Bergstra and Yoshua Bengio. Random search for hyper-parameter optimization. *Journal of Machine Learning Research*, 13(Feb):281–305, 2012.

[2] Lars Buitinck, Gilles Louppe, Mathieu Blondel, Fabian Pedregosa, Andreas Mueller, Olivier Grisel, Vlad Niculae, Peter Prettenhofer, Alexandre Gramfort, Jaques Grobler, Robert Layton, Jake VanderPlas, Arnaud Joly, Brian Holt, and Gaël Varoquaux. API design for machine learning software: experiences from the scikit-learn project. In *ECML PKDD Workshop: Languages for Data Mining and Machine Learning*, pages 108–122, 2013.

[3] Morten Hjorth-Jensen. Neural networks, from simple perceptron to deep learning. `https://compphysics.github.io/MachineLearning/doc/pub/NeuralNet/pdf/NeuralNet-minted.pdf`, 2019. Retrieved: 07-11-2019.

[4] Bernhard Nornes Lotsberg and Anh-Nguyet Lise Nguyen. *Project 1: Regression analysis and resampling methods*. FYS-STK3155/4155 Applied Data Analysis and Machine Learning. 2019.

[5] Stephen Marsland. *Machine Learning: An Algorithmic Perspective, Second Edition*, pages 71–107. Chapman and Hall/CRC, 2014.

[6] UCI Machine Learning Repository. Default of credit card clients Data Set. `https://archive.ics.uci.edu/ml/datasets/default+of+credit+card+clients`. Retrieved: 08-10-2019.

[7] I-Cheng Yeh and Che-hui Lien. The comparisons of data mining techniques for the predictive accuracy of probability of default of credit card clients. *Expert Systems with Applications*, 36(2):2473–2480, 2009.