Uncertainty Quantification with Split Conformal Prediction

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Motivation

- Machine learning appears to be able to solve most problems
- However we don't know how certain we are about the predictions we make
- Can we do this?

The Goal

- Given any supervised machine learning algorithm that maps paired training examples to a function:

$$(X_1, Y_1), \ldots, (X_n, Y_n) \mapsto \hat{f}_{1:n} \tag{1}$$

- For a new data point X_{n+1}, we would like to construct a 95% "confidence set" for Y_{n+1}
- This is a (random) set $C(X_{n+1})$ where we have that

$$\mathbb{P}(Y_{n+1} \in C(X_{n+1})) = 0.95$$

- Without any assumptions on our learning algorithm, or underlying model this seems impossible!

Motivation: Ranks of Random Variables

- Consider some i.i.d. real valued random variables $Z_1, \ldots, Z_{n+1}$
- What is the probability that Z_{n+1} is the k-th largest?
- By symmetry (exchangeability), all the orderings are equally likely
- Therefore:

$$\mathbb{P}(\mathrm{Rank}(Z_{n+1}) = k) = \frac{1}{n+1} \tag{2}$$

- This holds regardless of the distribution of Z_i!

A Note on Exchangeability

- Actually, we didn't need the i.i.d. assumption
- We only need exchangeability for any permutation π:

$$(Z_1, \ldots, Z_{n+1}) \stackrel{d}{=} (Z_{\pi(1)}, \ldots, Z_{\pi(n+1)})$$

- This is much weaker than i.i.d.
- Example: Drawing without replacement from an urn
  - Not independent (draws affect future probabilities)
  - But exchangeable (order doesn't matter)

Building Confidence Intervals from Ranks

- If we have $n + 1$ exchangeable random variables, we know their ranks are uniform
- Key insight: We can use this to build confidence intervals!
- For a $(1 - \alpha)$ confidence interval:
  - We want Z_{n+1} to be between the $\lceil \frac{\alpha}{2}(n+1) \rceil$-th and $\lfloor (1 - \frac{\alpha}{2})(n+1) \rfloor$-th order statistics
- Example: With n = 99 calibration points and $\alpha = 0.05$
  - Lower bound: 3rd smallest value
  - Upper bound: 97th smallest value
  - Probability new point falls in this interval $= 1 - \alpha = 0.95$
- This works regardless of the underlying distribution!

Building Exchangeable Variables

- Let's apply this to machine learning predictions by trying to build some exchangeable random variables - let's look at regression first.
- We split our training pairs into "pure training data" $\mathcal{I}_1$ and "conformal calibrating data" $\mathcal{I}_2$
- Let's train out model on $\mathcal{I}_1$ to get $\hat{f}(x)$
  and then we can evaluate our model on $\mathcal{I}_2$ to generate

$$R_i = |\hat{f}(X_i) - Y_i| \text{ for } (X_i, Y_i) \in \mathcal{I}_2$$

- These R_i are now exchangeable!!! So we can build a confidence interval for our next prediction using the ranking technique as before.

The Split Conformal Prediction Algorithm

- For a new point X_{n+1}, compute $R_{n+1}(y) = |\hat{f}(X_{n+1}) - y|$ for candidate values y
- Our confidence set $C(X_{n+1})$ is all values of y where $R_{n+1}(y)$ is "not too large" compared to the calibration scores
- Specifically: $y \in C(X_{n+1})$ if $R_{n+1}(y)$ is smaller than the $\lceil (1-\alpha)(n+1) \rceil$-th largest calibration score
- This gives us valid $(1-\alpha)$ coverage by the rank arguments above!