Uncertainty Quantification with Split Conformal Prediction

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Edinburgh AI Society Advanced Workshop

November 4, 2024

Motivation

- Machine learning appears hugely effective across many different problems
- However we don't know how certain we are about the predictions we make
  - A self-driving car needs to know when it's uncertain about an object
  - Medical diagnosis systems must express uncertainty in critical decisions
- Deep learning is notorious for being overly confident[1][2]
- Can we quantify uncertainty with minimal assumptions?

[1] Guo et al. "On Calibration of Modern Neural Networks"

[2] Begoli et al. "The need for uncertainty quantification in machine-assisted medical decision making"

What is a Confidence Interval?

- Informally a confidence interval is an interval which is expected to typically contain the parameter being estimated.
- The confidence level (e.g. 95%) tells us how often the interval contains the true value
- If we repeat the experiment many times, 95% of the intervals will contain the true value
- A wider interval gives you more "confidence" but gives you less precision about the location of the parameter

The Goal

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

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

- 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!

The Classical MLE Approach

- If we know the underlying distribution family, we can use Maximum Likelihood Estimation
- For example, with linear regression we assume:

$$Y = X\beta + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2)$$

- The MLE gives us asymptotically valid confidence intervals:

$$\hat{Y} \pm z_{1-\alpha/2}\hat{\sigma}$$

- But what if our distributional assumptions are wrong?
  - Non-normal errors
  - Non constant variance
  - Model misspecification

No Asymptotic Results Needed!

These results also need infinite amounts of data for the confidence interval to be valid

To Infinity and Beyond!

We can do better!

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:

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

- 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:

$$(Z_1, \dots, Z_{n+1}) \overset{d}{=} (Z_{\pi(1)}, \dots, Z_{\pi(n+1)})$$

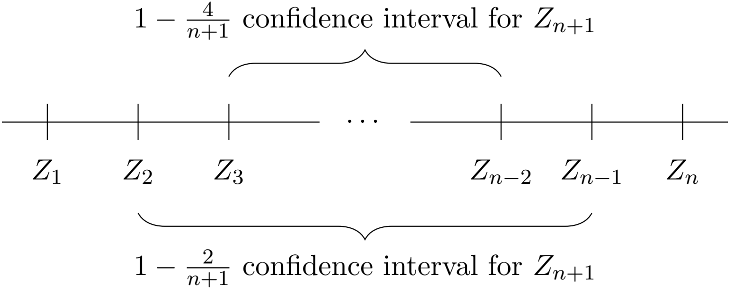
- This is much weaker than i.i.d.
- Example: Drawing without replacement from an urn
  - Not independent (draws affect future probabilities)
  - But exchangeable (order doesn't matter)

Building Confidence Intervals from Ranks

- If we have $n+1$ exchangeable random variables, we know their ranks are uniform
- 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
- This works regardless of the underlying distribution!

Visualizing the Interval

- Assuming the variables are ordered as $Z_1, Z_2, \ldots, Z_n$ we can visualise this as.



$1 - \frac{4}{n+1}$ confidence interval for Z_{n+1}

Z_1 Z_2 Z_3 $\ldots$ Z_{n-2} Z_{n-1} Z_n

$1 - \frac{2}{n+1}$ confidence interval for Z_{n+1}

An 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 gives us a concrete way to build prediction intervals!
- And we still maintain our distribution-free guarantee

Building Exchangeable Variables

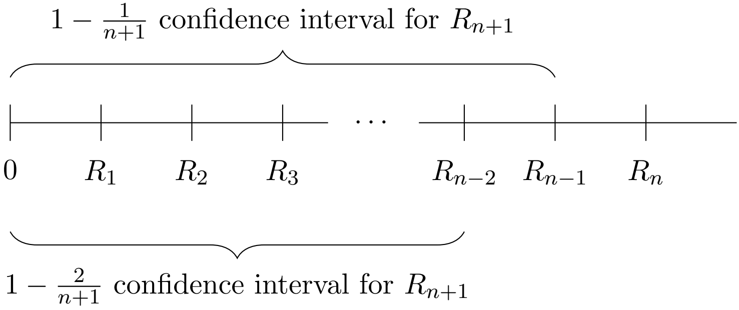
- Let's apply this to machine learning predictions by trying to build some exchangeable random variables - let's look at regression first.
- We split our training pairs into "pure training data" $\mathcal{I}_1$ and "conformal calibrating data" $\mathcal{I}_2$
- Let's train our model on $\mathcal{I}_1$ 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.

Visualizing the Residuals

- We know that the residuals must be positive so we only need to worry about one side of the interval.
- Assuming the residuals are ordered as $0, R_1, R_2, \ldots, R_n$ we can visualise this as.



$1 - \frac{1}{n+1}$ confidence interval for R_{n+1}

0 R_1 R_2 R_3 $\cdots$ R_{n-2} R_{n-1} R_n

$1 - \frac{2}{n+1}$ confidence interval for R_{n+1}

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!

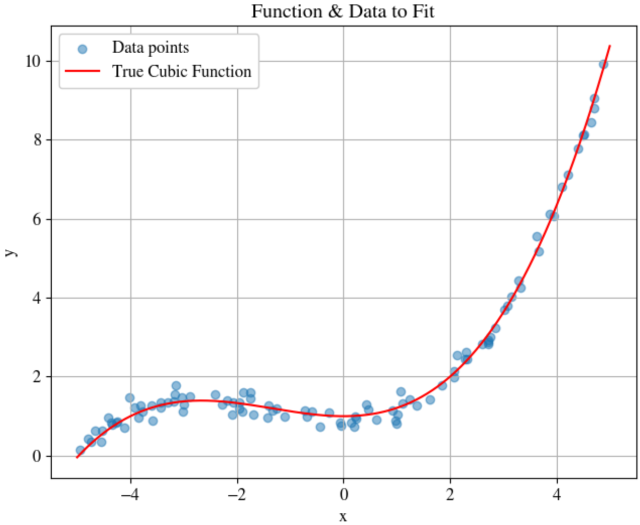
A Toy Example

- Let’s run a synthetic experiment to demonstrate conformal prediction
- We’ll generate data from:
  - X drawn from Uniform(-5, 5)
  - Y follows a cubic relationship with noise:

$$Y = 1 + \frac{1}{6}X^2 + \frac{1}{24}X^3 + \epsilon$$

  where $\epsilon \sim \mathcal{N}(0, 0.2)$
- This gives us ground truth to test drive our prediction intervals

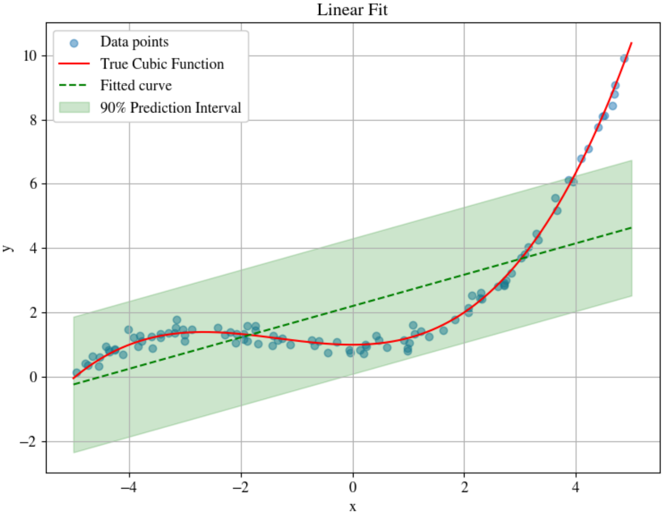
Visualizing the Data



Linear Model with Conformal Intervals

- Let's fit a linear model to this data - deliberately underfit!
- We should see that our conformal confidence interval gives a reasonably large interval
- The green region shows the 90% prediction interval
- Notice how:
  - The intervals are valid despite model misspecification
  - The intervals are very wide - we can't predict well so have high uncertainty

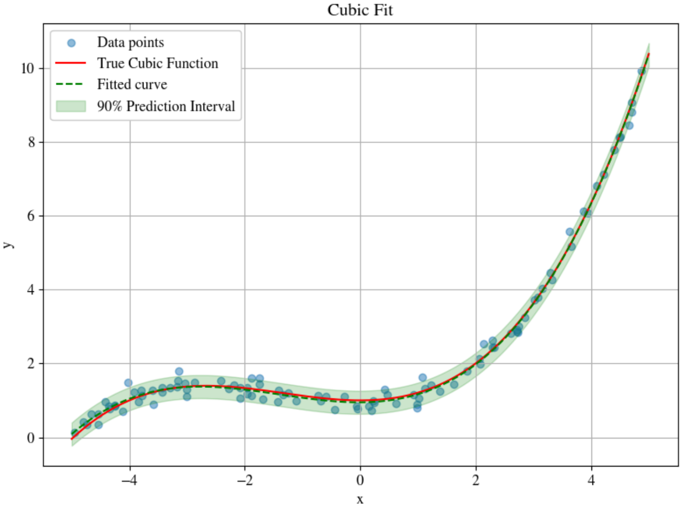
Linear Fit with Conformal Intervals



Linear Model with Conformal Intervals

- Let's now fit a cubic model to this data - this should give a much better fit
- We should see a small prediction interval

Cubic Fit with Conformal Intervals



Confidence Interval Size vs Model Complexity

Polynomial Degree	CI Width (lower is better)
0 (Constant)	5.03
1 (Linear)	3.82
2 (Quadratic)	2.40
3 (Cubic)	0.552
4 (Quartic)	0.583
5 (Quintic)	0.601

- Notice how the confidence interval width:
  - Decreases as we move from underfitting (degree 0) to good fit (degree 3)
  - Starts increasing again with higher degrees due to overfitting
- This shows that we can indeed use this to do model selection!

Code

All of the conformal prediction was 9 lines of code!

```
def get_conformal_predictor(x, y, degree=3):
    x_train, x_calib, y_train, y_calib = train_test_split(
        x, y, test_size=0.5, random_state=42
    )

    coeffs = np.polyfit(x_train, y_train, degree)

    y_pred_calib = np.polyval(coeffs, x_calib)
    residuals = np.abs(y_calib - y_pred_calib)

    def confinterval(x_new, alpha=0.9):
        y_pred = np.polyval(coeffs, x_new)
        q = np.quantile(residuals, alpha)
        return y_pred - q, y_pred + q

    return coeffs, confinterval
```

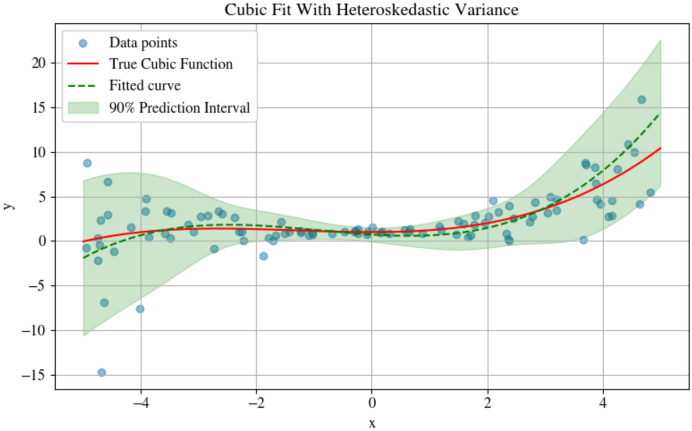
What's Next?

- We can generalise our R_is to be measures of a general "conformity score" $V(x,y)$ and then
$$R_i = V(X_i, Y_i) \left(= |\hat{f}(X_i) - Y_i| \text{ in this talk}\right)$$
- All of our results still hold - there is nothing special about the absolute value. We can use this to build x adaptive predictive intervals (this is called Locally-Weighted Conformal Inference)[3].
- Full Conformal Regression
- Leave one covariate out (LOCO) Conformal Regression

[3] Lei et al. "Distribution-Free Predictive Inference For Regression"

Locally Adaptive Conformal Inference

Setup is the same as before, however now the noise (ϵ) has non constant variance.


Cubic Fit With Heteroskedastic Variance
Data points
True Cubic Function
Fitted curve
90% Prediction Interval
y
x