

Non-linear regression and classification with MLPs

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Regression

In this problem, the objective is to approximate a non-linear function using a feedforward artificial neural network. The first step is to build the dataset.

Define the dataset

First, The dataset must be constructed using the digits of the student number. The largest five digits in descending order are used, this is, **86541**, to build a target T_{new} . This target is built using the following formula:

$$T_{new} = (8T_1 + 6T_2 + 5T_3 + 4T_4 + 1T_5) / (8 + 6 + 5 + 4 + 1)$$

where T_1, T_2, \dots, T_5 are located in the input data file and represents 5 independent nonlinear functions.

The dataset to use consists of X_1, X_2 and T_{new} . To draw 3 independent samples of 1000 points each, a vector from 1 to 13600 is created. This vector represents the indices of the dataset. Then, the content of this vector is randomized, and 1000 items are selected from X_1, X_2 and T_{new} using this randomized vector. This new dataset is now the training set, validation set, and test set, respectively.

Classification

Classification is a key problem in machine learning. This problem proposes a binary classification using a real-life dataset containing characteristics and quality of red and white wine.

Dataset

Given my student number, r0650814, the dataset is constructed in the following way using the white wine data:

- For the positive class, $C_+ = 4$
- For the negative class, $C_- = 5 + 6$

The last column of the data set, indicating the original class, is removed, and the new data is labeled using 1 for the positive class, and -1 for the negative class.

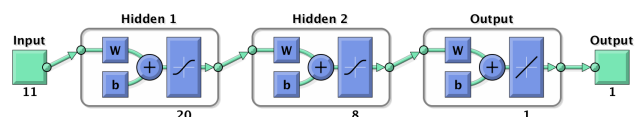
The number of instances in each class differs considerably, containing the positive class 163 instances and the negative class 3655.

Classify

First of all, as the classes are unbalanced, it is necessary to determine whether a result is considered good or not. If the majority category is always predicted, this is, the prediction is always C_- an accuracy in the classification of 95,73% is obtained. This result can be considered as our baseline data.

Then, a feedforward neural network is created. Different algorithms and network architectures has been tried, and the obtained results are presented:

- **Number of hidden layers** - Our experiments has shown that with two hidden layers, the best results are achieved. Although other architectures with one and three hidden layers has been tested, the results did not shown an increase in the network performance.
- **Number of neurons in the hidden layers** - The selected number of neurons for the first hidden layer is 20, and 8 for the second one. The purpose of this is to generalize and find underlying patterns in the data, and use this patterns to concretize.
- **Epochs** - The number of epochs has been set to 400.
- **Transfer function** - The transfer function used for the second layer is **tansig**, as the results obtained are slightly better than the ones using **purelin**.



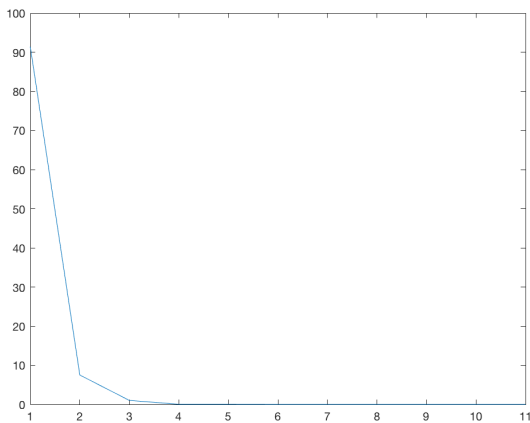
Using this network architecture, different training algorithm has been used:

- **traingd** - Gradient descent is a well-known algorithm that has been studied in previous assignments. The main problem of this algorithm is that it is prone to get stuck in local minima. In this case, it returns an accuracy of 95.73%, which is the one obtained using ZeroR.
- **trainlm** - Levenberg-Marquardt slightly improves Gradient descent with a performance of 95.96%.

- **trainbr** - Bayesian regularization shows the best results, obtaining an accuracy of 98.9%

Dimensionality reduction

To increase the performance of the network and reduce the complexity of the data set, Principal Component Analysis is applied. This method reduces the dimensionality of the data. First, we have to see which dimensions contains most of the variance, this is, separates the data better. It can be done calculating the eigenvalues of the covariance matrix of the data, and plotting them.



It can be seen that the first 4 dimensions holds the majority of the variance, which means that the dataset can be reduced from 11 dimensions to 4 without loss of generality.

Now, or dataset has been reduced to 4 dimensions, and a feedforward neural network is applied to classify the new dataset.

First, the same network with the same parameters and options used before is applied, to see the impact of dimensionality reduction in the results. Training and executing the network with the reduced dataset returns an accuracy of 97.73%, which is slightly worse than the one obtained with the original dataset, but better than the results obtained with ZeroR.

The network parameters and architecture have been changed, and other approaches to improve generalization and avoid overfitting have been tried, such as retraining the neural network and using multiple neural networks averaging their outputs, but it has not been appreciated an improvement in the accuracy.

Appendix