Reliable Calibrated Probability Estimation in Classification

MLDM Workshop

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Motivation

- Probability calibration: Expected probability of correct guesses differs from real proportions.
- Reliable probability and confidence estimation is crucial in many applications: (i) assessment of risks and costs, (ii) robust integration with background knowledge, (iii) multi classifiers – bad local estimations distort the global result.
- Binning method and isotonic regression are often used calibration methods.
- **Problem:** Binning and isotonic regression give poor results on small and noisy calibration sets.
  - Inappropriate intervals (too many or too few bins).
  - Boundary generalization (poor performance on the edges of bins).
  - Errors in examples distribute to all examples in the section.
- **Solution:** Calibrate with isotonic regression and binning method by using bootstrapping technique (**Boot-Binning, Boot-Isotonic Regression**). Use confidence intervals for merging unreliable or too narrow calibration intervals.

Univariate Calibration Methods

- **Simple Normalization**
  - (Non) linear transformations for pre-calibration.
  - E-calibration, Softmax calibration.
- **Calibration Using Mapping**
  - Mapping function from membership value p_i to a calibrated conditional probability for positive class $\widehat{f_i}$.
  - Binning, Platt's logistic regression, Piecewise (Full) logistic regression, Isotonic regression.
- **Calibration via Bayes Rule**
  - Positive unnormalized class scores are split into two groups according to their true class. Membership probabilities are determined with Bayes theorem to class conditional probabilities and class priors.
  - Choice of the distribution type for the class conditional probabilities: Gaussian, Laplacian.
- **Calibration Using Assignment Values**
  - Membership values are partitioned according to their assignment. Modelled separately in each partition as Beta distributed random variables.

Calibration Quality Measures

- (i) mean squared error (MSE), (ii) LogLoss, (iii) calibration by overlapping bins (CalBin), (iv) calibration loss (CalLoss), (v) H-hat and (vi) chi-squared test through Hosmer-Lemeshow C-hat.
- **Pure** measures: CalBin, CalLoss.
- Brier score was originally not a calibration measure. It was decomposed in terms of calibration and refinement loss.
- **Impure** measures: MSE, LogLoss.
- **Insensitive to calibration:** qualitative – CA, F-measure; ranking – AUC.

Boot-Binning and Boot-Isotonic Regression

1. Construct bootstrapped data set:
   - training set (sampled examples, 63%),
   - calibration set (37%).

2.1 Classification model.

2.2 Calibration. Binning (**Boot-Binning**)/isotonic regression (**Boot-Isotonic Regression**).

3 Repeat 1 and 2 r times. Record calibrated probabilities.

4 Final calibration.
   - Non parametric confidence interval and a pseudomedian estimate for each example x_i with Wilcoxon signed-rank test.
   - Continually merge two sets of intervals obtained from 3. Probabilities are merged accordingly.

- Parametric methods. (i) r, the number of iterations; (ii) T_{count}, confidence interval threshold; (iii) T_{in}, intersection between confidence interval and an individual bin.

Experimental Configuration

- **10 data sets** from the UCI repository: (i) Monks1, (ii) Mushroom, (iii) Adult, (iv) House voting, (v) Tic-Tac, (vi) Marketing, (vii) Yeast, (viii) Breast Cancer, (ix) Ionosphere, (x) Breast cancer Wisc.
- **5 classifiers:** (i) decision trees (DT), (ii) support vector machines (SVM), (iii) random forests (RF), (iv) boosting (Boost), and (v) naive Bayes (NB).
- **5 calibration methods:** (i) binning (Binn), (ii) isotonic regression (IR), (iii) boot-isotonic regression (B-IR) and (iv) boot-binning (B-Binn), (v) Base.
- **2 quality measures:** CalBin and MSE.
- 30 repetitions for each combination of data set, classification, calibration – $(7500 = 30 \cdot 10 \cdot 5 \cdot 5)$ tests. Final CalBin and MSE measures averaged over 30 repetitions.

Experimental Evaluation

- Differences exist in results, evaluated with CalBin/MSE measure. This arises from the different nature of the measures.
- Observations confirm previous knowledge.
  - Isotonic regression is more powerful than binning. Binning and boot-binning methods are outperformed by isotonic regression and boot-isotonic regression.
  - Substantial differences between learning algorithms.
- Two-sided paired Wilcoxon signed-rank test for comparison of two classifiers over multiple data sets.
- Null hypothesis: Binning (isotonic regression) and boot-binning (boot-isotonic regression) perform equally well.
- 10 hypotheses: 5 classifiers and 2 proposed methods.

Classifier	Binning
DT	0.00195; [0.0043, 0.0205]
SVM	0.00977; [0.0026, 0.0158]
RF	0.01898; [-0.0103, -0.0008]
Boost	0.02734; [0.0021, 0.0349]
NB	0.01953; [0.0010, 0.0158]

Table: Boot-Binning. $\alpha = 0.05$.

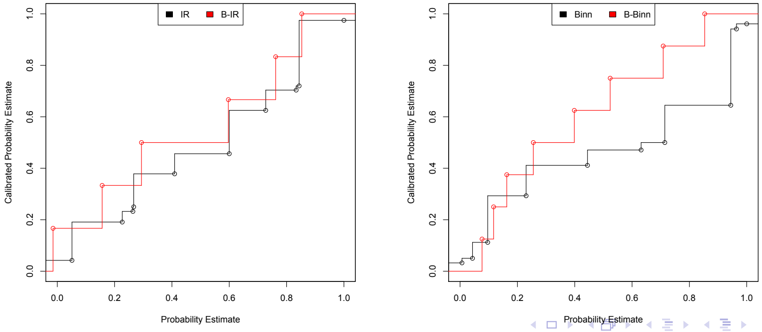
Classifier	Isotonic regression
DT	0.03711; [0.0015, 0.0288]
SVM	0.06251; [0.0195, 0.0488]
RF	0.05413; [0.0076, 0.0254]
Boost	0.04409; [0.0010, 0.0329]
NB	0.03091; [0.0019, 0.0291]

Table: Boot-Isotonic reg. $\alpha = 0.05$.

Anomalies Detection and Removal

- Evaluation on 6 artificial data sets. **A.** Gradual addition of noise. **B.** Proportion of positive class increases linearly with respect to the probability estimate + added class labels for 1.

Figure: **Left. Reliability diagram for (boot-) isotonic regression for A. Right.** Reliability diagram for (boot-) binning for B.



Conclusion and Future Work

- The problems of poor calibration results on small or noisy calibration sets have been eliminated.
- Calibration results show significant improvement using the bootstrapping approach.
- Null hypotheses, that binning (isotonic regression) and boot-binning (boot-isotonic regression) perform equally well is rejected for majority of classifiers.
- Unable to reject the null hypotheses of equal performance between isotonic regression and its bootstrapping improvement for SVMs and random forests.
- Future work.
  - Multi class problems.
  - Reduce complexity due to careful choice of parameters.