From Uncertainty to Precision: Challenging Binary Classifier Performance through Calibration.

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Séminaire d'été d'actuariat et de statistique

1. Introduction
2. Calibration
3. Impact of Poor Calibration
4. Score Heterogeneity and Tree-Based Methods

Calibration: intuition (1/2)

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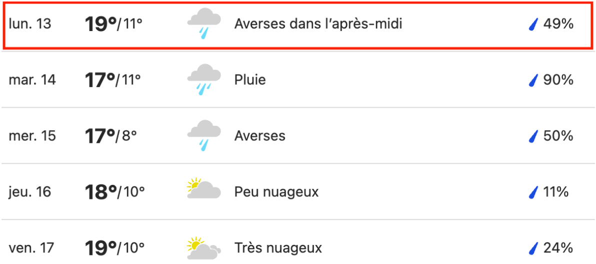

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mar. 14	17°/11°	Pluie	90%
mer. 15	17°/8°	Averses	50%
jeu. 16	18°/10°	Peu nuageux	11%
ven. 17	19°/10°	Très nuageux	24%

Figure 1: Weather Forecasts on Tuesday, March 2024. Source: The Weather Channel.

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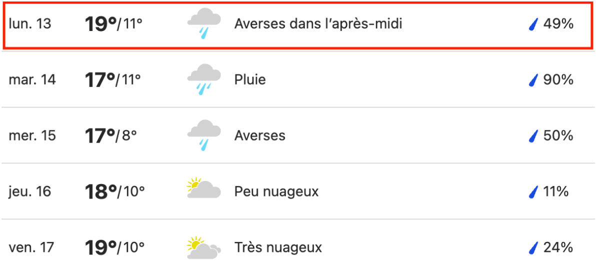

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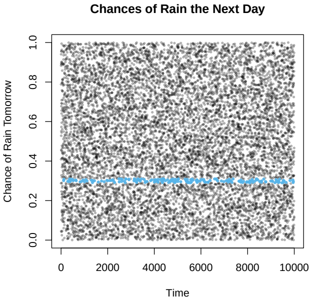
Consider a sequence of weather forecasts $\hat{s}(\mathbf{x}_t)$, where $t = 1, \ldots, T$ denotes the days of forecast and $\mathbf{x}$ represents characteristics used in forecasting.

Calibration: intuition (2/2)

Within this sequence, we focus on days where $\hat{s}(\mathbf{x}_i)$ closely approximates 30%.
By assuming an infinite sequence, we can determine the long-term proportion p of days where the forecasted event actually occurred.



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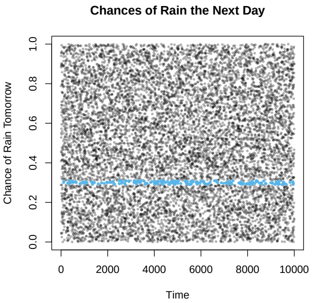

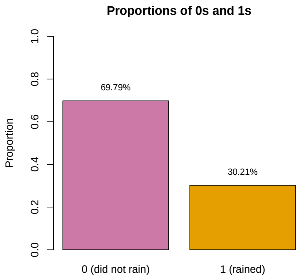

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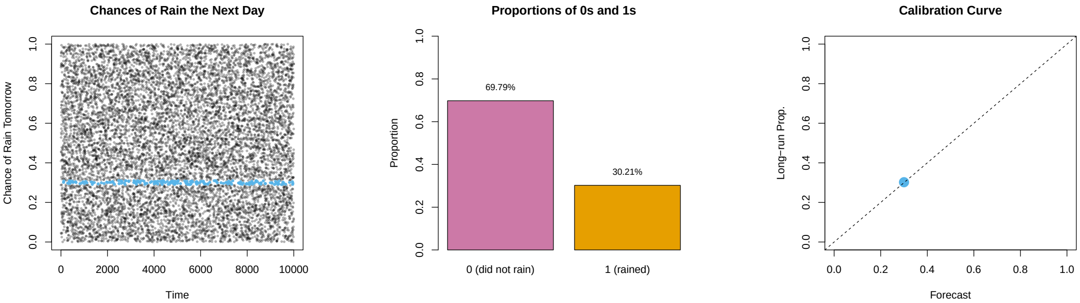

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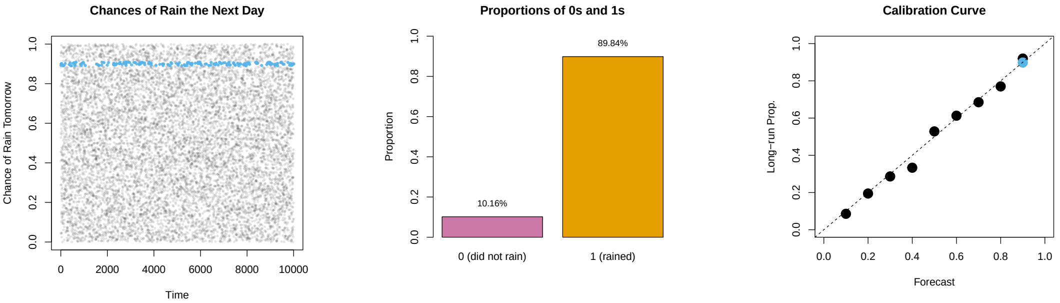

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- In such cases, it is important that the **estimated scores** can be interpreted as **probabilities**.
- This might become a problem when using **tree-based classifiers** (Niculescu-Mizil and Caruana, 2005; Park and Ho, 2020; Hänsch, 2020) rather than **logistic regression models** (Machado et al., 2024).

Roadmap

1. Introduction
2. Calibration
   - Definition
   - Measuring Calibration
3. Impact of Poor Calibration
4. Score Heterogeneity and Tree-Based Methods
   - Simulated Environment
   - Real-world scenario in insurance

1 Introduction

2 Calibration

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Measuring Calibration

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  where, with sample size $n > 0$, $i = 1, \ldots, n$ represents individuals, and $\mathbf{x}_i$ the characteristics.
- To **estimate this probability**, we can use a statistical model (*e.g.*, a GLM) or a machine learning model (*e.g.*, a random forest).

Definition

Calibration of a Binary Classifier (Schervish (1989))

For a binary variable D, a model is well-calibrated when

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Note: conditioning by $\{\hat{s}(\mathbf{x}) = p\}$ leads to the concept of (local) calibration; however, as discussed by Bai et al. (2021), $\{\hat{s}(\mathbf{x}) = p\}$ is *a.s.* a null mass event. Thus, calibration should be understood in the sense that

$$\mathbb{E}[D \mid \hat{s}(\mathbf{X}) = p] \overset{a.s.}{\to} p \text{ when } n \to \infty \ ,$$

meaning that, asymptotically, the model is well-calibrated, or locally well-calibrated in p, for any p.

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Visual approach: calibration curve

- Estimation of $\mathrm{g}(\cdot)$ (which measures **miscalibration** on predicted scores $\hat{s}(\mathbf{x})$):

$$\mathrm{g}:\begin{cases}[0,1]\to[0,1]\\ p\mapsto \mathrm{g}(p):=\mathbb{E}[D\mid \hat{s}(\mathbf{x})=p]\end{cases}. \tag{2}$$

- **Challenge**: having enough observations with identical scores is difficult.
- **Solution**: grouping obs. into B **bins**, defined by the **quantiles** of predicted scores:
  - The average of observed values ($\bar{d}_b$ with $b\in\{1,\ldots,B\}$), in each bin b can then be compared with the central value of the bin.
  - **Calibration curve** (reliability diagram (Wilks (1990)): middle of each bin on the x-axis, averages of corresponding observations on the y-axis.
  - When the model is **well-calibrated**, all B points lie on the **bisector**.

Metrics (1/2)

Expected Calibration Error or ECE (Pakdaman Naeini et al. (2015))

$$\text{ECE} = \sum_{b=1}^{B} \frac{n_b}{n} \mid \text{acc}(b) - \text{conf}(b) \mid$$

where n is the sample size, n_b is the number of observations in bin $b \in \{1, \ldots, B\}$.

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Accuracy $\text{acc}(b)$: The average of empirical probabilities or fractions of correctly predicted classes.

$$\text{acc}(b) = \frac{1}{n_b} \sum_{i \in \mathcal{I}_b} \mathbb{1}_{\hat{d}_i = d_i} \qquad (3)$$

The predicted class $\hat{d}_i$ for observation i is determined based on a classification threshold $\tau \in [0, 1]$ where $\hat{d}_i = 1$ if $\hat{s}(\mathbf{x}_i) \geq \tau$ and 0 otherwise.

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Confidence $\mathrm{conf}(b)$: Indicates the model's average confidence within bin b by averaging predicted scores.

$$\mathrm{conf}(b) = \frac{1}{n_b} \sum_{i \in \mathcal{I}_b} \hat{s}(\mathbf{x}_i)$$

Metrics (2/2)

Brier Score (Brier (1950))

The **Brier Score** does not depend on bins and is defined as:

$$BS = \frac{1}{n}\sum_{i=1}^{n}(d_i - \hat{s}(\mathbf{x}_i))^2 \tag{4}$$

where d_i is the observed event and $\hat{s}(\mathbf{x}_i)$ the estimated score.

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Mean Squared Error (MSE)

By substituting the observed event d_i by the true probability p_i (which can only be observed in an experimental setup), the metric becomes the MSE:

$$\text{True MSE} = \frac{1}{n}\sum_{i=1}^{n}(p_i - \hat{s}(\mathbf{x}_i))^2 \tag{5}$$

Smoother Visualization Technique

We prefer an alternative approach to visualize model calibration, aiming for a **smoother representation**: **local regression** (Loader (1999); Denuit et al. (2021)).

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- Given the number of data points, the precision of quantile binning can be suboptimal when determining the appropriate bin count.
- By contrast, with local regression, one can specify the percentage of nearest neighbors, providing greater flexibility.

Our new metric: LCS

Local Calibration Score (LCS)

A local regression of degree 0, denoted as $\hat{g}$, is fitted to the predicted scores $\hat{s}(\mathbf{x})$.
This fit is then applied to a vector of **linearly spaced values** within the interval $[0, 1]$.
Each of these points is denoted by l_j, where $j \in \{1, \ldots, J\}$, with J being the target number of points on the visualization curve.
The LCS is defined as:

$$\text{LCS} = \sum_{j=1}^{J} w_j \big(\hat{g}(l_j) - l_j\big)^2, \tag{6}$$

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Note: Austin and Steyerberg (2019) defined a similar metric using a L1 norm, called the Integrated Calibration Index (ICI).

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Data Generating Process

We **simulate** binary observations as in Gutman et al. (2022):

$$D_i \sim \mathcal{B}(p_i),$$

where individual probabilities are obtained using a logistic sigmoid function:

$$p_i = \frac{1}{1 + \exp(-\eta_i)},$$
$$\eta_i = \mathbf{a}\mathbf{x}_i + \varepsilon_i$$

with $\mathbf{a} = \begin{bmatrix} a_1 & a_2 & a_3 & a_4 \end{bmatrix} = \begin{bmatrix} 0.1 & 0.05 & 0.2 & -0.05 \end{bmatrix}$ and $\mathbf{x}_i = \begin{bmatrix} x_{1,i} & x_{2,i} & x_{3,i} & x_{4,i} \end{bmatrix}^\top$.
The observations $\mathbf{x}_i$ are drawn from a $\mathcal{U}(0,1)$ and $\varepsilon_i \sim \mathcal{N}(0, 0.5^2)$.

Forcing Poor Calibration

To simulate **uncalibration**, we generate samples of $2,000$ observations and we apply (monotonous) transformations to the true probabilities, either on:

1. the latent probability p_i:

$$p_i^u = \left(\frac{1}{1+\exp(-\eta_i)}\right)^{\alpha} \quad . \tag{7}$$

2. the linear predictor η_i:

$$\eta_i^u = \gamma \times ((-0.1)x_1 + 0.05x_2 + 0.2x_3 - 0.05x_4 + \varepsilon_i) \quad . \tag{8}$$

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The resulting transformed probabilities are considered as the scores: $\hat{s}(\mathbf{x}) := p_i^u$

Distortions

- We examine variations in $\{1/3, 1, 3\}$ for α and γ
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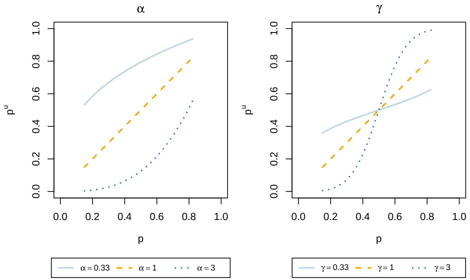

Figure 2: Distorted Prob. as a Function of True Prob., Depending on the Value of α (left) or γ (right)

Impacts: Calibration Metrics

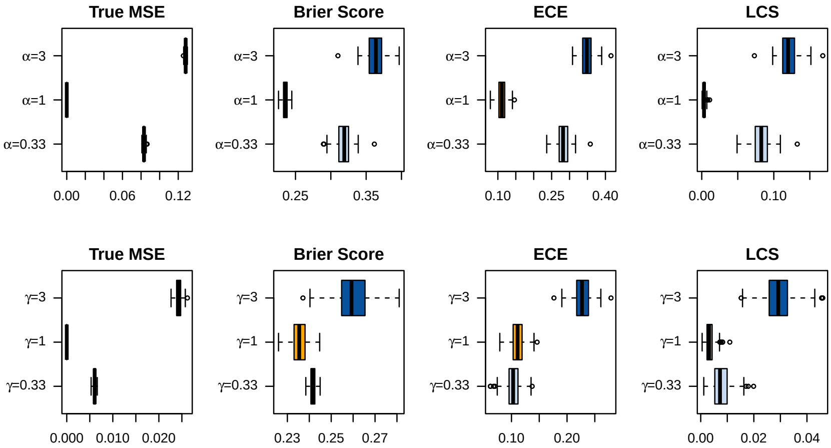

Figure 3: Calibration Metrics on 200 Simulations for each Value of α (top) or γ (bottom).

Impacts: Calibration Curves

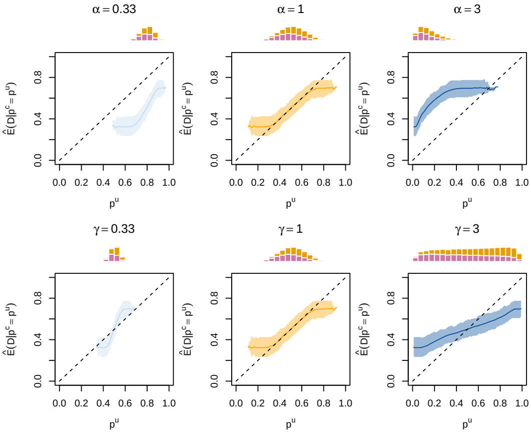

Figure 4: Calibration Curve Obtained with Local Regression, on 200 simulations for each Value of α (top) or γ (bottom). Distribution of the true probabilities are shown in the histograms (gold for $d = 1$, purple for $d = 0$).

(Mis-)Calibration and standard metrics

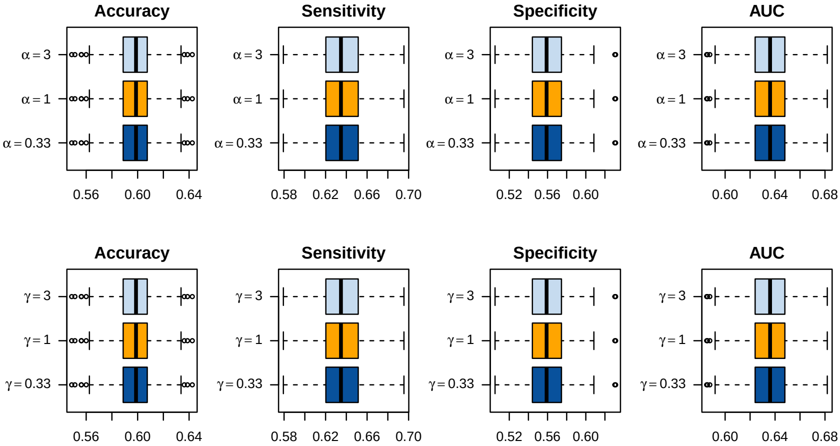

Figure 5: Standard Goodness of Fit Metrics on 200 Simulations for each Value of α (top) or γ (bottom). The probability threshold is set to $\tau = 0.5$.

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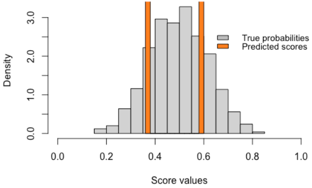

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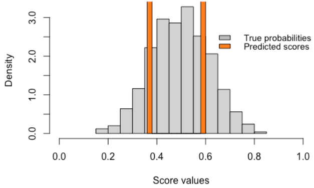

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Predicted score	Empirical frequency
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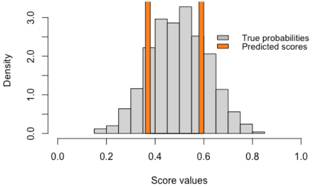

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→ **Perfect calibration curve**

Kullback-Leibler Divergence

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- In a **simulated environment**, we can optimize the hyperparameters of our ensemble method by **minimizing the KL divergence** from the distribution of predicted scores $\hat{s}(\boldsymbol{x})$ w.r.t. the true probability distribution p.

Overview for decision trees

Here, we consider a **simulated environment** for $D_i \sim \mathcal{B}(p_i)$, with p_i the **true underlying probability distribution**.

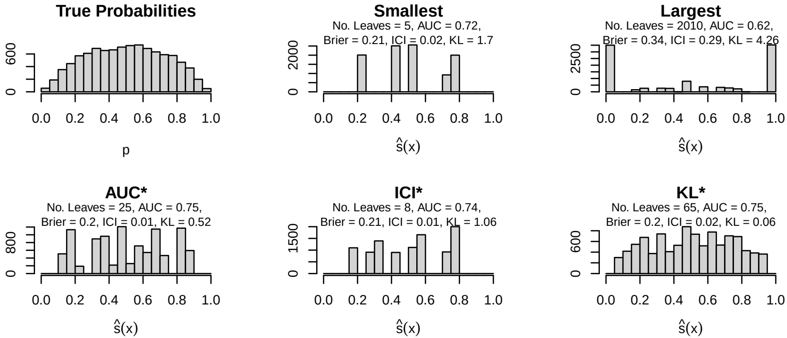

Figure 7: Distribution of true probabilities and estimated scores for trees of interest.

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Random Forest Optimization

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- We trained three different **random forests**, for which we have chosen hyperparameters optimized either for **AUC** (reference), **ICI**, or **KL divergence**.

Results for Random Forest

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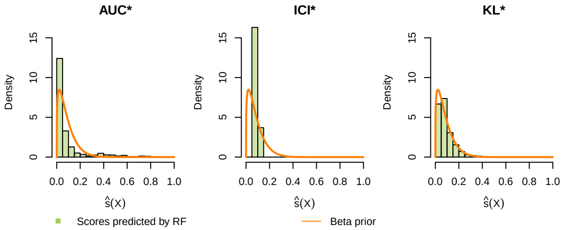

Figure 8: Distribution of RF predicted scores when optimizing hyperparameters for AUC (**AUC***), ICI (**ICI***) and KL (**KL***).

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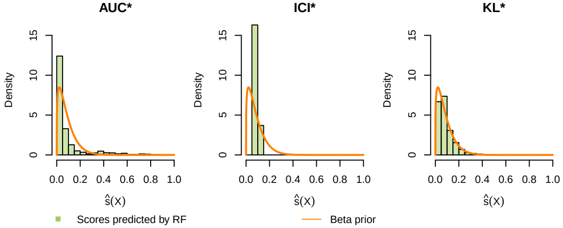

Figure 8: Distribution of RF predicted scores when optimizing hyperparameters for AUC (**AUC***), ICI (**ICI***) and KL (**KL***).

Table 2: Difference in validation set metrics between **ICI***, **KL*** and the reference model: **AUC***.

Optim.	ΔAUC	ΔICI	ΔKL
ICI*	-0.23	-0.02	$+0.44$
KL*	-0.05	$+0.01$	-0.77

Wrap up

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- **Calibration may not be sufficient** for **tree-based methods**: for RF, when score heterogeneity is lacking, metrics such as KL should complement the commonly used calibration metrics.

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5 Appendix

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(Mis-)Calibration and standard metrics

What are the impacts of miscalibration on standard metrics?
We will consider metrics based on the predictive performances calculated using a confusion table:

Table 3: Confusion Table

Actual/Predicted	**Positive**	**Negative**
Positive	TP	FN
Negative	FP	TN

where

$$\text{TPR} = \frac{\text{TP}}{\text{TP} + \text{FN}}; \quad \text{FPR} = \frac{\text{FP}}{\text{FP} + \text{TN}}$$

(Mis-)Calibration and standard metrics

$$\text{Accuracy} = \frac{\text{TP} + \text{TN}}{\text{N}}$$

Overall correctness of the model

$$\text{Sensitivity} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

Ability to correctly identify positive class

$$\text{Specificity} = TPR = \frac{\text{TN}}{\text{TN} + \text{FP}}$$

Ability to correctly identify negative class

AUC (Area Under Curve)

TPR and TFP for various prob. threshold τ