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Calibration of probabilistic predictive models

Machine Learning Journal Club, Gatsby Unit

David Widmann

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Centre for Interdisciplinary Mathematics, Uppsala University, Sweden

28 March 2022

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About me

TL;DR 📖

- 31 year old PhD student at Uppsala University
- On parental leave since September 2021
- Research on uncertainty quantification of probabilistic models
- Active member in the Julia community

About me

Education 🎓

2017—now: PhD student (Uppsala University)

2016—2017: MSc Mathematics (TU Munich)

2013—2016: BSc Mathematics (TU Munich)

2007—2013: Human medicine (LMU and TU Munich)

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Research interests 🔬

- Research topic: ”Uncertainty-aware deep learning”
- Statistics, probability theory, scientific machine learning, and computer science
- Julia programming, e.g., SciML and Turing

Papers

- J. Vaicenavicius et al. “Evaluating model calibration in classification.” In: *Proceedings of the Twenty-Second International Conference on Artificial Intelligence and Statistics.* Vol. 89. Apr. 2019
  - Focus on multi-class classification, calibration lenses, calibration estimation and tests with ECE

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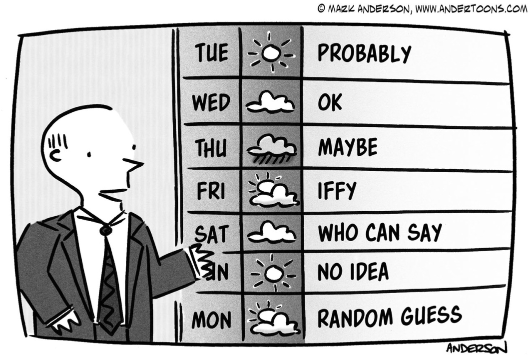
  - Calibration errors and tests for probabilistic predictive models based on scalar-valued kernels

Calibration: Motivation and definition

Example: Weather forecasts



"And now the 7-day forecast..."

E. Cooke. "Weighting forecasts." In: *Monthly Weather Review* 34.6 (June 1906), pp. 274–275

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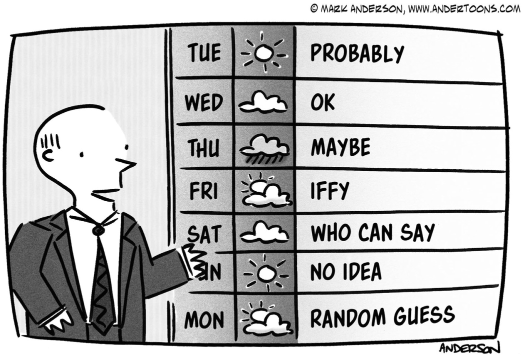

"And now the 7-day forecast..."

"Those forecasts which were marked 'doubtful' were the *best I could frame* under the circumstances. [...] If I make no distinction between these and others, I degrade the whole."

—E. Cooke

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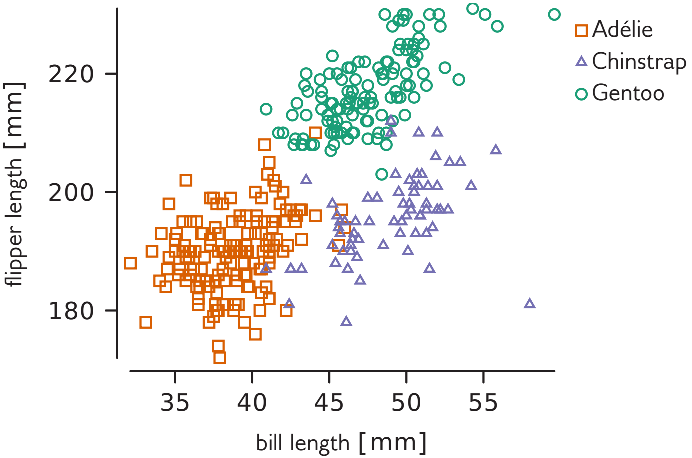
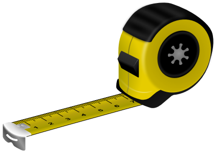
Motivation: Classification example



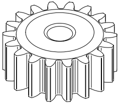
K. B. Gorman, T. D. Williams, and W. R. Fraser. "Ecological Sexual Dimorphism and Environmental Variability within a Community of Antarctic Penguins (Genus Pygoscelis)." In: *PLoS ONE* 9.3 (Mar. 2014), e90081

Motivation: Classification example

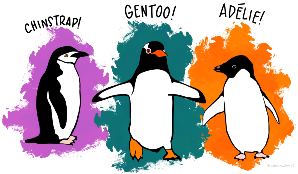
Input X



Model P



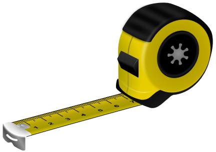
Prediction P_X (distribution of target Y)

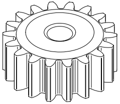


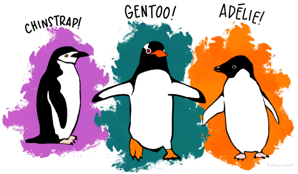
Artwork by @allison_horst

Motivation: Classification example

Input X | **Model P** | **Prediction P_X (distribution of target Y)**







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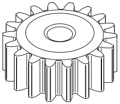
Example: Prediction P_X

Adélie	Chinstrap	Gentoo
80%	10%	10%

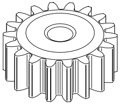
Calibration: Intuition

Model P



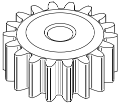
Calibration: Intuition

Model P

Input x_1 $\longrightarrow$ 

Calibration: Intuition

Model P **Prediction P_{x_1}**

Input x_1 →  →

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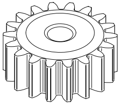
Input x_1 →  →

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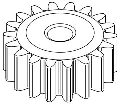
Empirical frequency

Adelie	Chinstrap	Gentoo
$\vert$		

Calibration: Intuition

Model P

Input x_2 → 

Empirical frequency

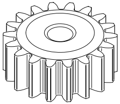
Adelie	Chinstrap	Gentoo
|		

Calibration: Intuition

Model P

Prediction P_{x_2}

Input x_2 →



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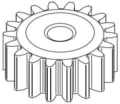
Input x_2 →  →

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Empirical frequency

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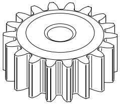
/	/	

Calibration: Intuition

Model P

Input x_3 $\longrightarrow$ 

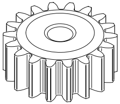
Empirical frequency

Adelie	Chinstrap	Gentoo
/	/	

Calibration: Intuition

Model P

Prediction P_{x_3}

Input x_3 →  →

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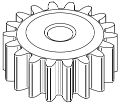
Input x_3 →  →

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Empirical frequency

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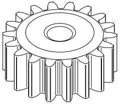
Calibration: Intuition

Model P **Prediction P_{x_i}**

Input x_i $\longrightarrow$



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Calibration

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Empirical frequency $\mathrm{law}(Y \mid P_X)$

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Calibration

Predictions consistent with empirically observed frequencies?

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Notion captures also weaker confidence calibration

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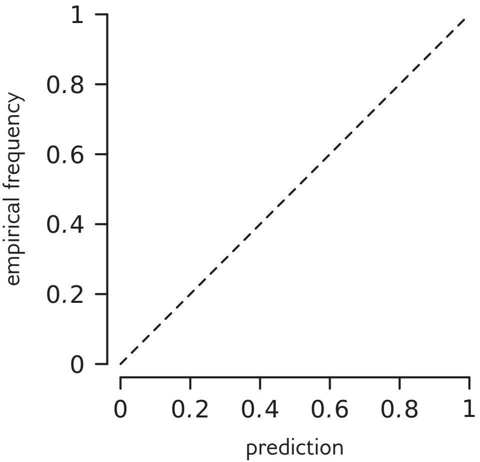
Binary classification: Reliability diagram



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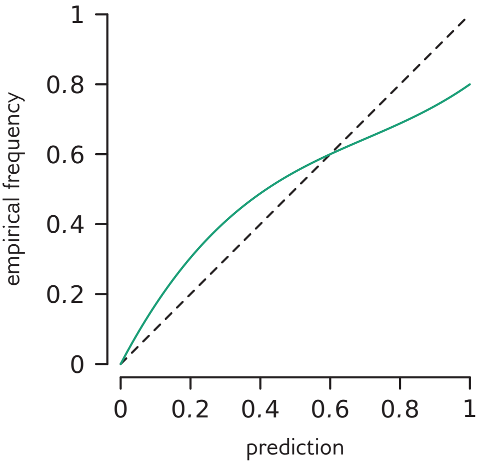

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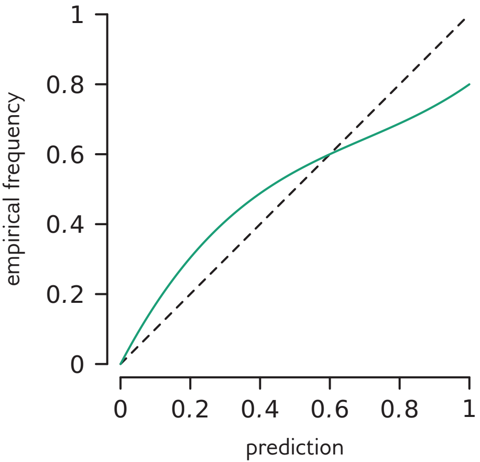

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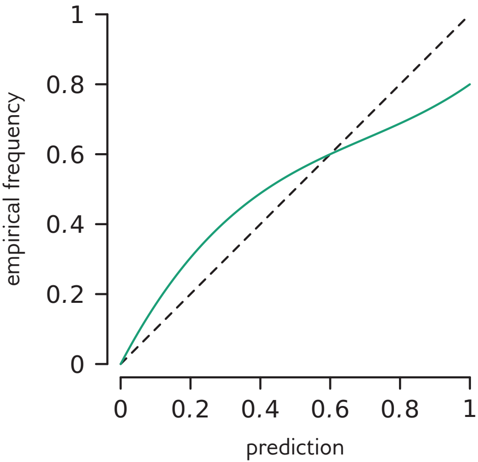

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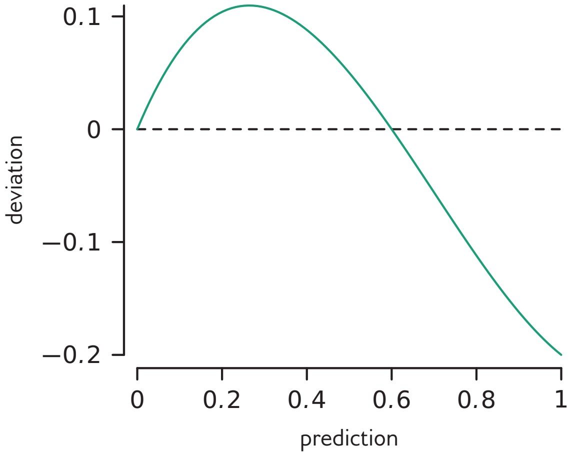

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Multi-class classification: All scores matter!

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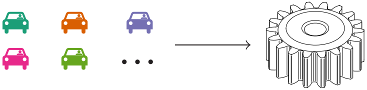

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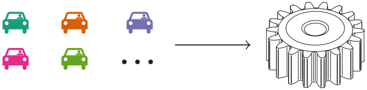

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80%	0%	20%

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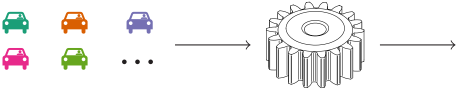

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Common calibration evaluation techniques consider only the most-confident score

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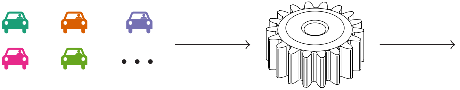

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Common calibration evaluation techniques consider only the most-confident score

Common approaches do not distinguish between the two predictions even though the control actions based on these might be very different!

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Weaker notions of calibration and calibration lenses

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Weaker notions of calibration such as confidence calibration or calibration of marginal classifiers can be analyzed by considering calibration of induced predictive models.

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Weaker notions of calibration and calibration lenses

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Definition (Calibration lenses)

Let ψ be a measureable function that defines targets $Z := \psi(Y, P_X)$. Then ψ induces a predictive model Q for targets Z with predictions

$$Q_X := \operatorname{law}\big(\psi(\tilde{Y}, P_X)\big)$$

where $\tilde{Y} \sim P_X$. Function ψ is called a *calibration lens*.

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Beyond classification

Definition (reminder)

A probabilistic predictive model P is calibrated if

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Beyond classification

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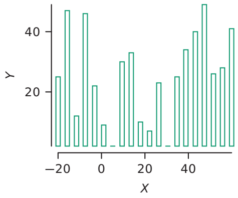
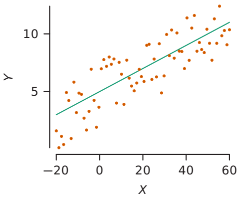
Examples of other target spaces

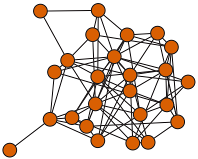
$\mathbb{N}_0$



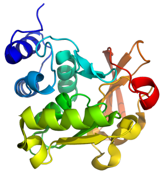
$\mathbb{R}^d$



graphs



protein structure



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Calibration errors

Expected calibration error (ECE)

Definition

The expected calibration error (ECE) with respect to distance measure d is defined as

$$\mathrm{ECE}_d := \mathbb{E}_{P_X} d\big(P_X, \mathrm{law}(Y \,|\, P_X)\big).$$

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Choice of distance measure d

- For classification typically (semi-)metrics on the probability simplex (e.g., cityblock, Euclidean, or squared Euclidean distance)

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Choice of distance measure d

- For classification typically (semi-)metrics on the probability simplex (e.g., cityblock, Euclidean, or squared Euclidean distance)
- For general probabilistic predictive models **statistical divergences**

Statistical divergences

Definition

Let $\mathcal{P}$ be a space of probability distributions. A function $d: \mathcal{P} \times \mathcal{P} \to \mathbb{R}$ that satisfies

- $d(P, Q) \geq 0$ for all $P, Q \in \mathcal{P}$,
- $d(P, Q) = 0$ if and only if $P = Q$,

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Note

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Examples

- f-divergences, e.g., Kullback-Leibler divergence or total variation distance
- Wasserstein distance

Scoring rules: Definition

Definition

The expected score of a probabilistic predictive model P is defined as

$$\mathbb{E}_{P_X,Y}\, s(P_X, Y)$$

where **scoring rule $s(p, y)$** is the reward of prediction p if the true outcome is y.

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Examples for classification

- Brier score: $s(p, y) = -\int_\Omega \left((\delta_y - p)^2\right)(\mathrm{d}\omega)$
- Logarithmic score: $s(p, y) = \log p\left(\{y\}\right)$

Scoring rules: Decomposition

For proper scoring rules

$$\mathbb{E}_{P_X,Y}\, s(P_X, Y) = \mathbb{E}_{P_X}\, d(\mathrm{law}(Y), \mathrm{law}(Y \mid P_X))$$

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Expected score of P under Q

$$S(P, Q) := \int_\Omega s(P, \omega)\, Q(\mathrm{d}\omega)$$

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J. Bröcker. "Reliability, sufficiency, and the decomposition of proper scores." In: *Quarterly Journal of the Royal Meteorological Society* 135.643 (July 2009)

Scoring rules: Decomposition

For proper scoring rules

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Models can trade off calibration for resolution!

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An alternative definition of calibration

Theorem

A probabilistic predictive model P is calibrated if

$$(P_X, Y) \stackrel{d}{=} (P_X, Z_X),$$

where $Z_X \sim P_X$.

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Calibration error as distance between $\mathrm{law}\big((P_X, Y)\big)$ and $\mathrm{law}\big((P_X, Z_X)\big)$

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Calibration error: Integral probability metric

$$\mathrm{CE}_{\mathcal{F}} := \sup_{f \in \mathcal{F}} \left| \mathbb{E}_{P_X,Y} f(P_X, Y) - \mathbb{E}_{P_X,Z_X} f(P_X, Z_X) \right|$$

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Examples

- 1-Wasserstein distance: $\mathcal{F} = \{f : \|f\|_{\mathrm{Lip}} \leq 1\}$
- Total variation distance: $\mathcal{F} = \{f : \|f\|_{\infty} \leq 1\}$

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Common choices of ECE_d in classification can be formulated in this way

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Kernel calibration error: Maximum mean discrepancy (MMD)

Choose $\mathcal{F} = \{f \in \mathcal{H} : \|f\|_{\mathcal{H}} \leq 1\}$ for some reproducing kernel Hilbert space $\mathcal{H}$

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- Hilbert space of functions that satisfy f close to $g \Rightarrow f(x)$ close to $g(x)$

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Definition

The kernel calibration error (KCE) of a model P with respect to kernel k is defined as

$$\mathrm{KCE}_k^2 := \mathrm{CE}_{\mathcal{F}}^2 = \int k\big((p, y), (\tilde{p}, \tilde{y})\big)\, \mu\big(\mathrm{d}(p, y)\big)\mu\big(\mathrm{d}(\tilde{p}, \tilde{y})\big),$$

where $\mu = \mathrm{law}\big((P_X, Y)\big) - \mathrm{law}\big((P_X, Z_X)\big)$.

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Choice of kernel

Observations

- Kernel k defined on the product space of predictions and targets

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- Otherwise numerical integration methods (e.g., Monte Carlo integration) can be used to integrate out Z_X
- Suggestive to use tensor product kernels $k = k_{\mathcal{P}} \otimes k_{\mathcal{Y}}$, where $k_{\mathcal{P}}$ and $k_{\mathcal{Y}}$ are kernels on the space of predictions and targets, respectively

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Tensor product kernel

Lemma

Let $k_{\mathcal{Y}}$ be a characteristic kernel on the target space and $k_{\mathcal{P}}$ be a kernel on the space of predictions that is non-zero almost surely. Then the KCE *of model P with respect to kernel $k = k_{\mathcal{P}} \otimes k_{\mathcal{Y}}$ is zero iff model P is calibrated.*

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Construction of $k_{\mathcal{P}}$ with Hilbertian metrics

- For Hilbertian metrics of form $d_{\mathcal{P}}(p, \tilde{p}) = \|\phi(p) - \phi(\tilde{p})\|_2$ for some $\phi \colon \mathcal{P} \to \mathbb{R}^d$,

$$k_{\mathcal{P}}(p, \tilde{p}) = \exp\big(-\lambda d_{\mathcal{P}}^{\nu}(p, \tilde{p})\big), \tag{1}$$

  is valid kernel on the space of predictions for $\lambda > 0$ and $\nu \in (0, 2]$

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- Parameterization of predictions gives rise to ϕ naturally
- For many mixture models, Hilbertian metrics of model components can be lifted to Hilbertian metric of mixture models

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Estimation of calibration errors

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Task

Estimate the calibration error of a model P from a validation dataset $(X_i, Y_i)_{i=1,\ldots,n}$ of features and corresponding targets.

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Dataset of predictions and targets sufficient

- Calibration (errors) defined based only on predictions and targets
- Estimation can be performed with dataset (P_{X_i}, Y_i) of predictions and corresponding targets instead
- Highlights that structure of features and model is not relevant for calibration estimation

ECE: Estimation

Problem

The estimation of $\operatorname{law}(Y \mid P_X)$ is challenging.

J. Vaicenavicius et al. "Evaluating model calibration in classification." In: *Proceedings of the Twenty-Second International Conference on Artificial Intelligence and Statistics*. Vol. 89. Apr. 2019

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ECE: Estimation

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The estimation of $\mathrm{law}(Y \mid P_X)$ is challenging.

Binning predictions

- Common approach in classification
- Often leads to **biased and inconsistent** estimators

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ECE: Experiments

10-class classification

For three models **M1**, **M2** and **M3**, 10^4 synthetic datasets $(P_{X_i}, Y_i)_{i=1,\ldots,250}$ are sampled according to

- $P_{X_i} = \mathrm{Cat}(p_i)$ with $p_i \sim \mathrm{Dir}(0.1, \ldots, 0.1)$,

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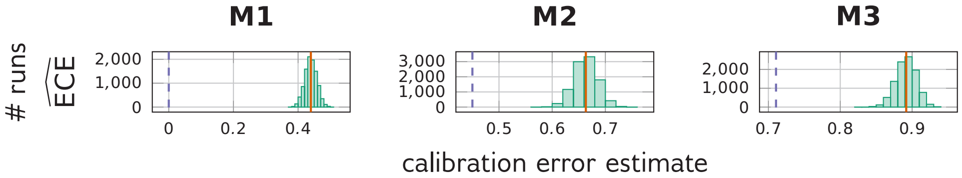

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Kernel calibration error: Estimation

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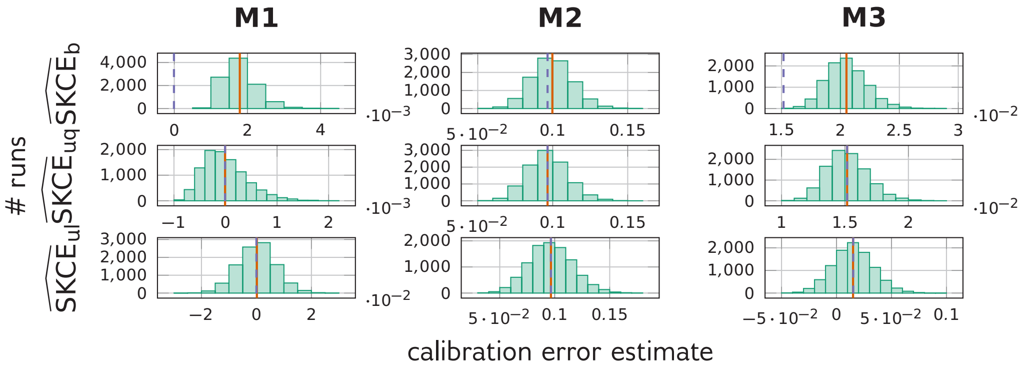

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Calibration tests

Problems with calibration errors

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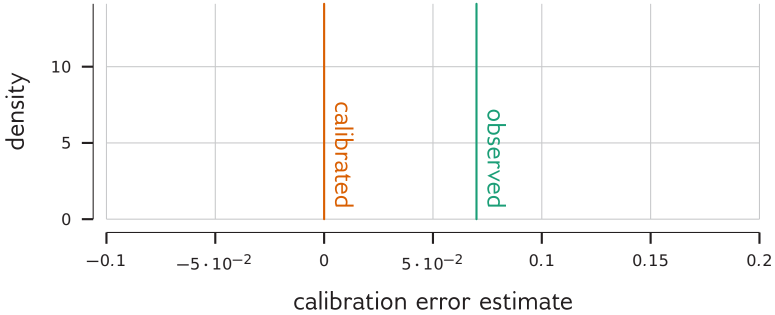
- Different calibration errors rank models differently
- Calibration error estimators are random variables

Calibration tests



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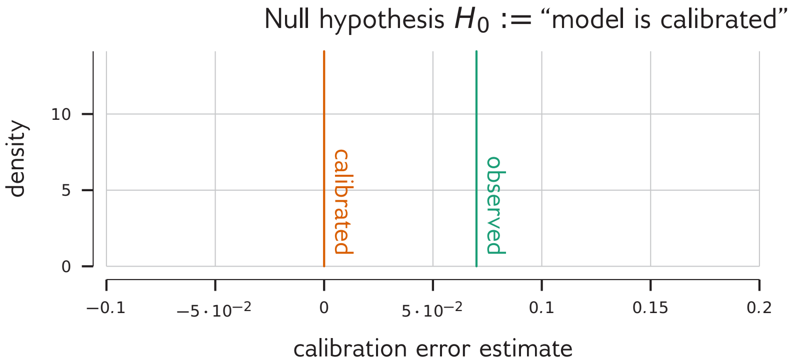

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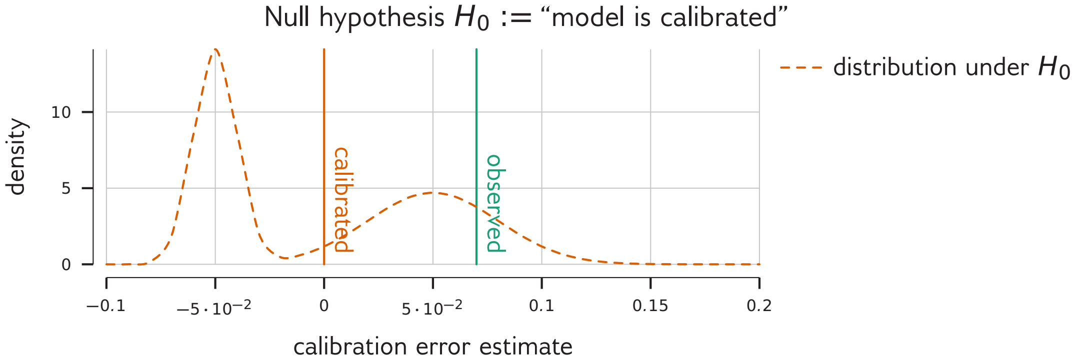

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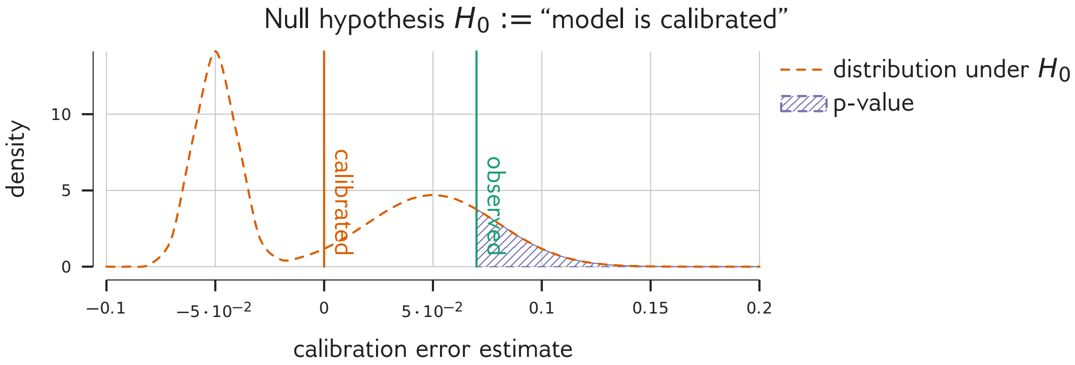

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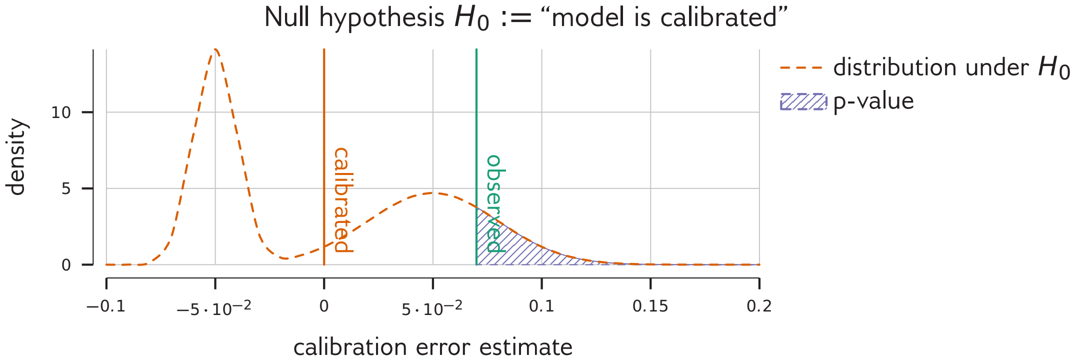

Reject H_0 if p-value is small

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Consistency resampling

Original dataset

$$\begin{array}{|cc|}\hline y_1 & P_{x_1} \\ \vdots & \vdots \\ y_n & P_{x_n} \\ \hline\end{array}$$

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Consistency resampling

Original dataset — Resampled dataset under H_0

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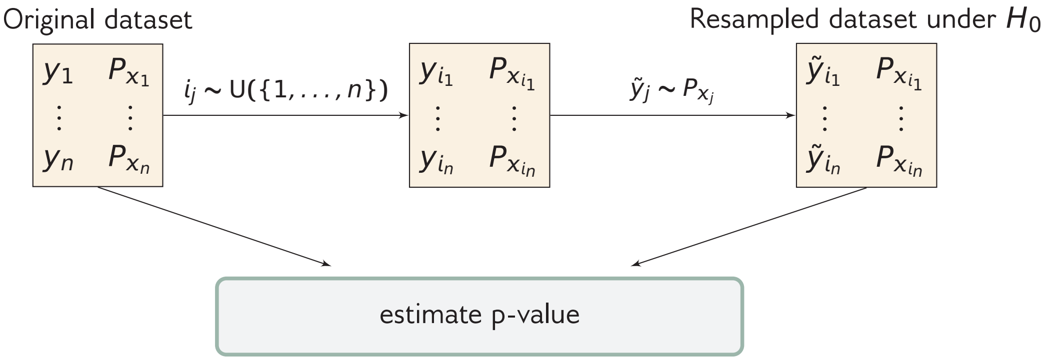

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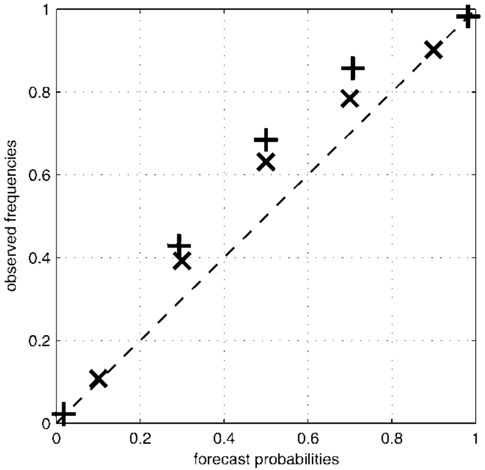
Consistency bars



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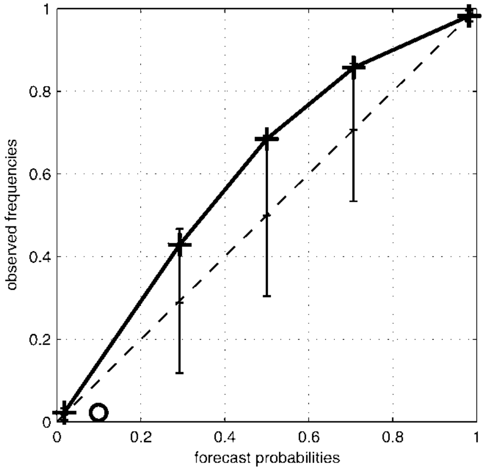
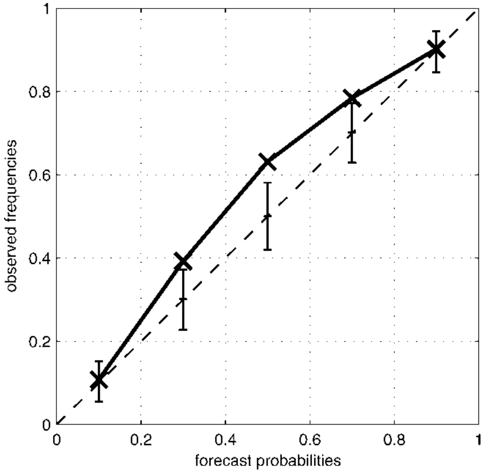
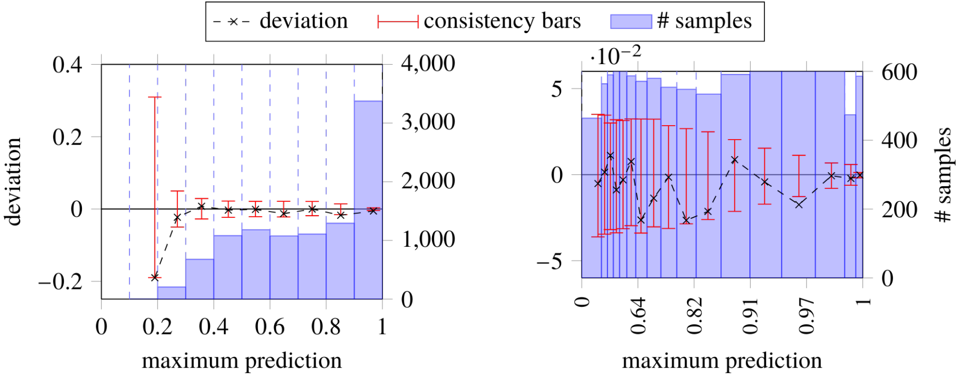




J. Bröcker and L. A. Smith. "Increasing the reliability of reliability diagrams." In: *Weather and Forecasting* (2007)

Variant



(a) Equally-sized bins

(b) Data-dependent bins

J. Vaicenavicius et al. "Evaluating model calibration in classification." In: *Proceedings of the Twenty-Second International Conference on Artificial Intelligence and Statistics*. Vol. 89. Apr. 2019

Kernel calibration error: Distribution-free tests

Upper bound the p-value

D. Widmann, F. Lindsten, and D. Zachariah. "Calibration tests in multi-class classification: A unifying framework." In: *Advances in Neural Information Processing Systems 32*. 2019

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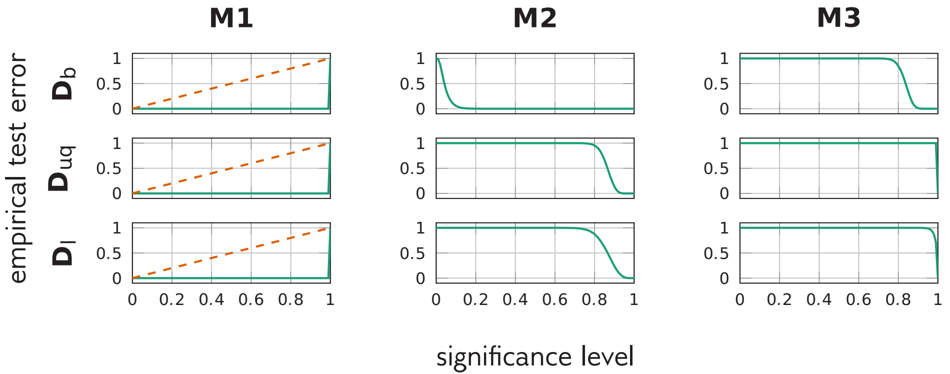

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Kernel calibration error: Asymptotic tests

Approximate the p-value based on the **asymptotic** distribution

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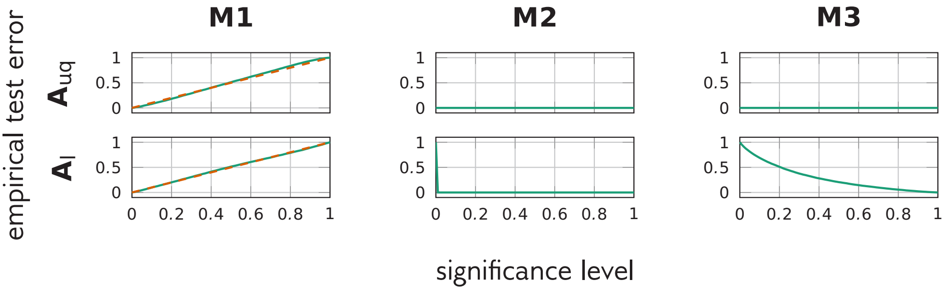

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Calibration: Software packages

`CalibrationAnalysis.jl`

Summary

- Suite for analyzing calibration of probabilistic predictive models
- Written in Julia, with interfaces in Python (`pycalibration`) and R (`rcalibration`)

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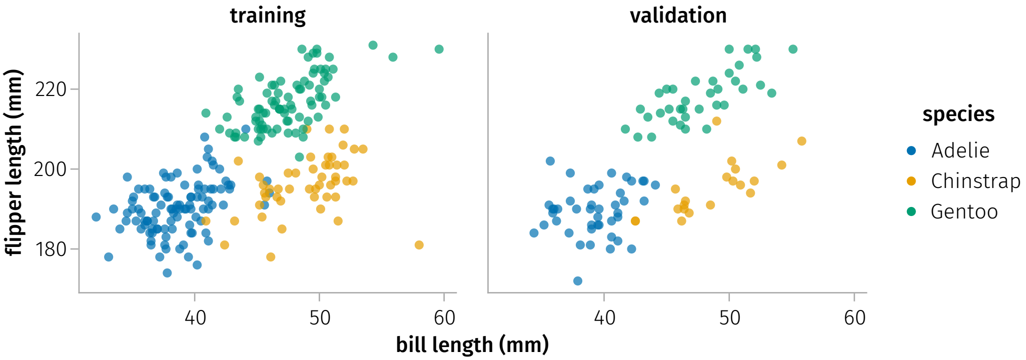
- Suite for analyzing calibration of probabilistic predictive models
- Written in Julia, with interfaces in Python (`pycalibration`) and R (`rcalibration`)

Features

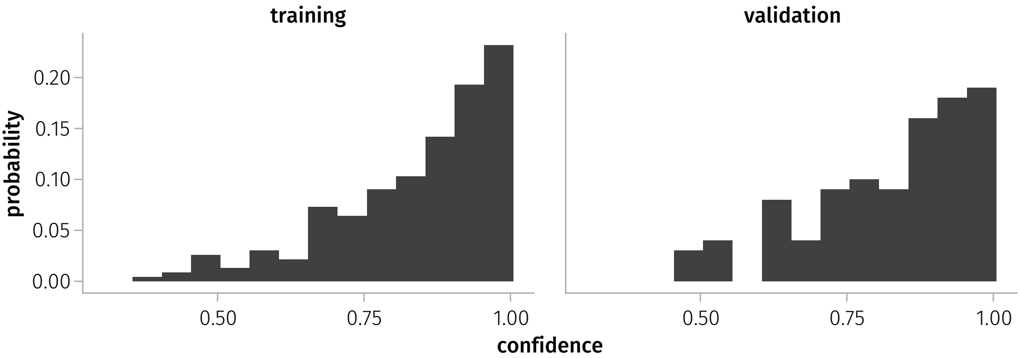
- Supports classification and regression models
- Reliability diagrams (`ReliabilityDiagrams.jl`)
- Estimation of calibration errors such as ECE and KCE (`CalibrationErrors.jl`)
- Calibration tests (`CalibrationTests.jl`)
- Integration with Julia ecosystem: Supports `Plots.jl` and `Makie.jl`, `KernelFunctions.jl`, and `HypothesisTests.jl`

Calibration analysis: Penguins example

We train a naive Bayes classifier of penguin species based on bill depth, bill length, flipper length, and body mass.



Binary predictions

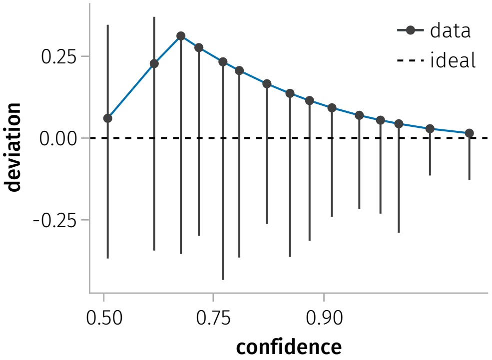


Reliability diagram

Code

```
julia> using CalibrationAnalysis, CairoMakie

julia> reliability(
           confidence,
           outcome;
           binning=EqualMass(; n=15),
           deviation=true,

           ↪  consistencybars=ConsistencyBars(),
       )
```

Polished result



Expected calibration error: Code

```julia
julia> ece = ECE(UniformBinning(5), TotalVariation());

julia> ece(confidence, outcome)
0.06594437403598197

julia> ece(predictions, observations)
0.15789651955832515
```

Kernel calibration error: Code

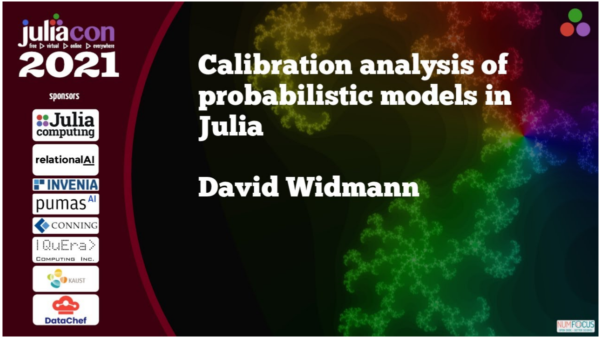
```julia
julia> kernel = GaussianKernel() ⊗ WhiteKernel();

julia> skce = SKCE(kernel);

julia> skce(predictions, observations)
0.003263144705774404

julia> skce = SKCE(kernel; unbiased=false);

julia> skce(predictions, observations)
0.004202113116841622

julia> skce = SKCE(kernel; blocksize=5);

julia> skce(predictions, observations)
-0.005037270862051889
```

Calibration test: Code

```
julia> AsymptoticSKCETest(kernel, predictions, observations)
Asymptotic SKCE test
--------------------
Population details:
    parameter of interest:   SKCE
    value under h_0:         0.0
    point estimate:          0.00326311

Test summary:
    outcome with 95% confidence: reject h_0
    one-sided p-value:           0.0150

Details:
    test statistic: -0.0009060378940361157

julia> test = ConsistencyTest(ece, predictions, observations);

julia> pvalue(test; bootstrap_iters=10_000)
0.0188
```

Additional resources

- Online documentation: `https://devmotion.github.io/CalibrationErrors.jl/`
- Talk at JuliaCon 2021: `https://youtu.be/PrLsXFvwzuA`



Slides available at `https://talks.widmann.dev/2021/07/calibration/`

Concluding remarks

Important takeaways

- More fine-grained analysis of calibration can be important
- MMD-like kernel calibration error can be applied to probabilistic models beyond classification
- Estimators of kernel calibration error have appealing properties
- Calibration errors and reliability diagrams can be misleading