Calibration Techniques for Binary Classification Problems: A Comparative Analysis

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Abstract: Calibrating a classification system consists in transforming the output scores, which somehow state the confidence of the classifier regarding the predicted output, into proper probability estimates. Having a well-calibrated classifier has a non-negligible impact on many real-world applications, for example decision making systems synthesis for anomaly detection/fault prediction. In such industrial scenarios, risk assessment is certainly related to costs which must be covered. In this paper we review three state-of-the-art calibration techniques (Platt's Scaling, Isotonic Regression and SplineCalib) and we propose three lightweight procedures based on a plain fitting of the reliability diagram. Computational results show that the three proposed techniques have comparable performances with respect to the three state-of-the-art approaches.

1 INTRODUCTION

Classification is one of the most important problems falling under the machine learning and, specifically, under the supervised learning umbrella. Generally speaking, it is possible to sketch three main families: clustering, regression/function approximation, classification. These problems mainly differ on the nature of the process to be modelled by the learning system (Martino et al., 2018a).

More into details, let $\mathcal{P} : \mathcal{X} \to \mathcal{Y}$ be an orientated process from the input space $\mathcal{X}$ (domain) towards the output space $\mathcal{Y}$ (codomain) and let $\langle x, y \rangle$ be a generic input-output pair drawn from $\mathcal{P}$, that is $y = \mathcal{P}(x)$.

In *supervised learning* a finite set $\mathcal{S} = \langle X, Y \rangle$ of input-output pairs is supposed to be known and common supervised learning tasks can be divided in *classification* and *function approximation*. In the former case, the output space $\mathcal{Y}$ is a non-normed space and output values usually belong to a finite categorical set of possible values. Conversely, in the latter case, the output space is a normed space (usually $\mathbb{R}$). In *unsupervised learning* there are no output values and regularities have to be discovered using only information from $\mathcal{X}$. The seminal example is data clustering, where aim of the learning system is to return groups (clusters) of data in such a way that patterns belonging to the same cluster are more similar with respect to patterns belonging to other clusters (Jain et al., 1999; Martino et al., 2017b; Martino et al., 2018b; Martino et al., 2019; Di Noia et al., 2019).

Synthesizing a classifier (predictive model) consists in feeding some $\langle x, y \rangle$ pairs to a training algorithm in such a way to automatically learn the underlying model structure. In other words, the classifier learns a decision function f that, given an input x, returns a predicted class label $\hat{y}$, i.e. a prediction regarding the class that pattern may belong to:

$$\hat{y} = f(x) \tag{1}$$

Eq. (1) is usually referred to as *hard classification*. Probabilistic classifiers can also return a posterior probability $P(\text{output}|\text{input})$ which can be useful for many real-world applications, for example condition-based maintenance, decision support systems or anomaly/fault detection as operators usually want to know the probability of a specific equipment to fail given some input (known) state/conditions (De Santis et al., 2018b). Trivially, probabilistic classifiers can be 'forced' to return hard predictions by letting

$$\hat{y} = \underset{y}{\operatorname{argmax}}\, P(Y = y|X) \tag{2}$$

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that is, for a given input pattern $x \in X$, the classifier assigns the output label $y \in Y$ which corresponds to the maximum posterior probability.

Albeit not all classifiers are probabilistic classifiers, some classifiers such as Support Vector Machine (SVM) (Boser et al., 1992; Cortes and Vapnik, 1995; Schölkopf and Smola, 2002; Cristianini and Shawe-Taylor, 2000) or Naïve Bayes may return a score $s(x)$ which somewhat states the 'confidence' in the prediction of a given pattern x. As regards Naïve Bayes, this score can be seen as the probability estimate for class membership. However, this score is not calibrated (Domingos and Pazzani, 1996). For SVMs, the score is basically the distance with respect to the separating hyperplane: the sign of $s(x)$ determines whether x has been classified as positive or negative, whereas the magnitude of $s(x)$ determines the distance with respect to the hyperplane. Conversely to Naïve Bayes, SVMs' scores not only are not calibrated, but also are not bounded in $[0,1]$, albeit some re-scaling can be performed (Zadrozny and Elkan, 2002).

Formally speaking, a classifier is said to be *well-calibrated* if $P(y|s(x) = s)$, that is, the probability for a pattern x to belong to a label y converges to the score $s(x) = s$ as the number of samples tends to infinity (Murphy and Winkler, 1977; Zadrozny and Elkan, 2002). In plain terms, the calibration of a classification system consists in mapping the scores (or not-calibrated probability estimates) into proper probability estimates bounded in range $[0,1]$ by definition.

The aim of this paper is to investigate amongst several calibration techniques by considering binary classification problems using SVM as classification system. The remainder of this paper is structured as follows: in Section 2 we give an overview of existing calibration techniques and figures of merit for addressing the goodness of the calibration along with three new lightweight procedures to be compared with state-of-the-art approaches; in Section 3 we describe the datasets used for experiments, along with comparative results amongst the considered methods; Section 4 concludes the paper, suggesting future research and applications.

2 AN OVERVIEW OF CALIBRATION TECHNIQUES

2.1 Current Approaches

In order to quantify the calibration of a given classifier the reliability diagram is usually employed (Murphy and Winkler, 1977). The reliability diagram is built as follows:

- scores/probabilities go on the x-axis
- empirical probabilities $P(y|s(x) = s)$, namely the ratio between the number of patterns in class y with score s and the total number of patterns with score s, go on the y-axis

and if the classifier is well-calibrated, then all points lie on the $y = x$ line (i.e., the scores are equal to the empirical probabilities). In case of binary classification, the empirical probabilities regard the positive instances only (i.e., the ratio between the number of positive instances having score s and the total number of instances with score s).

Since scores are normally real-valued scalars, it is quite impossible to quantify the number of data points sharing the same score[1]. In this case, a binning procedure is needed:

- on the x-axis, the average score value within the bin is considered
- on the y-axis, we get the ratio between the number of patterns in class y lying in a given bin and the total number of patterns lying in the same bin.

In works such as (Zadrozny and Elkan, 2002) and (Niculescu-Mizil and Caruana, 2005) the authors proposed to consider 10 equally-spaced bins in range $[0,1]$, regardless of the distribution of the scores within that range. For some datasets, however, this might not be a good choice and suitable alternatives which somewhat consider the available samples are:

- The Scott's rule (Scott, 1979) evaluates the bin width according to the number of samples (scores) n and their standard deviation σ as
$$\text{bin witdh} = \frac{3.5 \cdot \sigma}{n^{1/3}}$$
- The Freedman–Diaconis rule (Freedman and Diaconis, 1981) evaluates the bin width as follows
$$\text{bin witdh} = \frac{2 \cdot IQR}{n^{1/3}}$$
where IQR is the inter-quantile range
- The Sturges' formula (Sturges, 1926) evaluates the number of bins as follows
$$\text{number of bins} = 1 + \lceil \log_2 n \rceil$$
where $\lceil \cdot \rceil$ denotes the ceiling function
- The square root choice, where the number of bins is given by
$$\text{number of bins} = \lceil \sqrt{n} \rceil$$

[1]This counting procedure will return the (trivial) value of 1 for any $s(x)$.

However, using a single binning, even if evaluated according to one of the four alternatives above, might not be a good choice, especially if data do not follow a specific underlying distribution (e.g., uniform distribution in case of uniform binning or normal distribution in case of the Sturges's formula). To this end, in (Naeini et al., 2015), the Authors proposed the Bayesian Binning into Quantiles technique, which considers different binning (and their combination) in order to make the calibration procedure more robust.

Let c denote the positive class and let us assume $P(c|x) = 1$ for positive patterns and $P(c|x) = 0$ otherwise. After training a classifier such as SVM, aim of the calibration procedure is to find a function f formally defined as

$$f : s(x) \rightarrow \hat{P}(c|x) \tag{3}$$

hence, in other words, a function (model) in charge of transforming score values into probability estimates.

One of the most famous techniques is the Platt's scaling (Platt, 2000; Niculescu-Mizil and Caruana, 2005), a parametric approach in order to estimate $P(y = 1|s(x))$, namely the probability that a given pattern x belongs to the positive class. Platt's discussion starts by using the Bayes' formula

$$P(y = 1|s(x)) = \frac{p(s(x)|y = 1)P(y = 1)}{\sum_{i=\{\pm 1\}} p(s(x)|y = i)P(y = i)} \tag{4}$$

where $P(y = i)$ are prior probabilities and $p(s(x)|y = i)$ are the class conditional densities (i.e., the probability density function for belonging to class i). In order to use Eq. (4), one can estimate the class conditional densities by considering the normalized histograms of the scores as returned by the SVM. Platt showed that if the margin between the histograms of the two classes have an exponential trend, then Bayes' rule leads to

$$P(y = 1|s(x)) = \frac{1}{1 + \exp\{As(x) + B\}} \tag{5}$$

which is a plain parametric sigmoid function and tuning the calibration model basically consists in finding the two parameters A and B. Platt suggests to minimize the negative log-likelihood on some training data by means of a model-trust optimization procedure based on the Levenberg-Marquardt algorithm. In (Lin et al., 2007) an improved optimization procedure based on Newton's method is proposed. Platt's scaling has been proved to be successful if the reliability diagram of the dataset shows a sigmoidal trend.

An alternative technique relies on isotonic regression (Zadrozny and Elkan, 2002; Zadrozny and Elkan, 2001). Pair-Adjacent Violators (Ayer et al., 1955) is one of the main algorithms in order to compute an isotonic regression. Given a real-valued vector $\mathbf{x} \in \mathbb{R}^n$ and a weights vector[2] $\mathbf{w} \in \mathbb{R}^n$ such that $\mathbf{x}_i \geq \mathbf{x}_{i-1}$ and $\mathbf{w}_i > 0$ for all $i = 1, \ldots, n$, then the isotonic regression of a function $f(\mathbf{x})$ consists in finding a function $g(\mathbf{x})$ according to a mean squared error criterion

$$\sum_{i=1}^{n} \mathbf{w}_i (g(\mathbf{x}_i) - f(\mathbf{x}_i))^2 \tag{6}$$

where $g(\mathbf{x})$ must be a piecewise non-decreasing (isotonic) function. By letting $\mathbf{y}$ and $\mathbf{s}$ be the vectors containing the output class labels and their respective scores, Pair-Adjacent Violators works as follows:

1. sort $\mathbf{y}$ according to $\mathbf{s}$: if $\mathbf{y}$ is already isotonic[3], then return the estimate $\hat{\mathbf{y}} \equiv \mathbf{y}$, otherwise initialize the estimate values as $\hat{\mathbf{y}} = \mathbf{y}$
2. if $\hat{\mathbf{y}}$ is not isotonic, there must exist an index i such that $\hat{\mathbf{y}}_i \leq \hat{\mathbf{y}}_{i-1}$: for these values[4] we estimate $\hat{\mathbf{y}}_i = \hat{\mathbf{y}}_{i-1} = \frac{\hat{\mathbf{y}}_i + \hat{\mathbf{y}}_{i-1}}{2}$
3. repeat step 2 until $\hat{\mathbf{y}}$ is isotonic.

At the end of this procedure, $\hat{\mathbf{y}}$ contains ordered values (probability estimates) for scores in $\mathbf{s}$. Further, due to the piecewise nature of isotonic regression, $\hat{\mathbf{y}}$ will contain few different values, each of which is repeated several times. Generally, Pair-Adjacent Violators returns more samples in the score space where patterns have been misclassified and less samples where patterns have been correctly classified.

A recently proposed method is called SplineCalib (Lucena, 2018) which aims at overcoming the major drawbacks of Platt's scaling and isotonic regression:

- the Platt's scaling is based on the empirical observation that the relationship between scores and probabilities are *often* well-fitted by a sigmoid function: obviously, this works well only when the data fit the model, but performs poorly when the calibration function is not well-approximated by a sigmoid function
- the Platt's scaling works well for few calibration data (less than 1000 instances), but the isotonic regression overcomes this limitation
- the nature of piecewise constant approximation given by isotonic regression opens to a wider family of calibration function; however, its coarseness can be a drawback.

[2]This most general form is usually referred to as weighted isotonic regression. However, in this work, the weights vector is omitted.

[3]All 0's followed by all 1's since we are considering binary classification.

[4]The properly-said "pair-adjacent violators" since they violate the isotonic trend.

As its name suggests, SplineCalib is based on (cubic) smoothing splines. Like isotonic regression, SplineCalib is a non-parametric approach and, at the same time, unlike isotonic regression, SplineCalib fits a cubic spline instead of a piecewise constant approximation. In standard spline interpolation, one chooses a set of knots and fits a polynomial (usually with degree 3 or 4) within each interval: the more knots, the better the fitting of the data but also high risk of overfitting. Smoothing splines (Wahba, 1990) may also use all of the available points as knots and perform a regularized penalty on the second derivative of the function. Given a relationship between predictors x and output y of the form $y = f(x)$, the smoothing spline estimate $\hat{f}$ of f is the function, amongst the twice-differentiable ones, that minimize

$$\sum_{i=1}^{n} \left(y_i - \hat{f}(x_i)\right)^2 + \lambda \int \hat{f}''(t)dt \tag{7}$$

In (Lucena, 2018), instead of minimizing the sum of squares, the Author proposes to employ a log-likelihood criterion instead

$$-\sum_{i=1}^{n} \left[(y_i \cdot \log\hat{f}(x_i)) + (1-y_i) \cdot \log(1-\hat{f}(x_i))\right] + \\ + \frac{1}{2}\lambda \int \hat{f}''(t)dt \tag{8}$$

which resembles logistic regression (Hastie et al., 2001). Both Eqs. (7) and (8) see the regularization term $\lambda \geq 0$ which weights the contribution between goodness of fit (leftmost term) and roughness (rightmost term). Specifically, if $\lambda \to 0$ no smoothing is tolerated, with risk of overfitting; conversely, if $\lambda \to \infty$ no curvature is tolerated, with risk of going towards an ordinary least squares interpolation.
The probability estimates via SplineCalib can be evaluated by the following steps:

1. sample K knots[5] from the unique items in the score vector $\mathbf{s}$
2. build the natural basis expansion matrix $\mathbf{X} \in \mathbb{R}^{n \times K}$ between values in $\mathbf{s}$ and the K knots. Given a set of ordered knots $\{\phi_1, \ldots, \phi_K\}$, the natural cubic spline basis is defined as

$$N_1(x) = 1 \\ N_2(x) = x \\ N_{k+2}(x) = d_k(x) - d_{K-1}(x) \quad \forall k = 1, \ldots, K-2 \tag{9}$$

   where $d_k = \frac{(x-\phi_k)_+^3 - (x-\phi_K)_+^3}{\phi_K - \phi_k}$
3. perform an ℓ_2-regularized logistic regression over the pair $\langle \mathbf{X}, \mathbf{y} \rangle$ by considering a candidate value set for λ and choose the best value, say $\lambda^\star$, as the one that returns the best cross-validation log-loss
4. re-fit $\langle \mathbf{X}, \mathbf{y} \rangle$ using $\lambda^\star$
5. return the calibration function $f(s)$ by composing the basis expansion of s and the fitted model from the previous step in order to return the probability estimate.

2.2 Proposed Techniques

All of the three methods explained so far share the common goal to properly fit the reliability diagram: the better the fit, the more reliable the resulting probability estimates. Whilst the three methods use the 'score–label' pairs in order to accomplish this task, we investigate an alternative exercise by fitting the points lying on the reliability diagram. Hence, instead of working with 'score–label' pairs, we work with 'average bin value–fraction of positive patterns in that bin' pairs. As will be clear in Section 3, a reliability diagram almost never shows a linear trend, hence this fitting shall rely on more sophisticated functions[6]. For these exercises we use:

1. polynomial fitting: the points lying on the reliability diagram are fitted by means of 3-degree and 4-degree polynomials
2. spline fitting: after choosing a suitable number of knots and considering the corresponding intervals, within each interval a natural cubic spline interpolation is performed.

2.3 Figures of Merit

It is important to quantify the goodness of the calibration, hence how the probability estimates are far from the empirical probabilities. To this end, two methods have been proposed in literature: the Brier score (Brier, 1950; DeGroot and Fienberg, 1983) and the Log-Loss score.

Given a series of N known events and the respective probability estimates, the Brier score is the mean squared error between the outcome o (1 if the event has been verified and 0 otherwise) and the probability $p \in [0,1]$ assigned to such event. Hence, in its most general form, the Brier score has the form:

$$BS = \frac{1}{N}\sum_{i=1}^{N}(o_i - p_i)^2 \tag{10}$$

[5] One can also use all the available points, yet the Author states that 200 points suffice.

[6] Indeed, none of the methods introduced so far (Platt's scaling, isotonic regression, SplineCalib) use a linear fitting.

In the context of binary classification, Eq. (10) can be specifically written as:

$$BS = \frac{1}{N}\sum_{i=1}^{N}(T(y_i = 1|x_i) - P(y_i = 1|x_i))^2 \quad (11)$$

where $T(y_i = 1|x_i) = 1$ if $y_i = 1$ and $T(y_i = 1|x_i) = 0$ otherwise and $P(y_i = 1|x_i)$ is the estimated probability for pattern x_i to belong to class 1. As the Brier score resembles the mean squared error, a lower value is preferred.

The Log-Loss for binary classification is defined as follows:

$$LL = -\frac{1}{N}\sum_{i=1}^{N}[y_i \log p_i + (1-y_i)\log(1-p_i)] \quad (12)$$

and, as per the Brier score, the lower, the better. The Log-Loss index matches the estimated probability with the class label with logarithmic penalty: for small deviations between y_i and p_i the penalty is low, whereas for large deviations the penalty is high.

3 TEST AND RESULTS

3.1 Datasets Description

For addressing the calibration performances of the three state-of-the-art methods, namely Platt's scaling (PS), isotonic regression (IR), SplineCalib (SC) and the three fitting methods from Section 2.2, namely 3-degree polynomial (Poly3), 4-degree polynomial (Poly4) and natural cubic spline (NCS), two benchmark datasets from the UCI Machine Learning repository (Dua and Graff, 2019) have been considered:

Adult: the ADULT dataset is composed by 48842 instances and 14 attributes and the goal is to predict whether a person earns more than 50000$ per year based on census data

Abalone: the ABALONE dataset is composed by 4177 instances and 8 attributes and the goal is to predict the age of abalone from physics measurements. Since the Abalone dataset is natively multiclass (or for regression problems), we considered the median age and all output values below the median have been marked as 1 and the remaining values have been marked as 0.

These two datasets are freely available and have been extensively used as benchmarks for a plethora of learning techniques. Further, ADULT has been used in all major works on calibration techniques, see (Zadrozny and Elkan, 2002) for IR, (Platt, 2000) for PS and (Lucena, 2018) for SC. Alongside these two benchmark datasets, an additional dataset (hereinafter PCN) has been considered as well, where aim of the classification system is to predict whether a protein is an enzyme or not. This is a striking example of real-world problem in which a good probability estimation plays a huge role (Minneci et al., 2013; Li et al., 2016). The 3-dimensional folded structure of a protein can be described by its Protein Contact Network (Di Paola et al., 2012), an undirected and unweighted graph where nodes correspond to residues' α-carbon atoms and edges are scored if the Euclidean distance between nodes' spatial arrangements is within $[4,8]$Å. However, proteins notably have different sizes and some pre-processing stages need to be performed in order to map graphs into real-valued vectors of the same length. Following (Maiorino et al., 2017) and (Martino et al., 2017a), let $\mathbf{A}$ and $\mathbf{D}$ be the adjacency and degree matrices for a given graph $\mathcal{G}$. The Laplacian matrix $\mathbf{L}$ is defined as

$$\mathbf{L} = \mathbf{D} - \mathbf{A} \quad (13)$$

and the normalized Laplacian matrix $\overline{\mathbf{L}}$ reads as

$$\overline{\mathbf{L}} = \mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2} \quad (14)$$

If the graph $\mathcal{G}$ has m nodes, then $\mathbf{A},\mathbf{D},\mathbf{L},\overline{\mathbf{L}} \in \mathbb{R}^{m\times m}$ and none of these matrices can directly be used in order to properly match two graphs having different sizes. In order to overcome this problem, we consider the following property (Butler, 2016): the eigenvalues of $\overline{\mathbf{L}}$ lie in range $[0,2]$ regardless of the underlying graph. However, the number of eigenvalues equals the number of nodes m, hence neither the spectrum of $\overline{\mathbf{L}}$ can be used in order to compare two graphs. The final step is to consider the spectral density of the graph $\mathcal{G}$ by using a kernel density estimator (Parzen, 1962) with Gaussian kernel. Given $\Lambda = \{\Lambda_1,\ldots,\Lambda_m\}$ as the spectrum of $\overline{\mathbf{L}}$, the corresponding graph spectral density can be evaluated as

$$p(x) = \frac{1}{m}\sum_{i=1}^{m}\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left\{\frac{-(x-\Lambda_i)^2}{2\sigma^2}\right\} \quad (15)$$

where σ determines the kernel bandwidth and in order to consider a suitable value that scales in a graph-wise fashion, we used the Scott's rule (cf. Section 2.1). The distance between two graphs, say $\mathcal{G}_1$ and $\mathcal{G}_2$, can be evaluated as the ℓ_2 norm between their respective spectral densities, say $p_1(x)$ and $p_2(x)$:

$$d(\mathcal{G}_1,\mathcal{G}_2) = \int_0^2 (p_1(x) - p_2(x))^2 dx \quad (16)$$

Finally, 100 samples linearly spaced in $[0,2]$ have been extracted from the density function evaluated with Eq. (15). Such final 100 samples unambiguously identify each graph which, to this stage, is a vector

in $\mathbb{R}^{100}$ and in turn the dissimilarity measure between patterns, formerly Eq. (16), collapses into the plain Euclidean distance. This preprocessing stage has been performed on a subset of the *Escherichia coli* str. K12 proteome. Initially, the entire proteome gathered from UniProt (The UniProt Consortium, 2017) has been considered. After cross-checking with the Protein Data Bank database (Berman et al., 2000), all unresolved proteins have been removed. Further, in order to consider only good quality and reliable atomic coordinates, proteins with no information about the measurement resolution and proteins whose measurement resolution is greater than 3Å have been removed. Networks with at least one isolated node have not been considered either since it is impossible to evaluate Eq. (14). Finally, very few large protein complexes with over 2000 nodes have been removed as well. These filtering procedures returned a total number of 6061 proteins which have been labelled 1 if they have been assigned to an Enzyme Commission number (Webb, 1992), so they show enzymatic properties, and 0 otherwise. Subsets of this dataset have already been analyzed in works such as (Martino et al., 2017a; De Santis et al., 2018a; Martino et al., 2018c).

3.2 Comparative Results

The three datasets (ADULT, ABALONE and PCN) have been split into training (70% of the available patterns) and test set (the remaining 30%). For all datasets a 3-fold cross-validation has been performed for hyperparameters tuning and model calibration tuning. For all experiments, we considered a SVM classifier because it is a well-known uncalibrated binary classifier. In Figure 1 we show the reliability diagrams for training and test set for the three datasets. The binning has been performed with 10 uniformly-spaced bins, a common strategy in related works. In all cases, the trend is way far from the $y = x$ diagonal line: a clear sign that the classifier is not well-calibrated. By considering the ADULT dataset (training set) as an example, it is possible to see that all points whose score is less than 0.7 lie below the $y = x$ line: this means that all points with score (as returned by SVM) less than or equal to 0.7 have probability to belong to class 1 way inferior with respect to the score itself; similarly, for all points with score greater than 0.7, the true probability to belong to class 1 is superior with respect to the score assigned by the classifier.

Figure 2 shows the results in terms of fitted curves over the reliability diagram on the test set for the three considered datasets. Conversely, in Figure 3 we show the reliability diagram after calibration. For ease of comparison, in Tables 1 and 2 we show the two figure of merits (Brier score and Log-Loss score, respectively) on both the training set and test set.

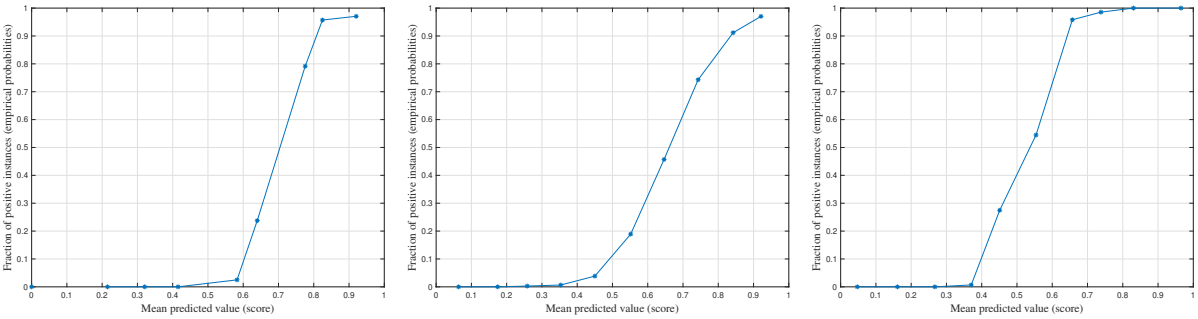
By considering the performances on test set, it is possible to see that the three alternative methods (Poly3, Poly4, NCS) have Brier score comparable to state-of-the-art techniques (PS, IR, SC): Poly4 is the best method for ABALONE, Poly3 and Poly4 equally outperform other methods for ADULT and Poly3 is the best method for PCN. In terms of Log-Loss, PS is the best method for ABALONE and ADULT, whereas SC is the best for PCN. Furthermore, the three alternative methods are featured by a lower computational burden, being a plain curve fitting over the reliability diagram.

4 CONCLUSIONS

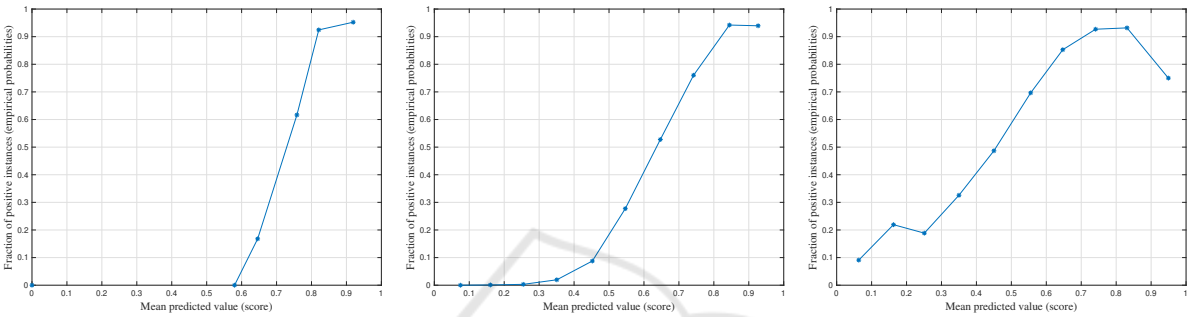
In this paper we reviewed three state-of-the-art techniques for calibrating a binary classifier in order to return reliable probability estimates on the resulting predictions. The three techniques (PS, IR and SC) have been benchmarked on two well-known datasets (ABALONE and ADULT) and an additional dataset (PCN) against three lightweight methods (Poly3, Poly4 and NSC), which basically perform a plain curve fitting on the reliability diagram. Computational results show that the three methods are comparable in terms of Brier score and Log-Loss score with respect to the three state-of-the-art approaches.

For these tests we used a SVM classifier due to its uncalibrated behaviour and in order to stress the comparison amongst calibration techniques rather than classification systems. Nonetheless, future research endeavours will consider the application of such techniques to different classification systems.

Indeed this study is part of a wider project concerning the design and implementation of a modelling and recognition system of faults and outages occurring in the real-world power grid managed by "Azienda Comunale Energia e Ambiente" (ACEA) company in Rome, Italy. The recognition system, based on a one-class classification approach as the main core of a larger system (De Santis et al., 2015), has been developed within the "ACEA Smart Grids project". A first task consists in modelling and recognizing faults in the power grid within a Decision Support System that provides support for the commanding and dispatching system, aiming at the implementation of Condition Based Maintenance programs. Another very important task consists in extracting from the learned fault classification model useful information for programming and control procedures, such as the estimation

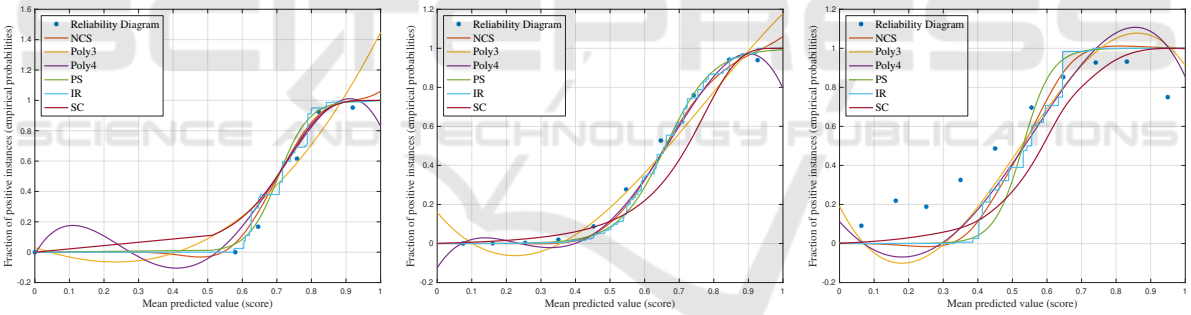


(a) ABALONE (training set) (b) ADULT (training set) (c) PCN (training set)



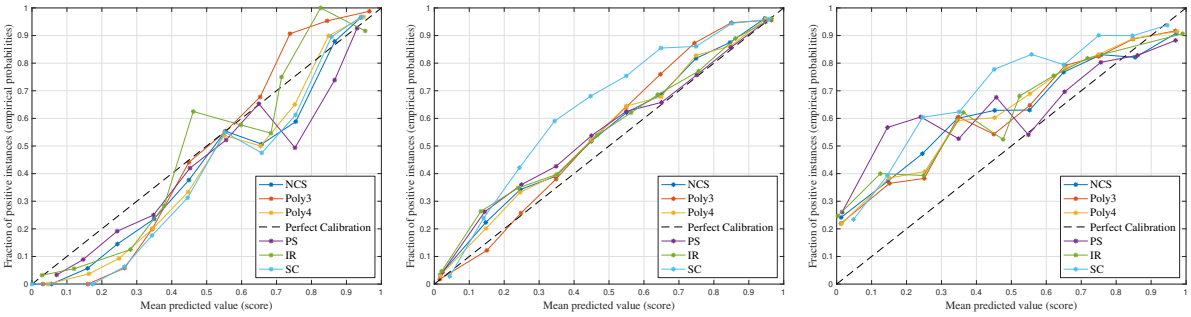
(d) ABALONE (test set) (e) ADULT (test set) (f) PCN (test set)

Figure 1: Reliability Diagrams.



(a) ABALONE (b) ADULT (c) PCN

Figure 2: Reliability Diagrams vs. fitted curves. For ABALONE we observe that for $x \in (0, 0.6)$ blue asterisks are missing, meaning that there are no scores in such bins.



(a) ABALONE (b) ADULT (c) PCN

Figure 3: Reliability Diagrams after Calibration.

Table 1: Brier Score.

Method	Abalone		Adult		PCN	
	Training Set	Test Set	Training Set	Test Set	Training Set	Test Set
uncalibrated	0.1788	0.1911	0.2028	0.1754	0.1302	0.1814
PS	0.1140	0.1209	0.1057	0.1084	0.0488	0.1977
IR	0.1083	0.1215	0.1050	0.1081	0.0442	0.1934
SC	0.1189	0.1263	0.1143	0.1179	0.0767	0.2073
Poly3	0.1368	0.1355	0.1095	0.1069	0.0582	0.1822
Poly4	0.1172	0.1236	0.1059	0.1069	0.0579	0.1847
NCS	0.1142	0.1207	0.1057	0.1070	0.0493	0.1878

Table 2: Log-Loss Score.

Method	Abalone		Adult		PCN	
	Training Set	Test Set	Training Set	Test Set	Training Set	Test Set
uncalibrated	0.5293	0.550	0.5919	0.5306	0.4404	0.5508
PS	0.3711	0.3901	0.3301	0.3395	0.1716	0.8451
IR	0.3503	0.3943	0.3274	0.3453	0.1476	2.3263
SC	0.3938	0.4080	0.3573	0.3626	0.2867	0.6486
Poly3	0.4572	0.4586	0.3613	0.3807	0.2260	1.8316
Poly4	0.3865	0.4184	0.3660	0.4416	0.2245	1.7577
NCS	0.3865	0.3909	0.3406	0.3718	0.1843	2.0713

of the financial risk associated to a set of power grid states and network resilience analysis. When dealing with risk assessment and cost benefit analysis for network expansion and maintenance planning, the availability of reliable probability estimates is of utmost importance.

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