IPML

IMPRECISE PROBABILISTIC MACHINE LEARNING

Lecture 9: Conformal Prediction and Calibration

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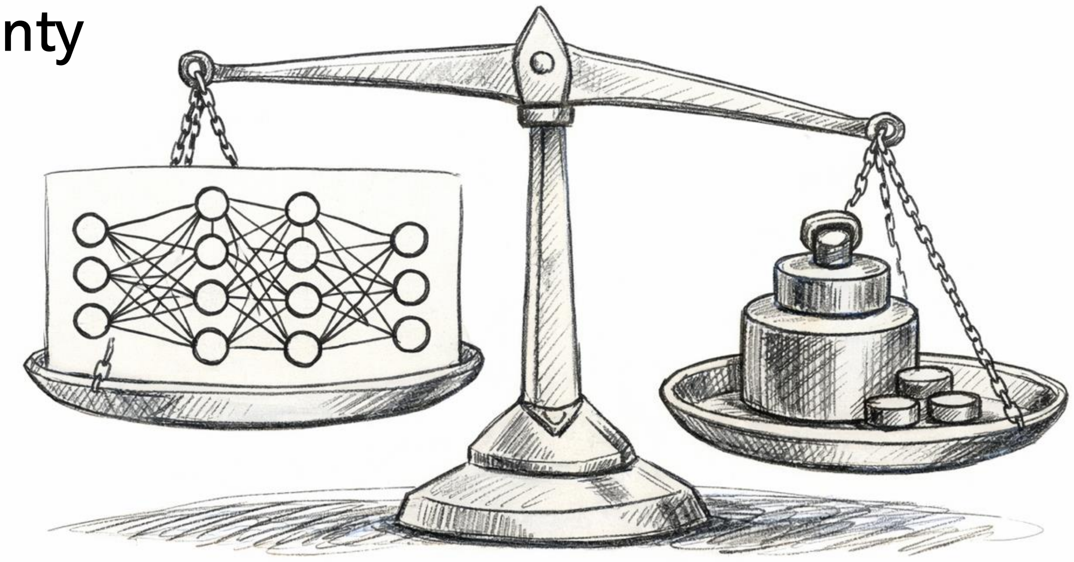
Outline

1. Conformal Prediction
2. Probabilistic Calibration
3. Applications

Conformal Prediction

Conformal Prediction

- Conformal prediction is a *frequentist* approach to **distribution-free** uncertainty quantification that is:
  1. Agnostic to the model
  2. Agnostic to data distribution
  3. Valid in finite sample



Heuristic Uncertainty → Conformal Prediction → Rigorous Uncertainty

Conformal Coverage Guarantee

- Given a predictive model $\hat{f}: \mathcal{X} \rightarrow \Delta(\mathcal{Y})$ and the test point $(X_{\text{test}}, Y_{\text{test}})$, we seek to construct a **prediction set** $C(X_{\text{test}}) \subset \mathcal{Y}$ that is **valid**, meaning

$$P(Y_{\text{test}} \in C(X_{\text{test}})) \geq 1 - \alpha$$

where $\alpha \in [0,1]$ is a user-chosen error rate.

- **Marginal coverage**: *The probability that the prediction set contains the correct label is almost exactly* $1 - \alpha$.

Conformal Coverage Guarantee

{ fox squirrel 0.99 }

{ fox squirrel 0.82, gray fox, 0.03, bucket, 0.02, rain barrel 0.02 }

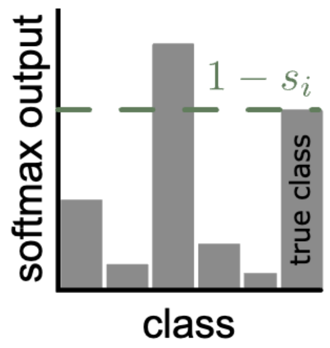
{ marmot, 0.30, fox squirrel, 0.22, mink, 0.18, weasel, 0.16, beaver, 0.03, polecat 0.01 }

We want the prediction set to contains the correct label **with high probability.**
The prediction set $C(X_{\text{test}})$ captures the model's uncertainty on the data X_{test}.

Split Conformal Prediction

Given a **calibration set** $(X_1, Y_1), \dots, (X_n, Y_n)$:

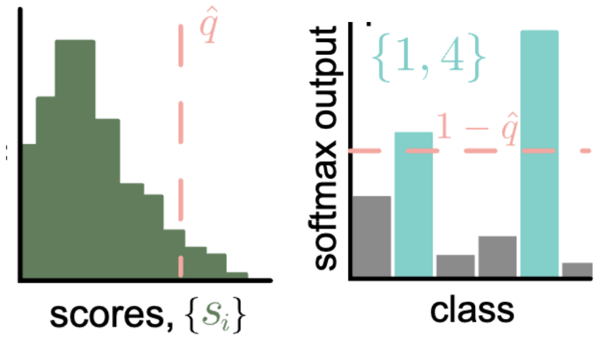
1. Identify a heuristic uncertainty using the pre-trained model
2. Define the **score function** $s(x, y) \in \mathbb{R}$
3. Compute $\hat{q}$ as the $\frac{\lceil (n+1)(1-\alpha) \rceil}{n}$ quantile of the calibration scores



$$s_1, s_2, \dots, s_n := s(X_1, Y_1), s(X_2, Y_2), \dots, s(X_n, Y_n)$$

4. Form the prediction sets of the new example X_{test} as

$$C(X_{\text{test}}) = \{y : s(X_{\text{test}}, y) \leq \hat{q}\}$$



Coverage Property

Suppose $(X_1, Y_1), \dots, (X_\mathrm{n}, Y_\mathrm{n})$ and $(X_\mathrm{test}, Y_\mathrm{test})$ are i.i.d and we define $\hat{q}$ as

$$\hat{q} = \inf\left\{q : \frac{|\{i : s(X_i, Y_i) \le q\}|}{n} \ge \frac{\lceil (n+1)(1-\alpha) \rceil}{n}\right\}$$

The prediction set $C(X) = \{\mathrm{y} : s(X, y) \le \hat{q}\}$ has a **valid marginal coverage**.

- WOLG, assume that the calibration scores are sorted: $s_1 < s_2 < \cdots < s_n$.
  1. If $\alpha < 1/(n+1)$, $\hat{q} = \infty$. Then, $C(X) = \mathcal{Y}$. **Valid!**
  2. If $\alpha \ge 1/(n+1)$, $\hat{q} = s_{\lceil (n+1)(1-\alpha) \rceil}$.
- Note that $\{Y_\mathrm{test} \in C(X_\mathrm{test})\} = \{s_\mathrm{test} \le \hat{q}\} = \{s_\mathrm{test} \le s_{\lceil (n+1)(1-\alpha) \rceil}\}$
- By exchangeability, $P(s_\mathrm{test} \le s_k) = k/(n+1)$.
- $P(s_\mathrm{test} \le s_{\lceil (n+1)(1-\alpha) \rceil}) = \lceil (n+1)(1-\alpha) \rceil/(n+1) \ge 1 - \alpha$.

Choice of Score Function

The **score function** $s(x, y) \in \mathbb{R}$ encodes *disagreement* between x and y. The larger the score $s(x, y)$, the worse the agreement between x and y.

Valid but useless ← bad — score s_i — good → *Reflect the uncertainty*

While the prediction set may provide a valid marginal coverage, the set can be useless if the score function is uninformative.

Adaptive Prediction Sets

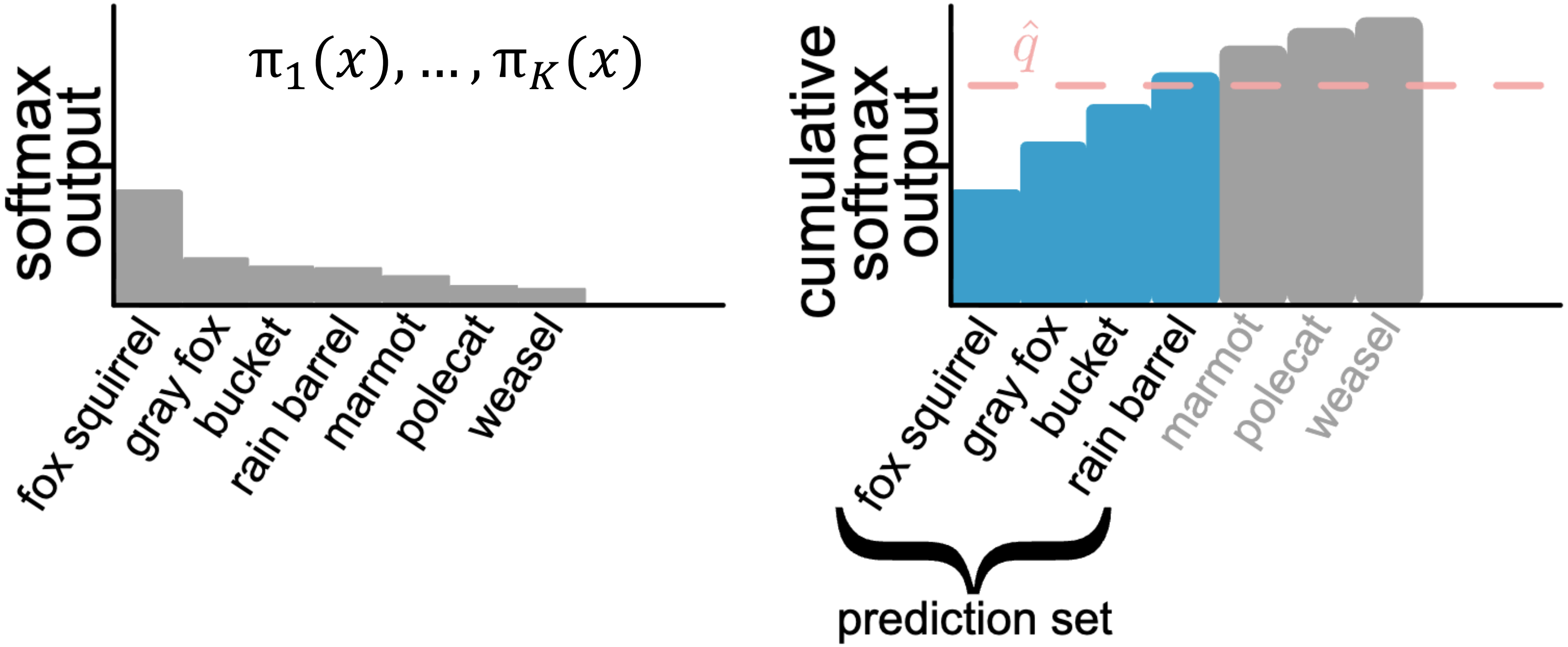
- Assume a predictive model $\hat{f}: \mathcal{X} \rightarrow \Delta(\mathcal{Y})$ where $\mathcal{Y} = \{1, \ldots, K\}$.
- Let $\pi_1(x), \ldots, \pi_K(x)$ be the permutation of $\{1, \ldots, K\}$ that sorts $\hat{f}(x)$ from most likely to least likely.
- Then, we define a score function as

$$s(x, y) = \sum_{j=1}^{k} \hat{f}(x)_{\pi_j(x)}, \qquad \text{with} \quad y = \pi_k(x)$$

- Calculate the quantile $\hat{q} = \text{quantile}\left(s_1, \ldots, s_n; \frac{\lceil (n+1)(1-\alpha) \rceil}{n}\right)$ and form the set

$$C(x) = \{\pi_1(x), \ldots, \pi_k(x)\}, \qquad k = \sup\left\{k' : \sum_{j=1}^{k'} \hat{f}(x)_{\pi_j(x)} < \hat{q}\right\} + 1$$

Adaptive Prediction Sets



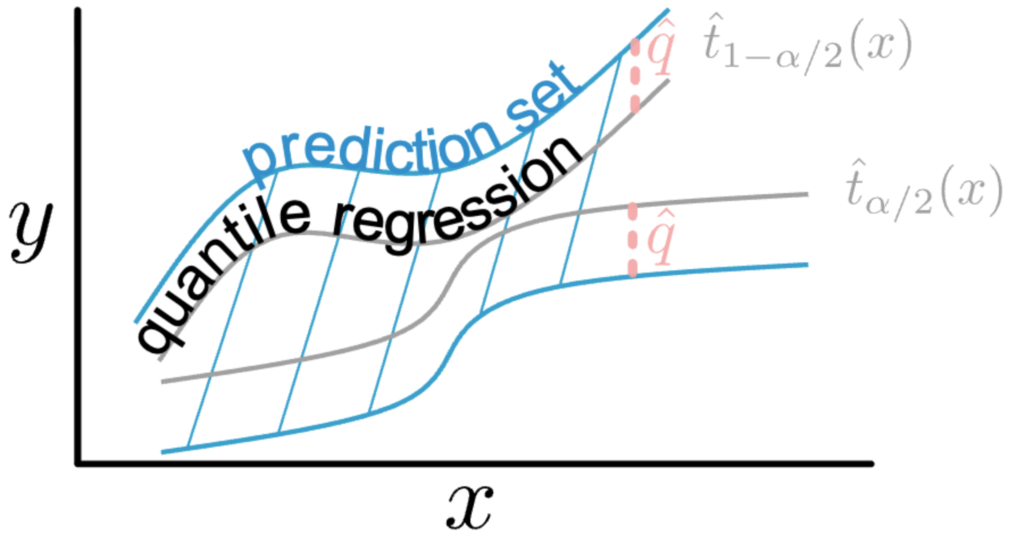
Conformalized Quantile Regression

- **Quantile regression:** learn the γ quantile t_γ of $Y_{\text{text}} \mid X_{\text{text}} = x$
- The quantile $[\hat{t}_{0.05}(x), \hat{t}_{0.95}(x)]$ has approximately 90% coverage.

$$s(x, y) = \max\{\hat{t}_{\alpha/2}(x) - y, y - \hat{t}_{1-\alpha/2}(x)\}$$

$$C(x) = [\hat{t}_{\alpha/2}(x) - \hat{q}, \hat{t}_{1-\alpha/2}(x) + \hat{q}]$$

$$\hat{q} = \text{Quantile}\left(s_1, \ldots, s_n; \frac{\lceil (n+1)(1-\alpha) \rceil}{n}\right)$$



Conformalized Uncertainty Estimates

Given some **point prediction** $\hat{f}(x)$ and some **uncertainty scalar** $u(x)$, we can provide a conformal guarantee:

- **Standard deviation** $\widehat{\sigma}(x)$: We can assume that

  $$Y_{\text{test}} \mid X_{\text{test}} = x \sim N(\mu(x), \sigma(x))$$

  with models $\hat{f}(x)$ and $\widehat{\sigma}(x)$. Conformal prediction gives $\hat{f}(x) \pm \hat{q}\widehat{\sigma}(x)$.

- **Magnitude of the residual** $\hat{r}(x)$: After fitting a model $\hat{f}$, we fit a second model $\hat{r}$ that predicts $\left|y - \hat{f}(x)\right|$.

$$s(x, y) = \frac{\left|y - \hat{f}(x)\right|}{u(x)}, \qquad C(x) = \left[\hat{f}(x) - u(x)\hat{q}, \hat{f}(x) + u(x)\hat{q}\right]$$

Example

Given a trained probabilistic classifier and a calibration set, compute a prediction set $C(x) \subseteq \{\mathrm{A}, \mathrm{B}, \mathrm{C}\}$ for a new input x_{test}, using split conformal in the multiclass classification setting.

- For a new x_{test}, the classifier outputs:
  - $\hat{p}(\mathrm{A} \mid x_{\text{test}}) = 0.50$
  - $\hat{p}(\mathrm{B} \mid x_{\text{test}}) = 0.35$
  - $\hat{p}(\mathrm{C} \mid x_{\text{test}}) = 0.15$

- We want 90% marginal coverage, so $\alpha = 0.1$.

i	True y_i	$\hat{p}(\mathrm{y}_i \vert x_i)$
1	A	0.80
2	B	0.55
3	C	0.60
4	A	0.40
5	B	0.70
6	C	0.30
7	A	0.90
8	B	0.20
9	C	0.45
10	A	0.65

Example

- Define the non-conformity score as

$$s(x, y) = 1 - \hat{p}(y \mid x)$$

- Let $n = 10$. Then, compute the index

$$k = \lceil (n+1)(1-\alpha) \rceil$$

- Sort $s_1, \ldots, s_{10}$ increasingly and set the threshold $\tau = s_{(k)}$ (the *k*-th smallest)
- For each label $y \in \{A, B, C\}$, compute $s(x_{test}, y)$ and include y in the set if $s(x_{test}, y) \leq \tau$.

i	**True** y_i	$\hat{p}(y_i \mid x_i)$	s_i
1	A	0.80	
2	B	0.55	
3	C	0.60	
4	A	0.40	
5	B	0.70	
6	C	0.30	
7	A	0.90	
8	B	0.20	
9	C	0.45	
10	A	0.65	

Adaptivity

The procedure should return large sets for harder inputs and smaller sets for easier inputs.

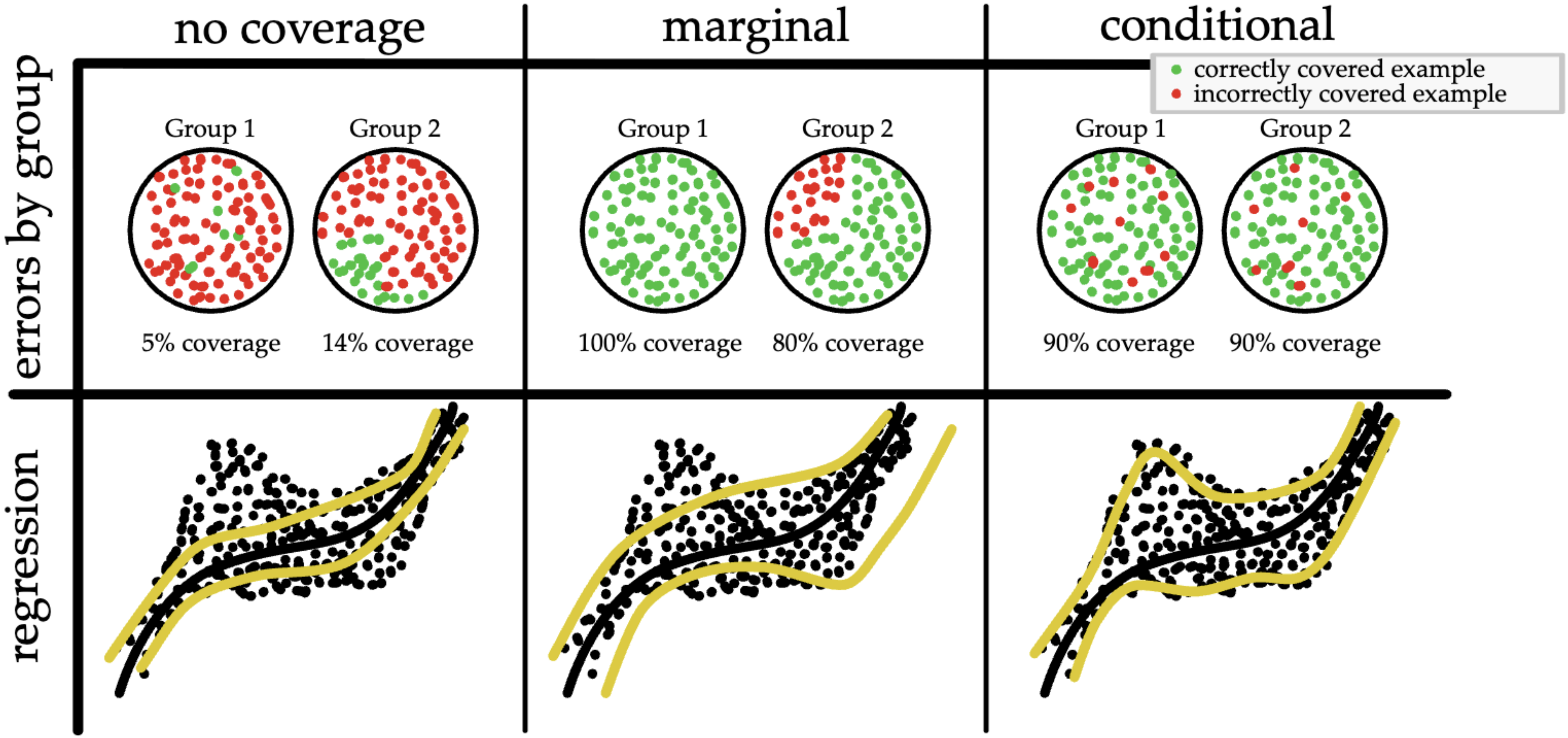
Conditional Coverage

- The **conditional coverage** property:

$$P(Y_{\text{test}} \in C(X_{\text{test}}) \mid X_{\text{test}}) \geq 1 - \alpha$$

- **Interpretation**: *for every value of the input X_{test}, we seek to return prediction sets with $1 - \alpha$ coverage*.
  - If we have two groups, A and B, comprising 90% and 10% of the population, conditional coverage requires that the prediction sets cover Y with at least 90% probability within each group.
- This is a stronger property than the *marginal coverage* property and is *impossible* to achieve in general.

Conditional Coverage



Extensions

- Group-balanced conformal prediction:

$$P(Y_{\text{test}} \in C(X_{\text{test}}) \mid X_{\text{test},1} = g) \geq 1 - \alpha, \qquad \forall g \in \{1, \dots, G\}$$

- Class-conditional conformal prediction:

$$P(Y_{\text{test}} \in C(X_{\text{test}}) \mid Y_{\text{test}} = y) \geq 1 - \alpha, \qquad \forall y \in \{1, \dots, K\}$$

- Conformal risk control:

$$\mathbb{E}[\ell(C(X_{\text{test}}), Y_{\text{test}})] \leq \alpha, \qquad \forall y \in \{1, \dots, K\}$$

- Conformal prediction under distribution shift

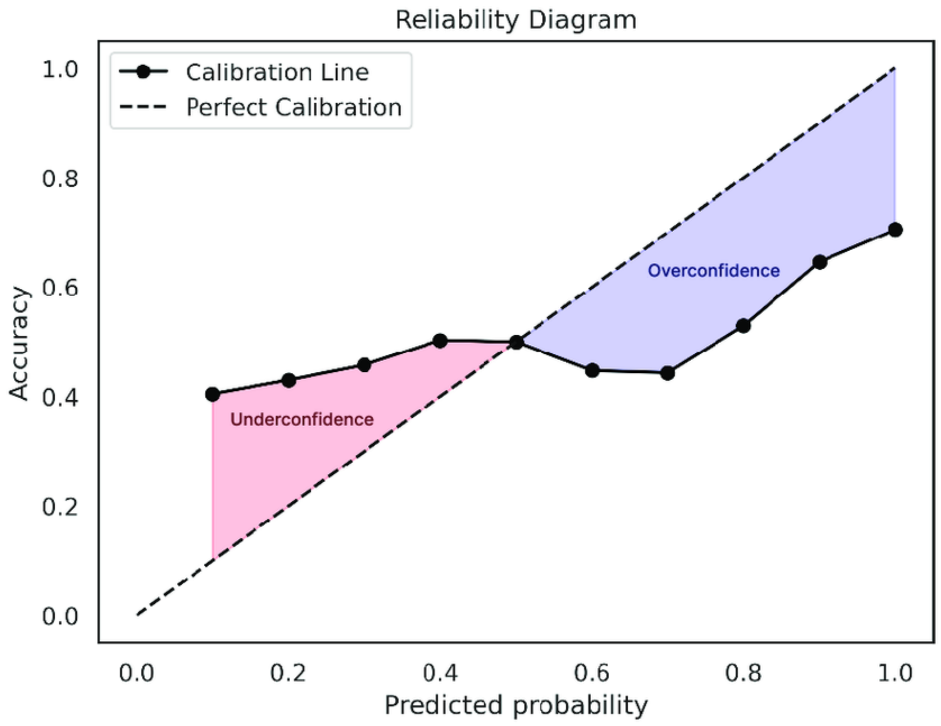
Probabilistic Calibration

Probabilistic Calibration

- Calibration ensures **honesty** in probability estimates overall.
- A probabilistic predictor $\hat{f}$ is *calibrated* if predicted probabilities match empirical frequencies:

$$P\left[Y = 1 \mid \hat{f}(x) = \rho\right] = \rho, \quad \forall \rho \in [0,1]$$

- **Interpretation**: *Among all instances predicted with probability ρ, about ρ fraction of them should be positive.*
- Violations indicate **systematic misrepresentation** of uncertainty.

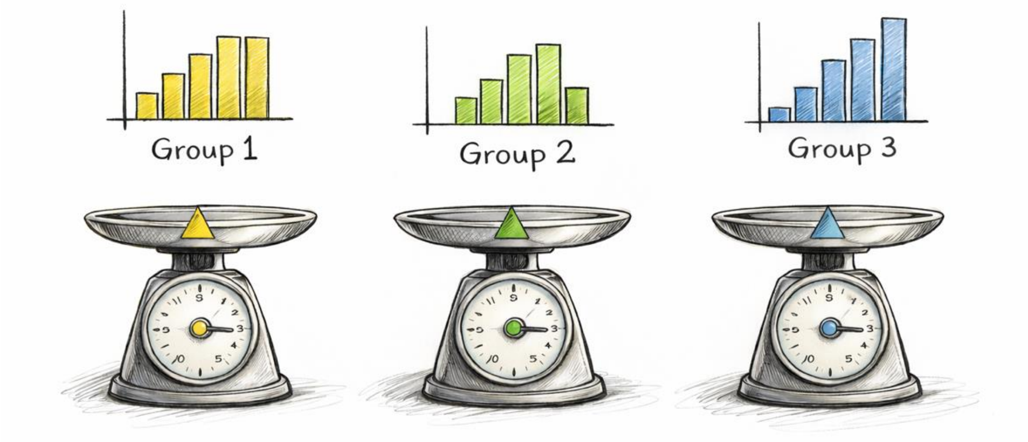


Multi-Calibration

- A predictor is *multi-calibrated* if it is calibrated **simultaneously** across many subpopulations:

$$P\left[Y = 1 \mid \hat{f}(x) = \rho, G = g\right] = \rho, \qquad \forall \rho \in [0,1], \forall g \in \{1, \dots, K\}$$

- Calibration holds not only overall, but for *every relevant group*.



Applications

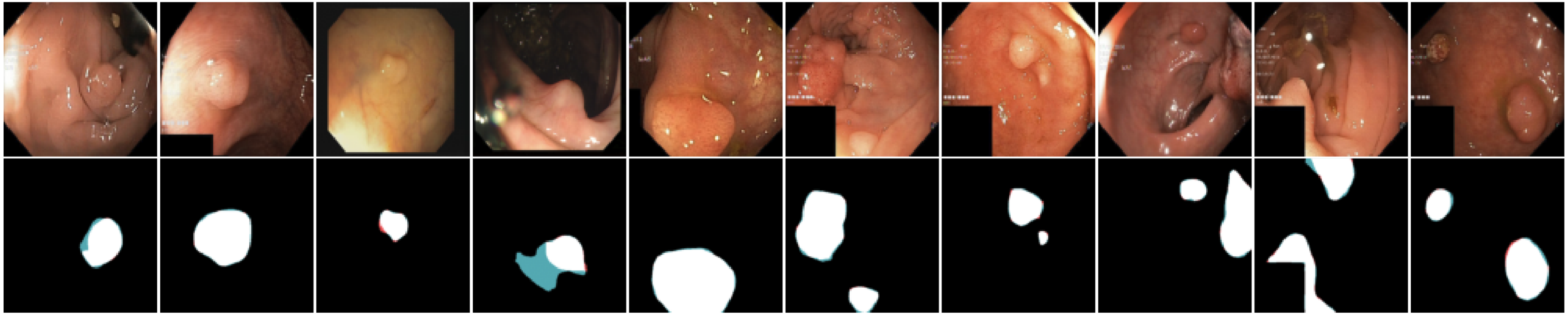
Multilabel Classification

The model's output is thresholded to get the subset of K classes, $C_\lambda(x) = \{y : \hat{f}(x) \geq \lambda\}$. The conformal risk control is used to pick the threshold λ certifying a low false negative rate (FNR).

Red = false negatives, Blue = false positives, Black = true positives

Tumor Segmentation

The model's output is thresholded to get the predicted binary mask, $C_\lambda(x) = \{(i,j) : \hat{f}(x)_{(i,j)} \geq \lambda\}$. The conformal risk control is used to pick the threshold λ certifying a low false negative rate (FNR).



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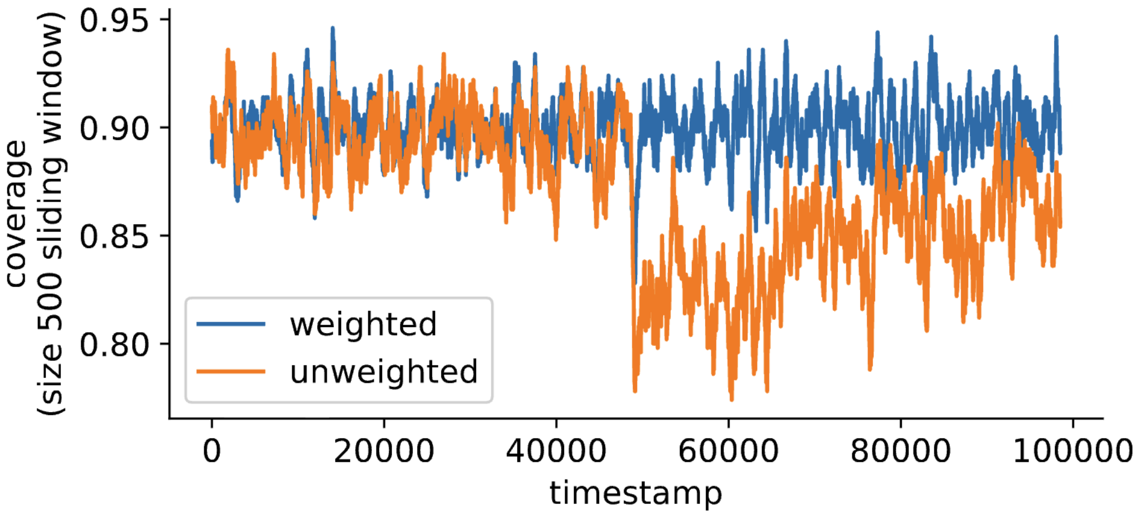
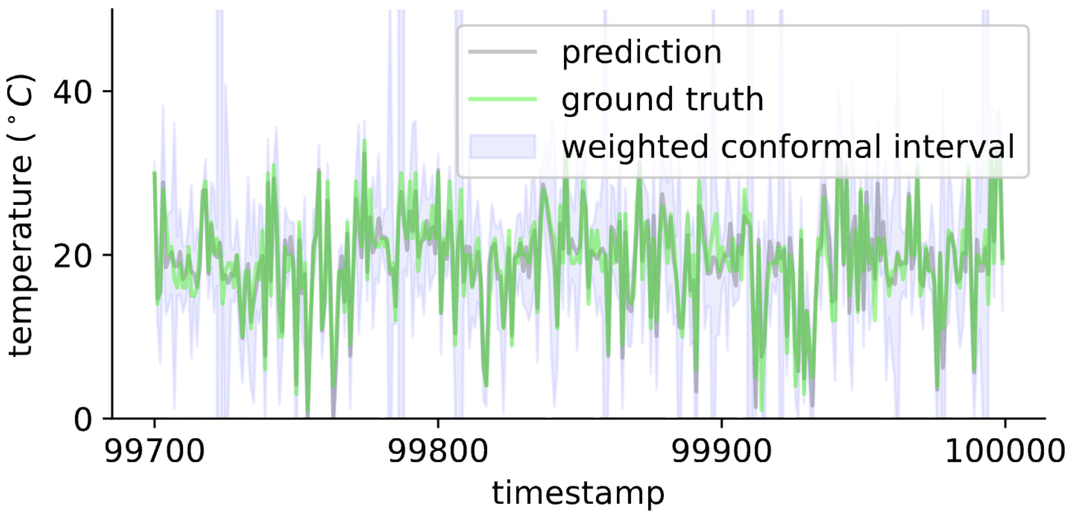
Weather Prediction with Time-Series

We seek to predict the temperature of different locations on Earth given covariates such as the latitude, longitude, altitude, atmospheric pressure, and so on.





Exchangeability is violated!

Recommended Reading

- Anastasios N. Angelopoulos and Stephen Bates. **A Gentle Introduction to Conformal Prediction and Distribution-Free Uncertainty Quantification**. arXiv:2107.07511 (2022).

Exercise

Given a trained probabilistic classifier and a calibration set, compute a conformal prediction set $C(x) \subseteq \{A, B, C\}$ for a new input x, using split conformal in the multiclass classification setting.

- For a new x_{test}, the classifier outputs:
  - $\hat{p}(A \mid x_{\text{test}}) = 0.40$
  - $\hat{p}(B \mid x_{\text{test}}) = 0.25$
  - $\hat{p}(C \mid x_{\text{test}}) = 0.35$
- We want 80% marginal coverage.

i	True y_i	$\hat{p}(y_i \mid \boldsymbol{x}_i)$
1	A	0.80
2	B	0.55
3	C	0.60
4	A	0.40
5	B	0.70
6	C	0.30
7	A	0.90
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