02450 Project 2

Report

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Technical University of Denmark Department of Applied Mathematics and Computer Science Introduction to Machine Learning and Data Mining Tue Herlau 3rd November 2014

Abstract

The objective of this second report is to apply the methods you have learned in the second section of the course on "Supervised learning: Classification and regression" in order to solve both a relevant classification and regression problem for your data.

Regression

1.1 Problem

Let D denote our data set that contains N observations:

$$D = \{(\mathbf{x}_i, y_i) | i = 1, 2, \dots, N\}$$

Each \mathbf{x}_i corresponds to the set of attributes of the *i*-th observation and y_i , corresponds to the target variable.

Regression is the task of learning a target function f that maps each attribute set \mathbf{x} into a continuous-valued output y. In particular, according to our dataset, the continuous-valued output corresponds to the letter index. Thus, the goal for our regression problem, is to find a target function, which describe the letter index, that can fit the input data with minimum error. The error function for a regression task will be expressed in terms of squared error.

The idea is to set an index for each letter (for example A=0, B=1..., Z=25) and then apply linear regression. If we apply linear regression for the whole data set (consider all the letters, equal to 26 classes) that will never work, linear regression is simply not sufficiently flexible, for instance, to understand that the differences in pixel intensities in a,b,c should result in y=1,2,3. Suppose x_a corresponds to the input of a and x_c the input of c. Then suppose you have trained the weights w such that:

$$1 = x_a * w$$

$$3 = x_c * w$$

it now follows that $2 = \frac{(x_a + x_a)}{2} * w$

That said, we are going to solve two different linear regression problem:

1. Considering a subset of our data corresponding to two letters. Then we have a proper two-class problem

2. Applying 1 out of K coding where K=26. We consider the one-against-rest scheme, where multiple classes are handled by decomposing the problem into K binary problems, where K is the number of classes. We train K classifiers, each fitted to classify one class against the rest of the classes lumped together.

1.2 TWO-CLASS LINEAR REGRESSION

Forward selection

We apply linear regression with forward selection considering a subset of data of two classes, where class 0 corresponds to the letter A while class 1 corresponds to the letter C. Since our output are purely binary $(y \in 0,1)$, we use logit function which maps the output in the regression analysis to the range (0,1). To measure how well we can predict the two letters, we will use the squared error between the true and the estimated error. In our estimation we use two level of cross-validation. On the outer level, we use 5-fold cross-validation to estimate the performance of our model computing the squared error averaged over 5 test sets. On the inner level, we use 10-fold cross-validation to perform sequential feature selection. Figure 1.1 shows that the most commonly selected features for letter recognition are width, x-bar, x2bar, y2bar, xy2br, xegvy, yegvx.

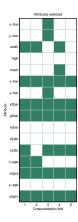
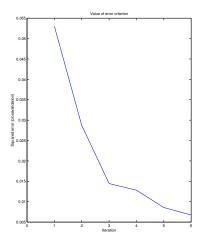


Figure 1.1: Linear regression with forward selection, attributes selected for all folds

The fold which requires the less number of feature for the linear regression is fold number 5. Figure 1.2 shows feature selection and crossvalidation error for the fold 5. We can see that the minimum squared error is reached with only six attributes.



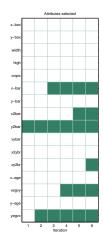


Figure 1.2: Feature selection and crossvalidation error for fold 5

We also find that in almost all cases there is no significant performance improvement (R^2 test score) between selecting all the features and the features suggested by the feature selection:

Linear regression without feature selection:

- Training error: 0.00 - Test error: 0.01 - R^2 train: 0.99 - R^2 test: 0.95

Linear regression with sequential feature selection:

- Training error: 0.00 - Test error: 0.01 - R^2 train: 0.98 - R^2 test: 0.96

However the feature selection allows to have a much simpler model with almost the same error performance.

Plotting the residual error vs. the attributes can give some insight into whether including a transformation of a variable can improve the model. If the points in a residual plot are randomly dispersed around the horizontal axis, a linear regression model is appropriate for the data; otherwise, a non-linear model is more appropriate. Looking the residual plot in figure 1.3, it shows a random pattern which indicates a good fit for a linear model. In fact, if we include transformation of some variable (for example the square of an attribute) we checked that there is no significant performance improvement.

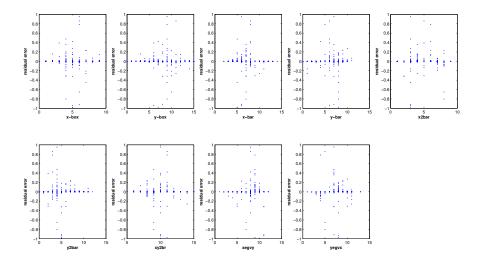


Figure 1.3: Residual error vs. the attributes

Attributes effects

Another approach to control for the complexity of the model is to regularize the parameters in the objective function. In linear regression we can regularize the parameter \mathbf{w} by the Frobenius norm. We run linear regression with regularization for the letter index attribute, with external 5-fold cross-validation and internal 10 fold cross-validation for estimating the optimal lambda value. Figure 1.4 shows that the optimal lambda = 10^{-2} , and how the attribute weights change due to regularization.

We calculate the average set of weights and we plot a bar chart to understand the contributions of the different attributes for the letter value (Figure 1.5). We see again that in order x-bar, y2bar, xegvy, yegvx are the most significant predictors.

The squared errors scores however show no significant improvement between the non regularized and the regularized models.

Artificial neural network

We fit an artificial neural network (ANN) to the data. We perform a 5 fold cross-validation to select the number of hidden units hyper-parameter. For each fold, we try to fit an ANN 5 times, and we select the ANN which produces the lowest train error. Just using only one hidden units and one train of neural network we obtain very interesting results, indeed, in this case, the train error and test error are approximately equal to 0% and 1% respectively. Increasing the number of re-train the errors remain pretty the same while increasing the number of hidden nodes (for instance equal to six), the train error and

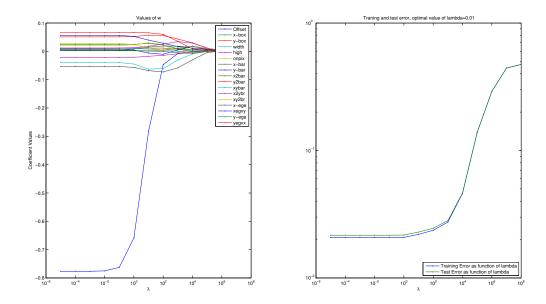


Figure 1.4: Linear regression with regularization, attribute weights and optimal λ

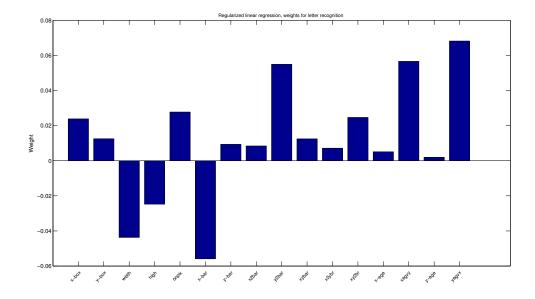


Figure 1.5: Linear regression with regularization, attribute weights

test error decrease and they are approximately equal to 0% and 0% (0.16%) respectively.

Figure 1.6 describe an ANN with 16 inputs(attributes) and one hidden layer that we have chosen as model to fit our data.

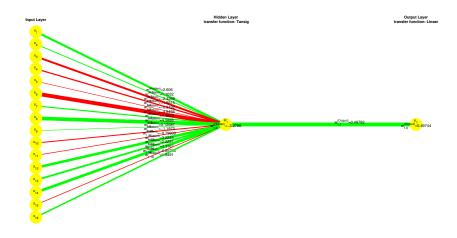


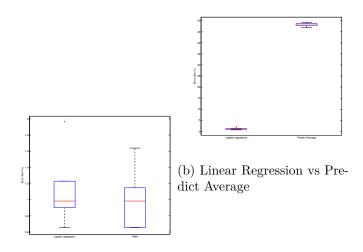
Figure 1.6: ANN with one hidden unit

Comparison

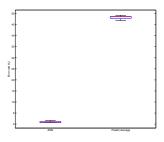
We perform a pairwise t-test between the regularized linear regression model, the ANN with one hidden node, and a baseline model predicting the average of the output variable (letter A or C). In order to compare the models we consider the error rate average of the five folds.

-	Error	rate	linear	regression	0.9%
-	Error	rate	ANN		1.1%
-	Error	rate	predict	average	48.3%

If we compare Linear regression vs ANN we note that the classifiers are NOT significantly different while if we compare linear regression vs predict average and ANN vs predict average it easy understand that the classifiers are significantly different. We can see the results also in Figure 1.7.



(a) Linear Regression vs ${\rm ANN}$



(c) ANN vs Predict Average

Figure 1.7: Box-Plots: Permormace of the models one against the other

1.3 MULTI-CLASS LOGISTIC REGRESSION

We run multi-class classification data set which fits logistic regression models to the training data using the one-against-rest strategy (each classifier trained to predict one class label vs. the remaining). Next, it computes the outputs of the C classifiers on the test data and classifies it according to the highest output. Our goal is classify, using multi-class regression model, all the letter indexes.

We use $\frac{2}{3}$ of the data set as training set and the remainder data for the test set and we obtain an error rate equals to 28%. Always considering the one-against-rest scheme, we fit 26 (number of outputs) neural networks with 2 hidden units. We use $\frac{2}{3}$ of the data set as training set and the remainder data for the test set and we obtain an error rate equals to 25%. Instead, considering a predict average model for all the 26 letters we obtain an error rate equals to 98%. Comparing these results we can say, even in multi-class classification, that the performance of multi-class regression vs multi-class ANN are not significantly different while if we consider predict average model vs regression or ANN obviously the performance are significantly different. This happens because predict average model is very inefficient when the number of classes is high.

Classification

2.4 Problem

The classification problem for our data we have chosen to solve is predicting a letter from the english alphabet (26 classes) using its attributes. Each record (letter) has 16 integer attributes in a range of 0 to 15.

2.5 Methods and parameters

We solved this problem using KNN, ANN and Naive Bayes methods. For every method we implemented two levels of cross-validation for estimating optimal parameters. For KNN it was a value of K, in ANN a number of nodes in the hidden layer, and i Naive Bayes method we estimated a number of features (best) used.

K-Nearest Neighbors

KNN algorithm predictions are very accurate for various values of K, but it appears that lower values are better. The lowest error rate is for k=1 despite of having no duplicates in our dataset. See figure 2.8

Naural Network

For an artifitial neural network method we use a perceptron with one hidden layer which uses softmax function on the output layer. We are optimizing number of nodes in a hidden layer. The lowest error rate occured with a hidden nodes count of approximetly 1.5 times a number of attributes, so about 26. This optimal number varies as the training subset changes in cross-validation, but still is close to that number. In the figure 2.9 we can see an average of error rates for various hidden neurons count.

Naive Bayes

For Naive Bayes method we tried to estimate optimal features set (number of features), however no matter of what classifier we used for feature selection

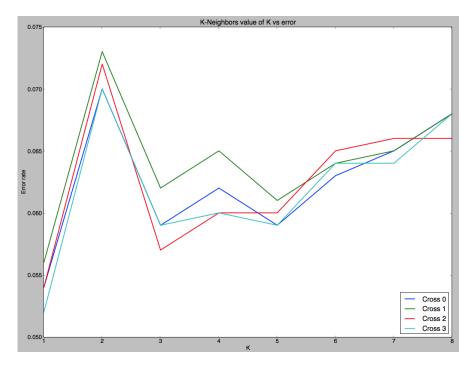


Figure 2.8: K-Nearest Neighbors - K vs error

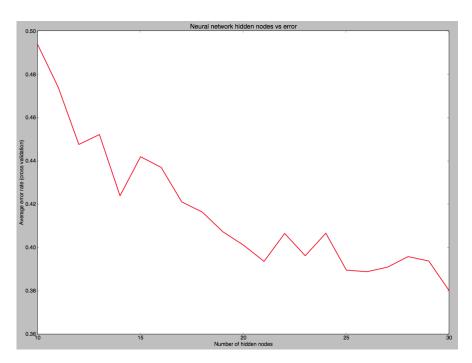


Figure 2.9: Neural Network - hidden nodes vs error

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using recursive feature elimination with cross-validation, the best accuracy was obtained with selecting all features. In a plot (figure 2.10) we can see how accuracy of the method depends on number of features.

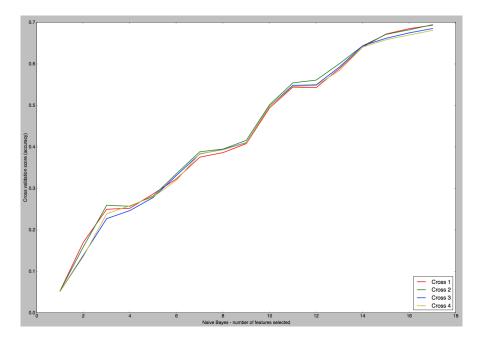


Figure 2.10: Naive Bayes - features vs accuracy

2.6 Results

For all methods, the error rate of predicting a letter basing of its attributes is below 50%, what is quite a good result for such a problem. The best results we got using K-Nearest Neighbors algorithm which with euclidesian mertic obtained less than 5% of bad answers (figure 2.11). Out error rate is calculated as:

error_rate = (predicted_letters != actual_letters) / number_of_tests

In the figure 2.12 we can see a plot describing how good letters are predicted by KNN method. From 5000 points used only a few are away from x = y line. Most of the points are on that line, which means that letters are predicted correctly.

Moreover, fitting our methods for all of the data (20000 records) we obtained on average 4% of an error rate for KNN and 35%, 44% for Neural Network and Naive Bayes accordingly. We used K-fold cross-validation using all that data which forced us to use parallelism computing every fold in a separate thread.

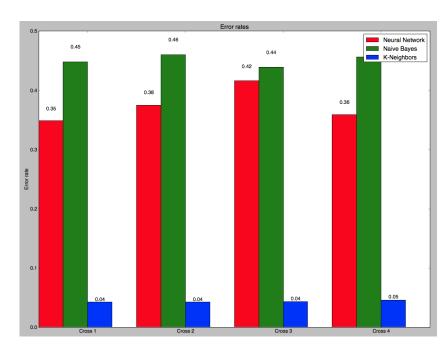


Figure 2.11: Performance of methods in outer cross-validation loop

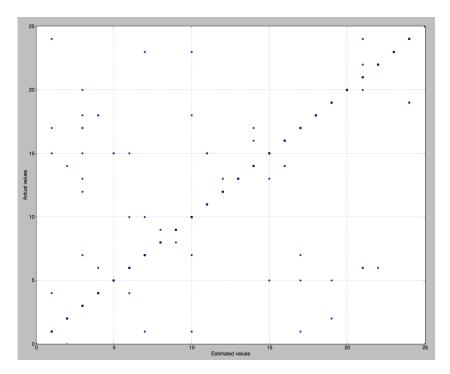


Figure 2.12: Predicted values vs actual values (KNN)

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2.7 Comparison

The boxplot below (figure 2.13) shows that there are great differences between a performance of used methods. We used also a paired t-test to compare

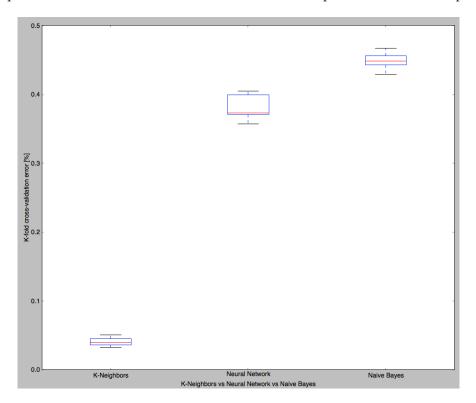


Figure 2.13: Cross-validation errors for all methods

selected methods with each other and additionally with a fake predictor, which classifies all outputs to be the largest class in the training data:

<u>*</u>	0		0
Compared alg.	t-test value	p-value	significantly
ANN vs Naive Bayes	-10.3	0.0	True
ANN vs KNN	57.8	0.0	True
Naive Bayes vs KNN	100.5	0.0	True
Biggest Class vs ANN	-100.4	0.0	True
Biggest Class vs KNN	-380.7	0.0	True
Biggest Class vs Naive Bayes	-133.3	0.0	True

The results shows us that all of the methods are significantly different in case of performance.

Related work 2.8

This dataset was used for letter recognition (classification) using Holland-style Adaptive Classifiers. The article is available on the following link:

http://download.springer.com/static/pdf/733/art%253A10.1007%252FBF00114162.pdf?auth66=1414859976_6267eff4e2e0779ac8c3bd5c7c57b61c&ext=.pdf The percentage of correct identifications they achieved varies between 50% to 80% depending on the settings, where the highest score is obtained with the most computationally demanding settings. Referring to that article we can assume that our results are successful.

Conclusions

Summing up our work, we observed that K-Nearest Neighbors algorithm is the best method for letter classification on our dataset. Neural networks also gained good results, however they could be made more precise applying deep neural networks with doing computations on GPU. Some of our methods were a way better than these presented by previous researchers.