Probability calibration methodologies with local expert ensembles

CPT Nick Normandin

Introduction

▶ Please ask questions as I go

- Please ask questions as I go
- ▶ I've assumed some audience proficiency in modern machine learning techniques, but I will alternatively try to provide a heuristic understanding of the concepts presented

- Please ask questions as I go
- ► I've assumed some audience proficiency in modern machine learning techniques, but I will alternatively try to provide a heuristic understanding of the concepts presented
- ▶ Full accompanying R code is available

- Please ask questions as I go
- I've assumed some audience proficiency in modern machine learning techniques, but I will alternatively try to provide a heuristic understanding of the concepts presented
- ▶ Full accompanying R code is available
- ► This work was funded by the Omar N. Bradley Officer Research Fellowship in Mathematics

What is local expert?

I created a new kind of ensemble forecasting method that I've called local expert regression. It involves the decomposition of a supervised learning task with a continuous target variable (regression) into a series of of many $\{0,1\}$ mappings corresponding to separate binary probabilistic classification tasks that produce estimates on the [0,1] interval.

Why is this useful ?!

Because you can aggregate the ensemble predictions to form a completely unique *probability distribution function* for each prediction. You can understand **risk** not just in terms of a model, but in terms of each individual forecast.

... see github.com/nnormandin/localexpeRt

What problem am I solving?

Local expert

Most classification methods produce scores for class membership which are interpereted as measures of class affiliation probability. This is the foundation of local expert regression. However, these 'probabilities' are not usually well-calibrated.

Definition:

For a model f and score s_i to be well-calibrated for class c_i , the empirical probability of a correct classification $P(c_i|f(c_i|x_i)=s_i)$ must converge to $f(c_i|x_i)=s_i$.

Example:

When $s_i = 0.9$, the probability of a correct classification should converge to $P(c_i|s_i = 0.9) = 0.9$. Otherwise, this isn't *really* a 'probability.'

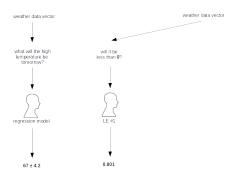
How do I propose to solve it?

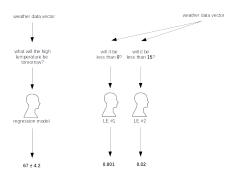
If probabilities aren't properly calibrated, the PDFs interpolated from them won't be reliable. How can we deal with this?

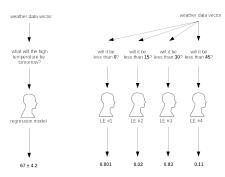
- 1. Change the loss function
- 2. Calibrate probabilities
 - isotonic regression, sigmoid transforms?

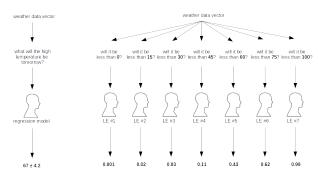
Local expert











Probability calibration

Why are some model scores poorly calibrated?

si dense around 0.5

- Maximal margin hyperplanes push scores away from extremes of distribution
- Common in support vector machines, boosted learners

s_i dense around 0, 1

- Model assumptions make class probabilites unrealistically confident
- Naive Bayes!

How can we visualize calibration?

Reliability plots!

- 1. Bin predictions by s_i (x-axis)
- 2. Calculate accuracy by bin (y-axis)

Method 1: Isotonic Regression

A strictly-nondecreasing piecewise linear function m, where $y_i = m(s_i) + \epsilon$ fit such that:

$$\hat{m} = \operatorname{argmin}_{z} \sum_{i} y_{i} - z(s_{i})^{2}$$

Method 2: Platt Scaling

Case study

Results

Conclusion

What have I demonstrated?

Which topics require more research?

- 1. Compensation for class imbalance (SMOTE?)
- 2. Kappa-based optimization methods
- 3. High-level parallelization

Questions