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calzone: A Python package for measuring calibration of probabilistic models for classification

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Summary

calzone is a Python package for evaluating the calibration of probabilistic outputs of classifier models. It provides a set of functions for visualizing calibration and computing of calibration metrics given a representative dataset with the model's predictions and the true class labels. The metrics provided in calzone include: Expected Calibration Error (ECE), Maximum Calibration Error (MCE), Hosmer-Lemeshow (HL) statistic, Integrated Calibration Index (ICI), Spiegelhalter's Z-statistics and Cox's calibration slope/intercept. The package is designed with versatility in mind. For many of the metrics, users can adjust the binning scheme and toggle between top-class or class-wise calculations.

Statement of need

Classification is one of the most common applications in machine learning. Examination of the discrimination performance (resolution), such as AUC or Se/Sp are also used to evaluate model performance. These metrics may be sufficient if the output of the model is not meant to be a calibrated probability.

Diamond (1992) showed that the resolution (i.e., high performance) of a model does not indicate the reliability/calibration of the model. Calibration is the agreement between predicted and true probabilities, $P(D = 1|\hat{p} = p) = p$, defined as moderate calibration by Van Calster & Steyerberg (2018) and also known as model reliability. Bröcker (2009) later showed that any proper scoring rule can be decomposed into the resolution and reliability. Thus, a model with high resolution may still lack reliability. In high-risk applications like medical diagnosis, reliability aids interpretability for treatment decisions.

The calzone package offers functions and classes for visualizing and evaluating calibration metrics with a representative dataset. Existing libraries like scikit-learn lack comprehensive calibration metrics, and others like uncertainty-toolbox focus on calibration methods rather than assessment (Chung et al., 2021).

Software description

Input data

To evaluate the calibration of a model, users need a representative dataset from the intended population. The dataset should contain the true class labels and the model's predicted probabilities. In calzone, the dataset can be a CSV file or two NumPy arrays containing true labels and predicted probabilities.

Reliability Diagram

The reliability diagram is a graphical representation of the calibration(Bröcker & Smith, 2007; Murphy & Winkler, 1977). It groups the predicted probabilities into bins and plots the mean predicted probability against the empirical frequency in each bin. The reliability diagram can be used to qualitatively assess the calibration of the model. The confidence intervals of the empirical frequency are calculated using the Wilson's score interval (Wilson, 1927).

```
from calzone.utils import reliability_diagram
from calzone.vis import plot_reliability_diagram
reliability, confidence, bin_edges, bin_counts = reliability_diagram(
    labels,
    probs,
    num_bins=15,
    class_to_plot=1
)

plot_reliability_diagram(
    reliability,
    confidence,
    bin_counts,
    error_bar=True,
    title='Reliability diagram'

)
```

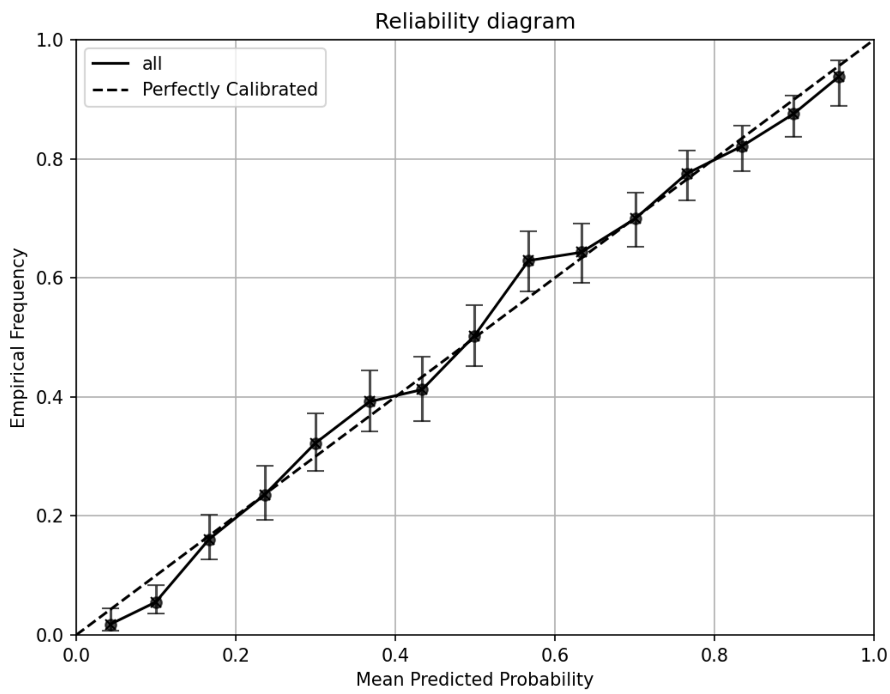

Figure 1: Reliability Diagram for class 1 with simulated data.

Calibration metrics

calzone provides functions to compute various calibration metrics. The `CalibrationMetrics()` class allows the user to compute the calibration metrics in a more convenient way. The following are metrics that are currently supported in calzone:

Expected Calibration Error (ECE) and Maximum Calibration Error (MCE)

Expected Calibration Error (ECE) and Maximum Calibration Error (MCE) (Guo et al., 2017; Pakdaman Naeini et al., 2015) measure the average and maximum deviation between predicted and true probabilities. calzone supports equal-width (ECE-H) and equal-count (ECE-C) binning. Users can compute these metrics for the top-class (highest probability) or class-of-interest (one-vs-rest classification).

Hosmer-Lemeshow statistic (HL)

The Hosmer-Lemeshow (HL) test (Hosmer & Lemesbow, 1980) evaluates model calibration using a chi-square test comparing observed and expected events in bins. The null hypothesis is that the model is well calibrated. calzone supports equal-width (ECE-H) and equal-count (ECE-C) binning. The test statistic is:

$$\text{HL} = \sum_{m=1}^{M} \frac{(O_{1,m} - E_{1,m})^2}{E_{1,m}\left(1 - \frac{E_{1,m}}{N_m}\right)} \sim \chi^2_{M-2}$$

where $E_{1,m}$ and $O_{1,m}$ are the expected and observed events in the m^{th} bin, N_m is the total observations in the bin, and M is the number of bins. For validation sets, the degrees of freedom change from $M-2$ to M (Hosmer Jr et al., 2013). The increase in degree of freedom for validation samples has often been overlooked but it is crucial for the test to maintain the correct type 1 error rate. In calzone, the default is $M-2$, adjustable via the `df` parameter.

Cox's calibration slope/intercept

Cox's calibration slope/intercept assesses model calibration without binning (Cox, 1958). A logistic regression is fit with predicted odds ($\frac{p}{1-p}$) as the independent variable and the outcome as the dependent variable. Perfect calibration is indicated by a slope of 1 and intercept of 0. To test calibration, fit the intercept with slope fixed at 1; if the intercept differs from 0, the model is not calibrated. Similarly, fit the slope with intercept fixed at 0; if the slope differs from 1, the model is not calibrated. Alternatively, fit both simultaneously using a bivariate distribution (McCullagh & Nelder, 1989). This feature is not in calzone, but users can manually test using the covariance matrix.

A slope >1 indicates overconfidence at high probabilities and underconfidence at low probabilities, while a slope <1 indicates the opposite. A positive intercept indicates general overconfidence. Even with ideal slope and intercept, non-linear miscalibration may still exist.

Integrated calibration index (ICI)

The Integrated Calibration Index (ICI) measures the average deviation between predicted and true probabilities using curve smoothing techniques (Austin & Steyerberg, 2019). It is calculated as:

$$\text{ICI} = \frac{1}{n}\sum_{i=1}^{n} |f(p_i) - p_i|$$

where f is the fitting function and p is the predicted probability. Typically, Locally Weighted Scatterplot Smoothing (LOWESS) is used, but any curve fitting method can be applied. calzone supports both Cox ICI and LOWESS ICI, allowing users to choose their preferred method. Users should visualize the fitting results to avoid overfitting or underfitting, as flexible methods like LOWESS are sensitive to span and delta parameters.

Spiegelhalter's Z-test

Spiegelhalter's Z-test is a test of calibration proposed by Spiegelhalter in 1986 (Spiegelhalter, 1986). It uses the fact that the Brier score can be decomposed into:

$$B = \frac{1}{N}\sum_{i=1}^{N}(x_i - p_i)^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i - p_i)(1-2p_i) + \frac{1}{N}\sum_{i=1}^{N}p_i(1-p_i)$$

And the test statistic (TS) of Z test is defined as:

$$Z = \frac{B - E(B)}{\sqrt{\mathrm{Var}(B)}} = \frac{\sum_{i=1}^{N}(x_i - p_i)(1-2p_i)}{\sum_{i=1}^{N}(1-2p_i)^2 p_i(1-p_i)}$$

and it is asymptotically distributed as a standard normal distribution.

Metrics class

calzone also provides a class called `CalibrationMetrics()` to calculate all the metrics mentioned above. The function will return a dictionary containing the metrics name and their values. The metrics can be specified as a list of strings. The string 'all' can be used to calculate all the metrics.

```python
from calzone.metrics import CalibrationMetrics

metrics = CalibrationMetrics(class_to_calculate=1)

metrics.calculate_metrics(
    labels,
    probs,
    metrics='all'
)
```

Other features

Confidence intervals

calzone also provides functionality to compute confidence intervals for all metrics using bootstrapping. The user can specify the number of bootstrap samples and the confidence level.

```python
from calzone.metrics import CalibrationMetrics

metrics = CalibrationMetrics(class_to_calculate=1)

CalibrationMetrics.bootstrap(
    labels,
    probs,
    metrics='all',
    n_samples=1000
)
```

and a structured NumPy array will be returned.

Subgroup analysis

calzone will perform subgroup analysis by default in the command line user interface. If the user input CSV file contains a subgroup column, the program will compute metrics for the entire dataset and for each subgroup. A detailed description of the input format can be found in the documentation.

Prevalence adjustment

calzone offers prevalence adjustment to correct for differences in disease prevalence between training and testing data. Calibration is based on posterior probability, so a shift in prevalence can cause miscalibration. The adjusted probability is calculated as:

$$P'(D=1|\hat{p}=p) = \frac{\eta'/(1-\eta')}{(1/p-1)(\eta/(1-\eta))} = p'$$

where η is the testing data prevalence, η' is the training data prevalence, and p is the predicted probability. The optimal η' is found by minimizing cross-entropy loss, or users can specify η' directly if known (Chen et al., 2018; Gu & Pepe, 2010; Horsch et al., 2008; Tian et al., 2020).

Multiclass extension

calzone supports multiclass classification using a 1-vs-rest approach or top-class calibration. In top-class calibration, class 1 probability is the highest predicted probability, and class 0 is 1 minus this probability. Metrics interpretation may change in this transformation.

Verification of methods

calzone results were compared with external packages for accuracy. Reliability diagrams were verified with `sklearn.calibration.calibration_curve()`(Pedregosa et al., 2011), top-class ECE and Spiegelhalter's Z scores with `MAPIE`(Taquet et al., 2022), and Hosmer-Lemeshow statistic with `ResourceSelection` (Lele et al., 2024) in R. Differences were within 0.1%, confirming consistency. Verification codes are in the documentation.

Command line interface

calzone offers a command line interface for visualizing calibration curves, calculating metrics, and confidence intervals. Run `python cal_metrics.py -h` for help.

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Conflicts of interest

The authors declare no conflicts of interest.

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