Getting More Out of Small Data Sets
Improving the Calibration Performance of Isotonic Regression by Generating More Data

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Keywords: Classification, Calibration.

Abstract: Often it is necessary to have an accurate estimate of the probability that a classifier prediction is indeed correct. Many classifiers output a prediction score that can be used as an estimate of that probability but for many classifiers these prediction scores are not well calibrated. If enough training data is available, it is possible to post process these scores by learning a mapping from the prediction scores to probabilities. One of the most used calibration algorithms is isotonic regression. This kind of calibration, however, requires a decent amount of training data to not overfit. But many real world data sets do not have excess amount of data that can be set aside for calibration. In this work, we have developed a data generation algorithm to produce more data from a limited sized training data set. We used two variations of this algorithm to generate the calibration data set for isotonic regression calibration and compared the results to the traditional approach of setting aside part of the training data for calibration. Our experimental results suggest that this can be a viable option for smaller data sets if good calibration is essential.

1 INTRODUCTION

In many predictive modeling applications, it is useful to not just provide a prediction but to also have an accurate estimate of the reliability of that prediction. This is especially true if classifier output is used as an input in another classifier or the decision is cost sensitive. For example, the reliability of individual samples in a spam filter application might be irrelevant as long as the overall classification rate remains high. A completely different case can be made for a machine learning system assisting a doctor in diagnosis. In this case, it is very important to have an accurate estimate of the reliability for the system outputs.

In the case of classification algorithms the reliability is measured by the posterior probability estimate, often called the prediction score. In other words, this is an estimate of the probability that the predicted example really belongs to the predicted class. However, classification algorithms' prediction scores do not generally estimate posterior probabilities very accurately and distribution of this error varies between data sets. Thus, calibration algorithms for the prediction scores of a classifier have been developed for this purpose. Several calibration algorithms have been used in the literature but they tend to require a somewhat large training data set to work well and they do not always produce good calibration.

Naïve Bayes is one commonly used learning algorithm because of several advantages it has. It is fast to train and to predict with and therefore not a lot of computing power is needed to run the algorithm (Kuhn and Johnson, 2013). The models produced by Naïve Bayes are easy to interpret (Kononenko, 1990) compared to many other commonly used learning algorithms such as Support Vector Machines or artificial neural networks. It can also handle missing values, which are common in many real world data sets, by simply ignoring them. The prediction performance is also usually surprisingly good (Domingos and Pazzani, 1997) given that the attribute independence assumption rarely holds. However, its prediction scores are not well calibrated (Domingos and Pazzani, 1997). Therefore we find Naïve Bayes to be a good candidate to demonstrate our calibration algorithm.

Calibration algorithms need training data to tune them. To avoid bias, a part of the overall training data set is set aside for calibration only while the rest is used for training the classification model. A large training set, which is obviously needed with this approach, is not always available, especially in

Alasalmi, T., Koskimäki, H., Suutala, J. and Röning, J.
Getting More Out of Small Data Sets - Improving the Calibration Performance of Isotonic Regression by Generating More Data.
DOI: 10.5220/0006576003790386
In *Proceedings of the 10th International Conference on Agents and Artificial Intelligence (ICAART 2018) - Volume 2*, pages 379-386
ISBN: 978-989-758-275-2

real world applications where the cost of collecting more data can be high, making it essential to develop algorithms for calibration that also work on smaller data sets. In this article we will present two novel approaches for generating more data to be used for calibrating the raw prediction scores of Naïve Bayes classifier on binary classification problems. These approaches work well also with smaller data sets.

This article is structured as follows. In Section 2 we will shortly review the literature on isotonic regression calibration and in Section 3 we will introduce the metrics that are used to evaluate calibration performance. Section 4 will present the calibration data generation algorithm that we have developed. In Section 5 we will explain our experimental setup and present the results of those experiments, and finally in Section 6 we will discuss the results and draw conclusions in Section 7.

2 ISOTONIC REGRESSION

As stated above, prediction scores of Naïve Bayes classifier are not well calibrated. Isotonic, i.e. monotically increasing, regression is one of the most commonly used algorithms for classifier calibration (Zhong and Kwok, 2013). Its use as a calibration algorithm is based on the assumption that the classifier ranks the examples correctly (Zadrozny and Elkan, 2002) so care needs to be taken to make sure this assumption is not violated. In practice this means that a higher prediction score translates into a higher probability of the prediction being correct. If this is indeed the case, as it often is in the case of Naïve Bayes (Zhang and Su, 2008), isotonic regression can be used to map the prediction scores into probabilities therefore improving the calibration. As isotonic regression is a non-parametric algorithm, the exact shape of the mapping does not need to be known, which is obviously an advantage compared to parametric algorithms.

Isotonic regression has been shown to perform well in many calibration tasks (Caruana et al., 2008; Niculescu-Mizil and Caruana, 2005; Zadrozny and Elkan, 2002). However, with small data sets, it might overfit. Also, using the same data for both training the prediction model and for calibrating the model can bias the calibration (Niculescu-Mizil and Caruana, 2005) which further increases the need for more data in the training set as the same data cannot be used for both purposes. If at least 1000 samples are available for calibration, isotonic regression calibration tends to work very well (Caruana et al., 2008).

Isotonic regression algorithms produces a piecewise constant function and can contain jumps. There are several techniques that can be used to smoothen these discontinuities (Zhong and Kwok, 2013). However, the problem of small training data sets remains with all these algorithms.

In this article, we will propose an algorithm for generating more calibration data when the data set is small to alleviate this problem.

3 EVALUATION METRICS

Classification model calibration can be visually evaluated with calibration plots or more objectively with some error metrics. We will introduce two commonly used error metrics below and these metrics will then be used to compare calibration performance of different calibration algorithms in our experiments.

Logarithmic loss (logloss) is an error metric that penalizes for being confident about a prediction while being wrong. Therefore it is a good metric for calibration performance. Logarithmic loss is defined in Equation (1) where N is the number of observations, M is the number of class labels, log is the natural logarithm, $y_{i,j}$ is 1 if observation i belongs to class j and 0 otherwise, and $p_{i,j}$ is the predicted probability that observation i belongs to class j. The prediction model being constant, logarithmic loss will decrease with better calibration.

Another error metric used to evaluate calibration performance is the mean squared error (MSE). MSE will also decrease with better calibration but is not as harsh for single confident but wrong decisions made by the classifier. It is defined in Equation (2) where N is the number of observations, y_i is 1 if observation i belongs to the positive class and 0 otherwise and p_i is the predicted probability that observation i belongs to the positive class.

$$logloss = -\frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{M} y_{i,j}log(p_{i,j}) \quad (1)$$

$$MSE = \frac{\sum_{i=1}^{N}(y_i - p_i)^2}{N} \quad (2)$$

Calibration plot is often used to get a quick glance at the calibration performance visually. In calibration plots, test data set predictions are grouped into bins according to their prediction scores. For each bin, the fraction of samples belonging to the positive class is determined. The fraction of positives is then plotted against the bin center values. If the bin center values and fraction of positives in the corresponding bins are close for each bin, the prediction scores are well calibrated. An example calibration plot can be seen in

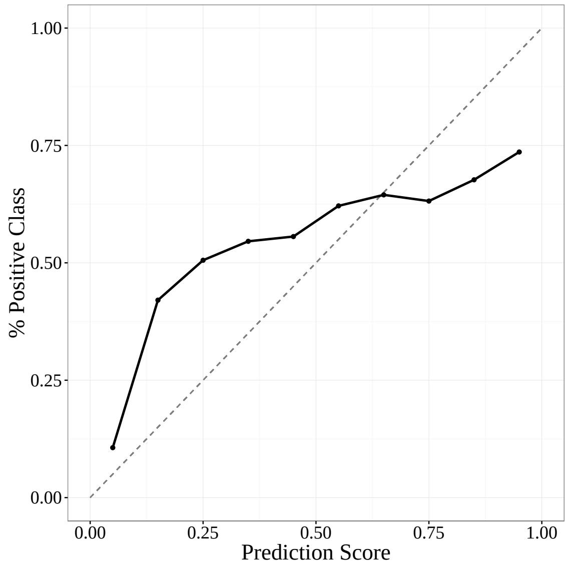


Figure 1: Calibration plot of the Adult data set classified with Naïve Bayes classifier. The dashed line represents perfect calibration.

Figure 1. The amount of data affects calibration plots as the amount of data in each bin needs to be sufficient to be a representative sample of the general calibration performance in that prediction score range. Interpretation of the calibration plot is obviously subjective and does not take into account the distribution of the prediction scores. It can, however, give valuable additional information to the modeler when used together with error metrics such as MSE and logloss.

4 GENERATING CALIBRATION DATA

Traditionally, calibration algorithms use a fraction of the training data set, separate from the data used to train the classifier, to tune the calibration model to avoid bias. Often, however, the amount of data available is limited. In addition, Naïve Bayes classifier tends to push uncalibrated prediction scores towards the extremes, leaving very little data to be used to tune the calibration model especially in the middle of the prediction score range.

If we knew the true probability distribution of our data, we could construct a perfect Bayesian model for classification and no calibration would be needed. As this is not possible in practice, we obviously cannot use the probability distribution to draw the calibration data from that, either. To get an estimate of the data distribution we can fit a classification model to the training data and use that model to generate more data that is used for calibration. As was stated above, the same data cannot, however, be used for training the model and for calibration to avoid bias. Therefore, in our approach, the calibration data is generated with cross-validation within the training data set. Hence we are not limited to a fraction of the training data and we can use the whole training data to train the prediction model which is obviously valuable. Of course, we cannot generate data out of nowhere but we argue that with our approach we can make better use of the existing information in our training data.

4.1 Traditional Approach

For the traditional isotonic regression, 10 % of the training data was split off to be used as the calibration data set and the rest was used to train the prediction model. A completely separate test data set was used to test the calibration performance.

4.2 Our Approach

In designing our calibration algorithm, two goals were in mind. First, the effect of training data set size on the calibration performance was to be reduced, and second, calibration performance was to be improved over traditional isotonic regression.

To achieve these goals, cross validation was used to generate the calibration data set. This generated data set was made available to the actual calibration algorithm, isotonic regression in this case. Similar approach to generate data was used by Alasalmi et al. (Alasalmi et al., 2016) for classification confidence estimation. Here we will use the same idea in the case of calibration. The procedure is shortly described below.

To generate the calibration data set, the training data was processed in a cross validation manner. 70 % of the training data was used to train a Naïve Bayes classifier and the rest of the training data set was then predicted with the model. Prediction scores as well as the true classes of those data points were added to the calibration data set. This procedure was then repeated with a different split of the data until at least the desired number of data, 5 000 samples in this case, was generated for the calibration data set. About 1 000 samples in the calibration data set has been suggested as the minimum for isotonic regression (Caruana et al., 2008; Niculescu-Mizil and Caruana, 2005). However, there seems to be improvement in isotonic regression calibration performance with more data (Niculescu-Mizil and Caruana, 2005). Therefore we chose to use 5 000 sample target in our calibration data generation.

Figure 2 summarizes the proposed algorithm for generating data for calibration. This generated data set was then used to train an isotonic regression model that was used for calibrating the prediction scores of previously unseen data. We call this the Data Generation (DG) calibration model. We also wanted to test if grouping together calibration data points with similar prediction scores before feeding them into isotonic regression would further increase the calibration performance. For this purpose, the 5 000 generated calibration data points were aggregated into groups of 100 data points and these aggregated data samples were instead fed to the calibration algorithm. We call this model the Data Generation and Grouping (DGG) calibration model. In essence, each aggregated sample represents an average calibration score and an associated fraction of positive samples in the aggregate. The amount of data points to aggregate into a sample is a compromise between the resolution of prediction scores and the resolution of the fraction of positives in the sample.

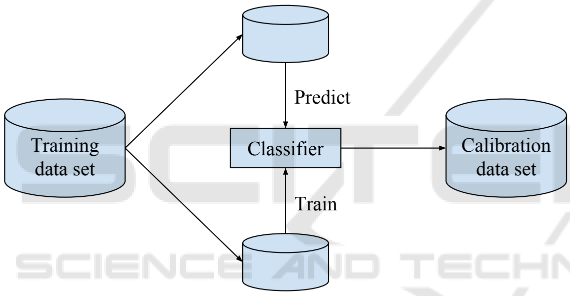


Figure 2: Calibration data set generation. Cross validation was repeated until the calibration data set size reached 5 000 samples.

5 EXPERIMENTS

To test the algorithm we developed, an experiment was set up as follows. Each data set was split into training and test data sets. 30 % of the samples were used as the test data while the rest served as the training data. Using the training data set only, a Naïve Bayes classifier was trained and four different calibration schemes were run using the training data set: control (no calibration, raw prediction scores), traditional isotonic regression calibration, and our two developed algorithms (DG and DGG). For the traditional isotonic regression, 10 % of the training data was put aside for calibration and the rest was used to train the prediction model. For our developed algorithms, cross validation was used to create the separate calibration dataset, as described in Section 4, and the whole training data set was used to train the prediction model. Next, the test data set samples were predicted and the prediction scores were calibrated using the algorithms tuned in the previous step. Threshold value used as prediction boundary was tuned with the calibrated training data to maximize classification rate. This was done separately for each calibration scheme. Using the threshold from the previous step as the cut off prediction score, the following metrics for classification and calibration performance were calculated for each calibration scheme: classification rate, logarithmic loss (logloss), and mean squared error (MSE). For each data set, this procedure was repeated 10 times with a different split into training and test data sets and the average performance is reported in the results to reduce the amount of chance in the results.

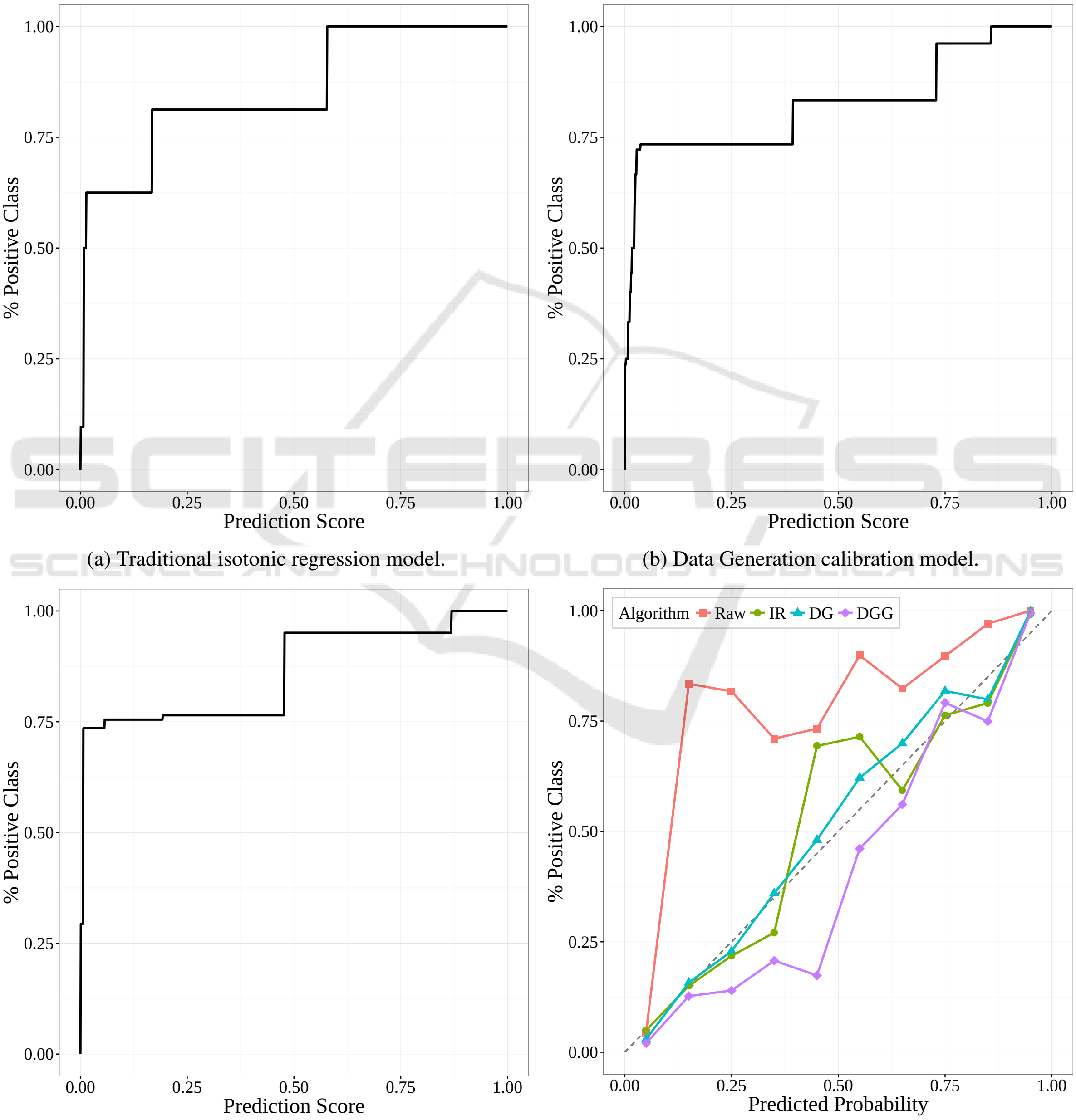
The experiments were run with the data sets whose properties are presented in Table 1. All of the problems were already or were converted into binary classification problems as described below. The prediction task with QSAR biodegradation data set (Mansouri et al., 2013) (Biodegradation) is to classify chemicals into ready or not ready biodegradable categories based on molecular descriptors. In Blood Transfusion Service Center data set (Yeh et al., 2009) (Blood donation), the task is to predict whether previous blood donors donated blood again in March 2007. Contraceptive Method Choice data set (Contraceptive) is a subset of the 1987 National Indonesia Contraceptive Prevalence Survey. The prediction task is to predict the current contraceptive method choice. A combination of classes short-term and long-term were used as the positive class while the no-use class served as the negative class. Letter Recognition data set (Letter) is a database for letter identification based on predetermined image features. We used a variation of the data set by reducing it down into two similar letters. The letter Q served as the positive class and the letter O as the negative class. The Mushroom data set contains descriptions of physical characteristics of mushrooms and the prediction task is to determine if the mushrooms are edible or poisonous. All data sets are freely available from the UCI machine learning repository (Lichman, 2013).

Comparison of traditional isotonic regression, Data Generation calibration, and Data Generation and Grouping calibration algorithms on the Mushroom data set is shown in Figure 3. Figures 3a-3c show the traditional isotonic regression, Data Generation, and Data Generation and Grouping calibration models, respectively. Also, a calibration plot with the four calibration algorithms is shown in Figure 3d.

Classification rates (CR), loglosses, and MSEs for each calibration scheme are presented in Tables 2-6.

Table 1: Data set properties.

Data set	Samples	Features	Positive class	Calibration samples
Biodegradation	1055	41	34 %	73
Blood donation	748	4	24 %	52
Contraceptive	1473	9	57 %	103
Letter	1536	16	51 %	107
Mushroom	8124	20	52 %	568



(a) Traditional isotonic regression model.

(b) Data Generation calibration model.

(c) Data Generation and Grouping calibration model.

(d) Calibration plot of all calibration schemes.

Figure 3: Calibration models and calibration plot for the Mushroom data set.

The results are reported as average values of 10 simulations. For logloss and MSE, the lowest values, i.e. the best calibration result according to that metric, are in boldface. Statistical significance of the difference in the mean values was calculated using a Welch t-test (Welch, 1947) and the significant differences are indicated in the Tables.

Table 2: Performance metrics on the Biodegradation data set. * Significantly lower than Raw, $p < 0.05$. ** Significantly lower than Raw, $p < 0.01$. † Significantly lower than IR, $p < 0.05$. ‡ Significantly lower than IR, $p < 0.01$.

Algorithm	CR	Logloss	MSE
Raw	84.6 %	13.77	0.570
IR	83.2 %	4.81 **	0.278 **
DG	84.5 %	3.42 **	0.268 **
DGG	84.7 %	**0.93** **‡	**0.246** **†

Table 3: Performance metrics on the Blood donation data set. * Significantly lower than Raw, $p < 0.05$. ** Significantly lower than Raw, $p < 0.01$. † Significantly lower than IR, $p < 0.05$. ‡ Significantly lower than IR, $p < 0.01$.

Algorithm	CR	Logloss	MSE
Raw	75.8 %	1.49†	0.381
IR	75.4 %	4.17	0.393
DG	75.6 %	1.21**‡	**0.342***‡
DGG	75.9 %	**1.04****‡	0.343*‡

Table 4: Performance metrics on the Contraceptive data set. * Significantly lower than Raw, $p < 0.05$. ** Significantly lower than Raw, $p < 0.01$. † Significantly lower than IR, $p < 0.05$. ‡ Significantly lower than IR, $p < 0.01$.

Algorithm	CR	Logloss	MSE
Raw	63.5 %	1.85†	0.515
IR	63.8 %	2.45	0.469**
DG	63.4 %	**1.28****‡	**0.450****‡
DGG	62.9 %	**1.28****‡	**0.450****‡

6 DISCUSSION

The calibration models for the different calibration schemes in Figures 3a-3c do not differ dramatically. The traditional isotonic regression model is more coarse because of the low amount of data available. However, as a significant portion of the prediction scores tend to be near zero and one with Naïve Bayes classifier, the differences in the calibration models near zero and one can become significant, especially when logloss is used as the error metric, as we will see later.

Table 5: Performance metrics on the Letter data set. * Significantly lower than Raw, $p < 0.05$. ** Significantly lower than Raw, $p < 0.01$. † Significantly lower than IR, $p < 0.05$. ‡ Significantly lower than IR, $p < 0.01$.

Algorithm	CR	Logloss	MSE
Raw	83.3 %	1.16	0.295
IR	82.3 %	1.68	0.239**
DG	83.2 %	**0.72****‡	**0.222****
DGG	83.0 %	**0.72****‡	0.223**

Table 6: Performance metrics on the Mushroom data set. * Significantly lower than Raw, $p < 0.05$. ** Significantly lower than Raw, $p < 0.01$. † Significantly lower than IR, $p < 0.05$. ‡ Significantly lower than IR, $p < 0.01$.

Algorithm	CR	Logloss	MSE
Raw	97.4 %	0.359	0.081
IR	97.2 %	0.376	0.046 **
DG	97.4 %	**0.192** **‡	**0.043** **
DGG	97.1 %	0.223 **‡	0.044 **

Visually inspected (Figure 3d), calibration of raw Naïve Bayes prediction scores with the Mushroom data set is not very good. However, all of the compared calibration algorithms were able improve the calibration with this data set based on the calibration plot. Based on the plot, DG calibration seems to perform best, i.e. it runs overall closest to the center line meaning that the predicted probability and the true fraction of positives are well correlated.

More objective measures for calibration performance are logloss and MSE. With only one of the data sets, traditional isotonic regression was able to improve the calibration of Naïve Bayes when using the logarithmic loss as the measure of calibration performance. On the other four data sets, however, logloss actually increased compared to the uncalibrated control although in two cases the difference was not statistically significant. This is not very surprising because the calibration data sets were very small and isotonic regression needs a decent amount of data to work properly in calibration without overfitting. On the other hand, by generating more data to be used for calibration, as suggested in this article, the logloss was lower with every tested data set than with raw prediction scores or prediction scores calibrated with traditional isotonic regression, sometimes drastically. The differences were statistically significant in every case when compared to uncalibrated control. When compared to isotonic regression, the differences were statistically significant with the exception of DG model on the Biodegradation data set.

When using the mean squared error metric for calibration success, it seems that isotonic regression may be able to improve the calibration over raw prediction scores in most cases. More specifically, MSE for isotonic regression was statistically significantly lower than than uncalibrated control with the exception of the Blood donation data set. By generating more calibration data we were able to decrease MSE with every tested data set and the differences were statistically significant in all cases for both DG and DGG model when compared to uncalibrated control. MSE with both DG and DGG were statistically significantly lower than with isotonic regression on Blood donation and Contraceptive data sets as well as for DGG on the Biodegradation data set.

Data sets with prediction scores that are very much pushed towards one and zero suffer from an unexpected problem regarding calibration. As the algorithm that is used to produce the isotonic regression function cannot handle several data points with the same prediction score, much of the calibration data can be lost and wrong conclusions can be made, especially on the smaller data sets. This can lead to mistakes in calibration particularly near one and zero where logloss will penalize errors hard. MSE, however, is not as much affected by the errors made in the extreme ends. The Biodegradation data set is one example of such problem. Histogram of the raw prediction scores with this data set is depicted in Figure 4. Our Data Generation and Grouping model tries to address this issue by aggregating calibration data into larger samples and averaging them. DGG performs best of all of the algorithms with the problematic Biodegradation data set and on par with DG on three other data sets. On the Mushroom data set DG works better than DGG, although the difference in logloss is not statistically significant. However, DGG can still beat uncalibrated prediction scores and traditional isotonic regression calibration by a clear margin. This result is somewhat surprising as we were using groups of 100 data points resulting in only 50 samples in the calibration data set which is actually smaller calibration data set than in any of the tested data sets. These samples better represent the true nature of the data set than the same amount of individual data points can.

It is impossible, of course, to correct for shortcomings of the data set itself just by sampling but we argue that our approach makes it possible to make better use of the data that is available. This is apparent from the error metrics. Clearly, using a very small data set for calibration can not be advised based on our results, as has been suggested in the literature, too. But generating more calibration data with either DG or DGG model can lower error metric figures indicating the calibration function is less biased towards the calibration data set making it better generalized for unseen data.

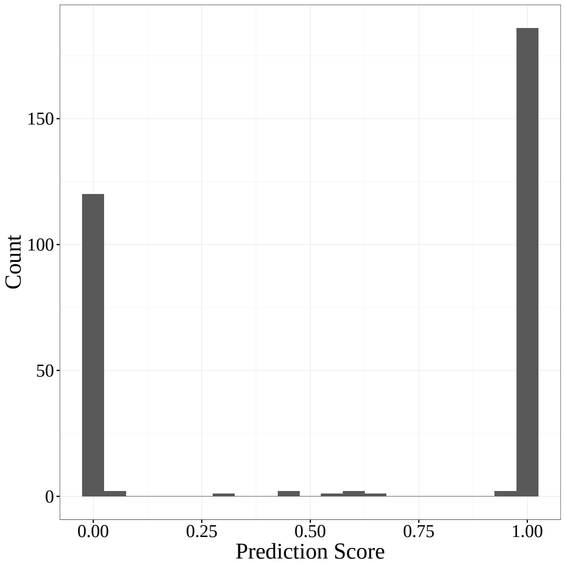


Figure 4: Histogram of the raw prediction scores in an extreme example, the Biodegradation data set.

The different calibration schemes do not have any significant effect on classification rate. This is expected as ranking of the predictions is not affected by calibration if the original ranking was somewhat close to being correct.

Classification rate is inversely associated with both logloss and MSE. This is because a correct classification will always lead to a smaller error than an incorrect one, however uncertain it was to begin with. The small differences in classification rate between calibration conditions cannot, however, explain the lower error metrics achieved with the calibration schemes. The differences are, therefore, explained by the performance differences between the tested calibration algorithms.

7 CONCLUSIONS

Small data sets are problematic for isotonic regression calibration and applying it might actually worsen the calibration of unseen data. Making better use of the information in the data by generating more calibration data can alleviate the problem. With the approach suggested in this article, we were able to improve calibration of Naïve Bayes over uncalibrated and traditional isotonic regression with every tested data set. In some cases, grouping the generated calibration data into small samples can lead to even better calibration than just using the generated data intact. Generating the calibration data is obviously computationally more complex than just splitting the training data set in two. The actual computational cost will depend on the classification model used. However, the calibration data generation only needs to be done once in the training phase and obtaining the calibrated prediction score for new data is very fast.

If the amount of training data available is limited and a good calibration of the used classifier is important, using the suggested approach for calibration can be a viable option.

ACKNOWLEDGEMENTS

The authors would like to thank Infotech Oulu, Jenny and Antti Wihuri Foundation, and Tauno Tönning Foundation for financial support of this work.

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