

Machine Learning Project 2
Supervised Learning: Classification and Regression

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Group 94

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(a) Group members.

| Task | Vincent | Diego | Albert |
|---------------------------------|---------|-------|--------|
| Training & test loops | 0% | 0% | 0% |
| Coding visualisations | 0% | 0% | 0% |
| Section 3 | 0% | 0% | 0% |
| L ^A T _E X | 0% | 0% | 0% |

(b) Contributions & responsibilities table.

Table 1: Group information & work distribution.

Introduction

The objective of this report is to apply the methods that were discussed during the second section of the course *Machine Learning* [1] to a chosen dataset. The aim is to perform relevant regression and classification to the data.

The particular dataset that is being investigated is – just like in Project 1 – the *Glass Identification* dataset from 1987 by B. German [2]. Table 1a lists our full names and student numbers, while Table 1b shows an overview of the contribution of each team member.

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| Outer fold | ANN | | Linear regression | | Baseline |
|------------|---------|------------------------|-------------------|-------------------------|------------------------|
| i | h_i^* | E_i^{test} | λ_i^* | E_i^{test} | E_i^{test} |
| 1 | 128 | 2.847×10^{-2} | 0.01 | 9.516×10^{-14} | 9.893×10^{-6} |
| 2 | 128 | 1.572×10^{-2} | 0.01 | 3.239×10^{-13} | 7.295×10^{-6} |
| 3 | 128 | 7.582×10^{-2} | 0.01 | 7.883×10^{-13} | 7.229×10^{-6} |
| 4 | 256 | 1.983×10^{-2} | 0.01 | 1.095×10^{-13} | 8.142×10^{-6} |
| 5 | 128 | 2.452×10^{-2} | 0.01 | 2.309×10^{-13} | 3.843×10^{-6} |
| 6 | 128 | 2.165×10^{-2} | 0.01 | 1.261×10^{-13} | 4.273×10^{-6} |
| 7 | 128 | 1.983×10^{-2} | 0.01 | 4.525×10^{-13} | 8.609×10^{-6} |
| 8 | 128 | 1.222×10^{-2} | 0.01 | 1.560×10^{-13} | 1.072×10^{-5} |
| 9 | 256 | 5.593×10^{-2} | 0.01 | 6.452×10^{-13} | 1.782×10^{-5} |
| 10 | 256 | 9.549×10^{-2} | 0.01 | 7.505×10^{-14} | 1.526×10^{-5} |

Table 2: Summary of two-level cross validation for predicting [TODO: see Python script]. Hyperparameters and test errors E_i^{test} on $\mathcal{D}_i^{\text{test}}$ per outer fold i , for each of the three considered models.

1 Regression

[TODO: Make visualisations of the results in Table reftable:e-test-regression]

1.1 Linear regression

1.1.1 Aim

[TODO: Explain what variable is predicted based on which other variables and what you hope to accomplish by the regression. Mention your feature transformation choices such as one-of- K coding. Since we will use regularization momentarily, apply a feature transformation to your data matrix X such that each column has mean 0 and standard deviation 1.]

[TODO: ...]

1.1.2 Regularization

[TODO: Introduce a regularization parameter λ as discussed in 14 of the lecture notes, and estimate the generalization error for different values of λ . Specifically, choose a reasonable range of values of λ (ideally one where the generalization error first drop and then increases), and for each value use $K = 10$ fold cross-validation (algorithm 5) to estimate the generalization error. Include a figure of the estimated generalization error as a function of λ in the report and briefly discuss the result.]

[TODO: Figure]

[TODO: Reference figure]

[TODO: ...]

1.1.3 Model interpretation

[TODO: Explain how the output, y , of the linear model with the lowest generalization error (as determined in the previous question) is computed for a given input x . What is the effect of an individual attribute in x on the output, y , of the linear model? Does the effect of individual attributes make sense based on your understanding of the problem?]

[TODO: Final equation]

| Outer fold | [TODO: Decision Tree?] | | Logistic regression | | Baseline |
|------------|------------------------|----------------------------|---------------------|----------------------------|----------------------------|
| i | h_i^* | E_i^{test} | λ_i^* | E_i^{test} | E_i^{test} |
| 1 | 10 | $1.363\,64 \times 10^{-1}$ | 0.001 | $2.272\,73 \times 10^{-1}$ | $6.363\,64 \times 10^{-1}$ |
| 2 | 6 | $4.090\,91 \times 10^{-1}$ | 0.008\,86 | $2.727\,27 \times 10^{-1}$ | $6.818\,18 \times 10^{-1}$ |
| 3 | 4 | $4.545\,45 \times 10^{-1}$ | 0.008\,86 | $4.090\,91 \times 10^{-1}$ | $5.909\,09 \times 10^{-1}$ |
| 4 | 4 | $5.000\,00 \times 10^{-1}$ | 0.008\,86 | $4.545\,45 \times 10^{-1}$ | $5.454\,55 \times 10^{-1}$ |
| 5 | 7 | $2.857\,14 \times 10^{-1}$ | 0.001 | $3.333\,33 \times 10^{-1}$ | $6.190\,48 \times 10^{-1}$ |
| 6 | 10 | $4.761\,90 \times 10^{-1}$ | 0.001 | $5.714\,29 \times 10^{-1}$ | $7.142\,86 \times 10^{-1}$ |
| 7 | 8 | $2.857\,14 \times 10^{-1}$ | 0.008\,86 | $3.333\,33 \times 10^{-1}$ | $7.142\,86 \times 10^{-1}$ |
| 8 | 5 | $1.428\,57 \times 10^{-1}$ | 0.0183 | $2.380\,95 \times 10^{-1}$ | $6.190\,48 \times 10^{-1}$ |
| 9 | 10 | $4.761\,90 \times 10^{-1}$ | 0.001 | $3.333\,33 \times 10^{-1}$ | $8.571\,43 \times 10^{-1}$ |
| 10 | 3 | $4.285\,71 \times 10^{-1}$ | 0.0183 | $4.761\,90 \times 10^{-1}$ | $8.095\,24 \times 10^{-1}$ |

Table 3: Summary of two-level cross validation for predicting the glass type. Hyperparameters and test errors E_i^{test} on $\mathcal{D}_i^{\text{test}}$ per outer fold i , for each of the three considered classification models. [TODO: Change λ to C ?]

[TODO: ...]

1.2 Regularized linear regression vs an Artificial Neural Network

[TODO: Rewrite this (concisely!) so that it isn't an exact copy of the assignment]

In this section, we will compare three models: the regularized linear regression model from the previous section, an artificial neural network (ANN) and a baseline. We are interested in two questions: Is one model better than the other? Is either model better than a trivial baseline?. We will attempt to answer these questions with two-level cross-validation.

[TODO: Create the table as in the assignment (Vincent)]

[TODO: Write the accompanying text on how we retrieved the data in the table.]

[TODO: Write out the statistical comparisons using data from the table.]

[TODO: TABLE: Include p-values and confidence intervals for the three pairwise tests in your report.]

[TODO: Conclude on the results from the values in the table and reference the table.]

2 Classification

[TODO: Choose method 2: ANN, CT, KNN, NB]

[TODO: Make visualisations of the results in 3]

2.1 Introduction

[TODO: Explain which classification problem you have chosen to solve. Is it a multi-class or binary classification problem?]

2.2 Logistic regression vs [...method 2...]

[TODO: Rewrite the assignment below such that it (consisely!) states what we will do in this section.]

We will compare logistic regression, method 2 and a baseline. For logistic regression, we will once more use λ as a complexity-controlling parameter, and for method 2 a relevant complexity controlling parameter and range of values. We recommend this choice is made based on a trial run, which you do not need to report. Describe which parameter you have chosen and the possible values of the parameters you will examine. The baseline will be a model which compute the largest class on the training data, and predict everything in the test-data as belonging to that class (corresponding to the optimal prediction by a logistic regression model with a bias term and no features).

[TODO: Perform a statistical evaluation of your three models similar to the previous section. That is, compare the three models pairwise.]

[TODO: TABLE: Include p-values and confidence intervals for the three pairwise tests in your report.]

[TODO: Conclude on the results from the values in the table and reference the table.]

2.3 Interpretation of the LR model

[TODO: Train a logistic regression model using a suitable value of λ (see previous exercise). Explain how the logistic regression model make a prediction. Are the same features deemed relevant as for the regression part of the report?]

Use of GenAI

...

References

- [1] Tue Herlau, Mikkel N. Schmidt, and Morten Mørup. *Introduction to Machine Learning and Data Mining*. Technical University of Denmark (DTU), Lyngby, Denmark, 2023. Lecture notes, Fall 2023, version 1.0. This document may not be redistributed. All rights belong to the authors and DTU.
- [2] B. German. Glass Identification. UCI Machine Learning Repository, 1987. DOI: <https://doi.org/10.24432/C5WW2P>.

Appendix

A Repository and supplementary materials

The full notebook, scripts, and generated figures for this project are available in the project repository:

https://github.com/schependom/DTU_machine-learning-projects/tree/main

This repository contains the data-loading and analysis code that produced the tables and figures cited above (see the `figures/` folder for the PDF outputs referenced in the report).