Adaptive Conformal Inference

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3/8/2023

Summary

With the increased prevalence of less-interpretable models like machine learning algorithms, the importance of distribution-free tools to quantify the prediction uncertainty has increased (especially since these classes of models are less explicit in what drives their predictions and where they might go wrong).

One of the most popular approaches to address this problem is conformal inference. Conformal inference allows us to measure the predictive power of otherwise non-transparent models by calculating a “conformity score” on model generated predictions and their observed counterparts. However, conformal inference relies quite heavily on exchangeability assumptions, which are often not met in real world applications, in particular settings that are heavily time dependent.

In response, Gibbs and Candès (I. Gibbs and E. Cand`es, “Adaptive conformal inference under distribution shift,” arXiv:2106.00170, 2021.) devise a new method: adaptive conformal inference (ACI). ACI works to measure predictive power of models in settings without exchangeability in which data is revealed incrementally, by adjusting the procedure based on the coverage rate in each time step.

They show that given a long enough time, ACI meets target coverage without additional assumptions in situations where standard conformal inference fails. Additionally they show that given small distribution assumptions, ACI is robust for most time steps.

The authors test their new procedure on two datasets, election predictions and stock price predictors. In both cases they confirm their theoretical results, ACI maintained approximately 90% coverage while conformal inference failed, often dramatically.

We seek to extend ACI for use on batch data, and test empirically the effects of allowing varying quantile and score functions.

Intuitive Explanation

The goal of conformal inference is to produce a confidence interval for a new prediction. (The authors’ equivalent formulation: determine if some value y is a “reasonable” estimate.) In essence, we are looking at where some percentage of the most “unusual” predictions have fallen so far, and stating that outside of that interval, the same percentage of future predictions should be similarly unusual. The split conformal inference process is to: (a) fit some “conformity score” on a subset of the data (“training set”) that characterizes how well each model prediction matches the corresponding actual value, (b) calculate conformity scores on the rest of the data (“holdout” or “calibration set”), (c) find the $(1-\alpha)^{th}$ quantile of the calibration conformity scores, and (d) infer the prediction interval as the range in which $S(X_{t+1}, y) \leq \hat{Q}(1-\alpha)$.

When new data points are generated from the same process, our quantile will still contain each new point's conformity score with the same probability. However, if new data points are generated from a different process – a distribution shift – then their conformity scores may be more or less likely to fall within our quantile. This paper suggests that we can account for this fact and maintain the same probability of coverage in the long term by updating our quantile cutoff based on whether or not we cover each new prediction.

The paper suggests making this update by decreasing our quantile by $\gamma\alpha$ if we covered the last prediction or increasing it by $\gamma(1-\alpha)$ if we do not, using some heuristically- or empirically-selected step size γ. Note that for low alpha, we increase our quantile cutoff much more quickly when we fail to cover than we decrease it when we do cover (for example, for $\alpha = 0.05, \gamma(1-0.05) = 0.95\gamma >> \gamma(0.05)$). This makes sense because, with correct $\alpha = 0.05$ coverage, we expect to cover 95% of the time and miss 5% of the time – so our adjustments in each direction should be weighted to reflect that a miss is more "surprising" than a cover.

This "adaptive conformal inference" procedure allows us to ensure that in the long run, we will achieve our targeted coverage frequency. Even in the short run, the local coverage rate will stay relatively close to the target as long as the distribution doesn't shift too drastically.

Main Theoretical Results

The authors define their adaptive conformal inference procedure as an online update to the quantile cutoff in the setting in which the true value Y_t is revealed after each prediction y. Specifically, the authors point out that there is a value α_t^* such that the miscoverage rate of the prediction set up to t is α when we use $1-\alpha_t^*$ as our quantile cutoff. The authors propose the following procedure to estimate α_t^* at each time step (with the estimate called α_t, initialized to α in their experiments):

$$\mathrm{err}_t := \begin{cases} 1 & \text{if } Y_t \notin \hat{C}_t(\alpha_t), \\ 0 & \text{otherwise} \end{cases}$$

where

$$\hat{C}_t(\alpha_t) := y : S_t(X_t, y) \leq \hat{Q}_t(1 - alpha_t)$$

Then, fixing a step size parameter $\gamma > 0$ we consider the simple online update

$$\alpha_{t+1} := \alpha_t + \gamma(\alpha - \mathrm{err}_t).$$

Substituting err_t into $1-\alpha_{t+1}$, this procedure sets the $t+1$ quantile cutoff as:
$1-\alpha_{t+1} = 1-(\alpha_t + \gamma(\alpha-1)) = 1-\alpha_t + \gamma(1-\alpha)$ when we fail to cover and
$1-\alpha_{t+1} = 1-(\alpha_t + \gamma(\alpha-0)) = 1-\alpha_t - \gamma\alpha$ when we do cover.

A higher step size γ makes the method more adaptive to distribution shifts but also can make local coverage more variable; lower γ makes the method less adaptive ($\gamma = 0$ is equivalent to standard split conformal inference) but moves more towards conditional coverage with respect to time. The authors do not propose a theory-based means of selecting γ (they do note that the optimal alpha is proportional to the square root of a quantification of distribution shift, but this is unobserved so is unhelpful in practice). However, they say that $\gamma = 0.005$ empirically worked well with their datasets.

The authors also note that the procedure can be easily modified to give some weight to previous coverage/noncoverage events in updating α_t, essentially adding some momentum to the update. Specifically:

$$\alpha_{t+1} = \alpha_t + \gamma(\alpha - \sum_{s=1}^{t} w_s \text{err}_s)$$

where weights are ∈ $[0, 1]$ and sum to 1. (Obviously, $w_t = 1$ is equivalent to the unweighted method.) However, the authors say that though weighting may somewhat smooth local coverage, in their experiments it produces similar results to unweighted updates.

The authors note that this adaptive inference procedure works for any choice of quantile and score functions (assuming those functions are definitionally valid, e.g. the quantile function must be nondecreasing). However, they also acknowledge that the procedure's performance is sensitive to quality of conformity scores. In particular, the closer to stationary the conformity score (despite shifts in the data distribution), the closer the procedure will stay to target coverage.

The authors do not spend much time addressing the choice of initial α_0, but it seems clear that $\alpha_0 = \alpha$ should be the best choice in the absence of any prior beliefs about the magnitude and direction of distribution shift.

The authors prove two main performance guarantees for the procedure. First, they show that over a long time interval, adaptive conformal inference converges on the targeted coverage frequency without any distributional assumptions:

$$\lim_{T\to\infty} \frac{1}{T} \sum_{t=1}^{T} \text{err}_t \overset{a.s.}{=} \alpha.$$

Then, they show that for a sufficiently small distribution shift (and appropriate initialization of α_1), the marginal coverage rate will stay close to 1-α in expectation. Specifically, the authors prove this result in the case in which the data originates from distributions associated with the states of a hidden Markov chain with a stationary distribution. The authors acknowledge that this model may not directly apply to the real world, but argue that the results are a good approximation of the procedure's behavior in many real-world settings.

(To analyze this claim a bit: Two cases in which this model would not be applicable are when the data distribution shifts seasonally or with a continual trend, as the corresponding Markov process would be periodic or contain infinite transient states, respectively, and so would have no stationary distribution. But note that these cases are where the data distribution has a trend or is seasonal; trend or seasonality in X and y is fine as long as their joint distribution remains the same. Also, predictable distribution shift could be handled in the long run by adding a time variable to X. A more problematic case is that of the infinite null recurrent Markov chain, eg a number line random walk.)

This second performance guarantee also requires a few other assumptions: that an initialization period has passed such that the Markov process has reached its stationary distribution, and that the quantile and score functions are fixed in time. The latter assumption is potentially rather limiting as this is not how the procedure would typically be implemented; in practice we would want to retrain the functions as we get additional data.

The actual result shown by the authors is the following:

$$E[(M(\alpha_t|A_t)-\alpha)^2] \leq \frac{L(1+\gamma)}{\gamma}E[|\alpha^*_{A_{t+1}}-\alpha^*_{A_t}|]+\frac{L}{2}\gamma$$

where M is the realized miscoverage rate, A indicates the hidden state of the underlying Markov model, and L is a positive constant such that

$$|M(\alpha_2|a)-M(\alpha_1|b)| \leq L|\alpha_2-\alpha_1|$$

for any α_1, α_2 and any Markov state a in the chain. (The authors also prove an intermediate result showing that the miscoverage rate's distance from α is bounded over sufficiently long time periods.) The left-hand side of the inequality result is the expected Euclidean distance between marginal misclassification rate and α. Since γ is typically small, the right-hand-side of the inequality will be small, bounding the misclassification rate near α. The right-hand-side expectation quantifies the distribution shift, showing that the distance between marginal coverage and alpha is bounded more tightly when the distribution shift is small.

Limitations

Gibbs and Candès point out three limitations with their method. First, their method is devised with the assumption that data is revealed in an online manner: the true value of each time step is revealed before prediction of the next time step. While this assumption is met in some cases (like stock market data), there are many settings in which data is received in batches. On top of making it hard to evaluate settings where data is irregular over time, it prevents the evaluation scheme from distinguishing between “bad” prediction subsets and “good” ones merely by conditioning on time.

Another limitation of the more strict theoretical performance result is that the authors assume a fixed quantile function, $\hat{Q}(\cdot)$, predetermined without influence from new data. Gibbs and Candès prove that fitting $\hat{Q}_t(\cdot)$ in an online fashion to the most recent data similar to α_t will provide correct coverage given sufficiently large time intervals. However, the proof of short term bounds given good initialization of α_1 relies on a fixed $\hat{Q}(\cdot)$, limiting the theoretical performance of the fully online method. The online method was used in their following experiments, showing that it does have practical success. We further investigate this discrepancy below.

A third limitation of the procedure is that the authors specify no theoretical guidelines for choosing an effective γ. A proper choice of step size for the data is extremely important, as too large values of γ induce volatility in the coverage produced at each step α_t. In their experiments they settle on a choice of $\gamma = 0.005$, but acknowledge that this has no guarantee of success in other applications.

A limitation not mentioned by the authors comes from common procedures to reduce the computational complexity of conformal inference methods. One such procedure is to limit the calculation of the prediction set to the interval observed in the data. In standard conformal inference, this simplification is guaranteed to not adjust the coverage by much for large n, as:

$$\hat{C}'(X_{n+1}) = \hat{C}(X_{n+1}) \cap \text{range}_{1\leq i\leq n}(Y_i)$$

$$P(Y_{n+1} \in \hat{C}'(X_{n+1})) \geq P(Y_{n+1} \in \hat{C}'(X_{n+1}) - P(Y_{n+1} \notin \text{range}_{1\leq i\leq n}(Y_i) \geq 1-\alpha-\frac{2}{n+1} \text{ by exchangeability}$$

But since

1. ACI does not assume exchangeability for all $(Y_1, \ldots, Y_{n+1})$, and
2. ACI calculates $\hat{C}_t(\cdot)$ in an online fashion, making the bound dependent on time even if exchangeability was met

ACI may not be able to make a similar time saving procedure, hampering practical performance unless some assumptions are conceded.

Extension: Batched Procedure

As pointed out previously, one limitation of the procedure is that it is unable to handle data received in delayed batches, and may mistreat data in cases without data collectable on uniform time increments.

An intuitive extension to ACI that may work better in these cases is a procedure that updates α based on coverage rate in chunks (either defined by intervals of discrete time or regularly spaced batches of data). Consider the following procedure:

Given data (X_{s_i}, Y_{s_i}) in discrete chunks enumerated (X_s, Y_s). Assume for each data point s_i we are given a fitted score function $S_{s_i}(\cdot)$ and a corresponding quantile function $\hat{Q}_{s_i}(\cdot)$. Then, in similar fashion to the old procedure define the realized miscoverage rate of the prediction set $\hat{C}_{s_i}(\alpha_s) := \{y : S_{s_i}(X_{s_i}, y) \leq \hat{Q}_{s_i}(1 - \alpha_s)\}$ as

$$M_s(\alpha_s) := P(S_s(X_s, Y_s) > \hat{Q}_s(1 - \alpha_s)).$$

Define the sequence α_s given a target α, fixing a step size parameters $\gamma > 0$ as:

$$\alpha_{s+1} := \alpha_s + \gamma(\alpha - \mathrm{err}_s).$$

for err_s:

$$\mathrm{err}_s := \frac{1}{\#\text{ i in s}} \sum_{i \in s} \mathbb{1}\{Y_{s_i} \notin \hat{C}_{s_i}(\alpha_s)\}$$

Intuitively what we are doing is rather than adjusting the value of α for every data point s_i, we are adjusting it per chunk of data s by the rate of coverage in that chunk.

An important note here regards the choice of γ for this procedure. A good rule of thumb is to select γ that is higher than the γ used in the original method by roughly a factor of the number of data points per time step, or slightly below. (Or, we could define the procedure such that each adjustment is proportional to the number of time steps in the relevant batch, which would be preferable for variable batch sizes but reduce flexibility for constant-size batches.) Otherwise, this procedure will adjust $alpha_t$ too slowly relative to the original procedure. The reason that we might select γ slightly lower than a simple multiple of original γ is that using the simple multiple, the batched procedure will adjust α_t by *more* than the online procedure, since the online procedure's updates will reduce as α_t approaches α_t^*.

A final note here: In the alternative setting in which we receive batches of data in which we *do* know the ordering of data in the batch, it is likely preferable to use the original online procedure in order to not "overshoot" α_t^* (though the online procedure is somewhat more computationally expensive).

Long term coverage for modified procedure

Following similar steps to the proof outlined for the standard ACI, we can get some long term coverage guarantee for our modified procedure. We will similarly assume that with probability one $\alpha_1 \in [0,1]$ and $\hat{Q}_{s_i}(\cdot)$ is non decreasing and is ∞ for inputs greater than one and $-\infty$ for inputs less than zero.

Lemma 4.1 adjusted: with probability one we have that $\forall s \in \mathbb{N}, \alpha_s \in [-\gamma, 1+\gamma]$.

Proof: assume towards a contradiction that with positive probability $\{\alpha_s\}_{s\in\mathbb{N}}$ is such that $\inf_s \alpha_s < -\gamma$ (the case where $\inf_s \alpha_s > 1+\gamma$ is identical). Note that $\sup_s |\alpha_{s+1} - \alpha_s| = \sup_s \gamma|\alpha - \text{err}_s| < \gamma$. Thus, with positive probability we may find $s \in \mathbb{N}$ such that $\alpha_s < 0$ and $\alpha_{s+1} < \alpha_s$. However,

$$\alpha_s < 0 \implies \hat{Q}_{s_i}(1-\alpha_s)\forall i \in s \implies \text{err}_s = 0 \implies \alpha_{s+1} = \alpha_s + \gamma(\alpha - \text{err}_s) \geq \alpha_s$$

and thus $P(\exists s \text{ such that } \alpha_{s+1} < \alpha_s < 0) = 0$, which is a contradiction.

Proposition 4.1 adjusted: with probability one we have that $\forall S \in \mathbb{N}$,

$$|\frac{1}{S}\sum_{s=1}^{S} \text{err}_s - \alpha| \leq \frac{\max\{\alpha_1, 1-\alpha_1\} + \gamma}{S\gamma}$$

which implies

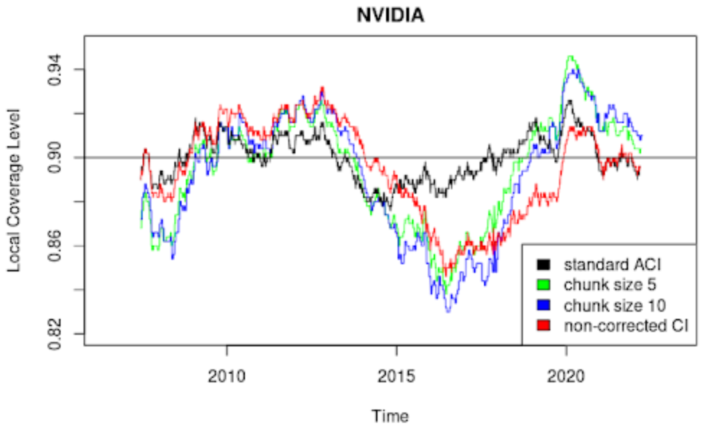
$$\lim_{S\to\infty} \frac{1}{S}\sum_{s=1}^{S} \text{err}_s \overset{a.s.}{=} \alpha$$

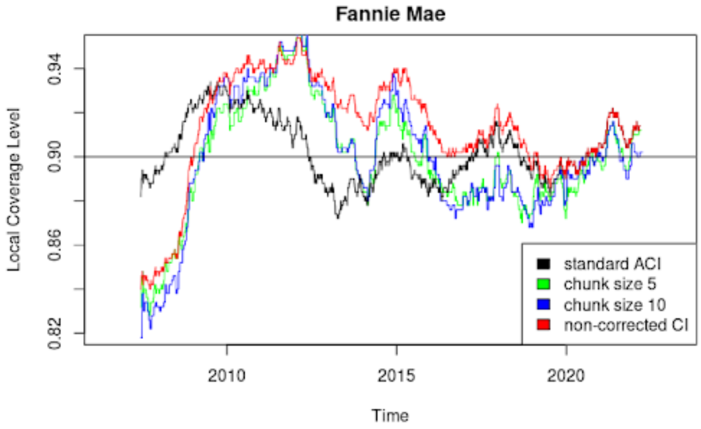
Proof: expanding the recursion for α_s and applying lemma 4.1 adjusted in the same way as for the original method yields the result, since the recursion for α_s and α_t share the same structure.

Thus our modified procedure has a similar agnostic guarantee of correct long-term coverage frequency as standard ACI.

Modified procedure in practice

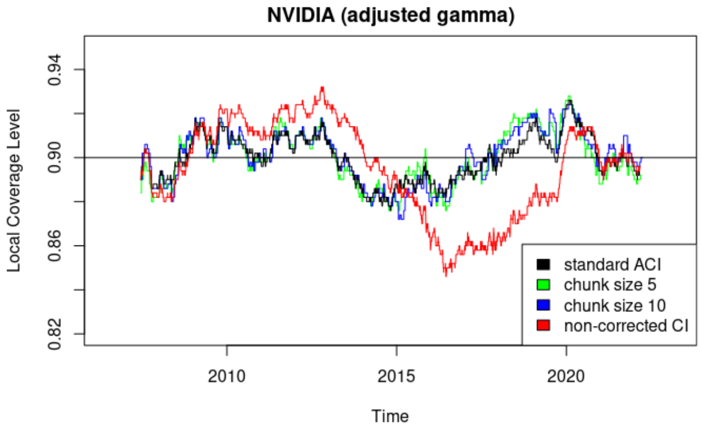
To get a quick comparison between the standard method and the modified one we ran the modified procedure on the same data set as those run for the standard procedure (NVIDIA and Fannie Mae stock data), with a target coverage level of 90%. To do this, we simply grouped the otherwise perfectly distributed data into specified chunk sizes for our two runs of the modified procedure. For some details on the author's code, see the caveat in the next section.

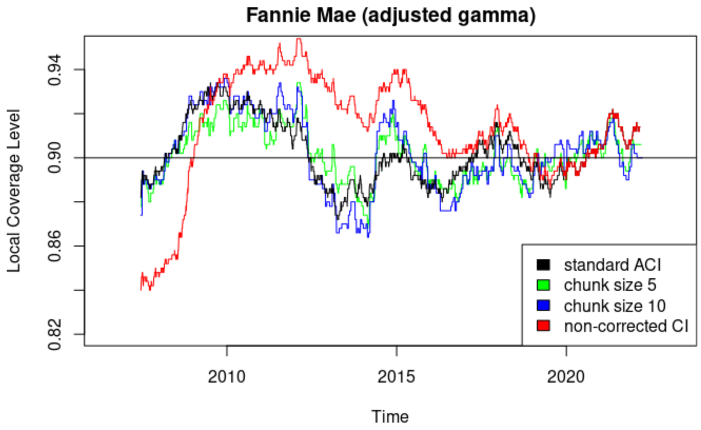




We do see less robustness with changes to time than standard ACI, but this is to be expected, as we have less effective time to converge to good values of alpha, and less points in time to adjust to shifts in the underlying distribution, however the effect is too large for this to be the only cause. A possible cause for this effect is that in taking large batches of data, we are effectively increasing the pressure that our small choice of γ has on the data. If the modified and standard ACI procedures choose the same γ, in the time interval of the batch the standard procedure will update with γ many times, where as the modified procedure will only update once.

If we correct our choice of γ to be scaled by the time size of the batch, we get results that are similarly robust to changes in time as standard ACI, confirming our hypothesis.





This reinforces how important appropriate γ selection is practice of both the modified and standard methods.

Experiment: How Applicable is the Fixed-QS Setting?

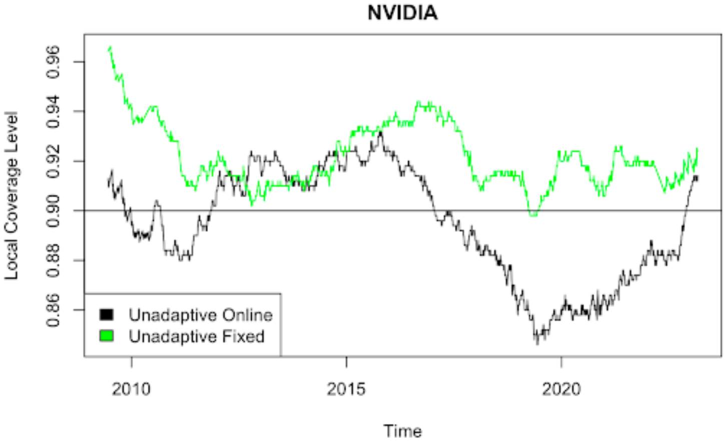
Intuitively, we might expect varying-QS to perform better than fixed-QS in a distribution-shifting setting, both because this provides a larger amount of training/calibration data and because it essentially adjusts S and Q in addition to α_t in response to distribution shift. On the other hand, it is possible that the approach used by the authors in their experiments – refitting S and Q on the previous `lookback` data points at each time step (they use `lookback=1250` in their stock analysis) – is subject to overfitting issues due to the reuse of the same data for score training and quantile calibration.

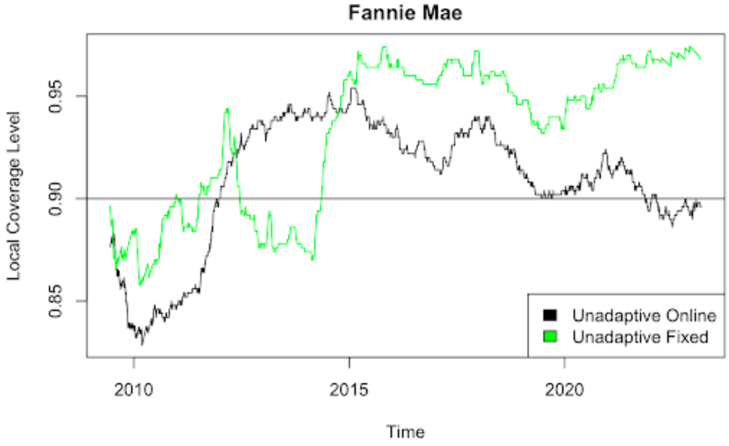
As the authors allude to, it's difficult to obtain analytical results for varying-QS performance. So, we used the same stock-volatility example as the authors to explore the differences in results between fixed-QS and varying-QS approaches.

Specifically, we replicate the authors' experimental results shown in Figure 1 for NVIDIA and Fannie Mae, then repeat the same analysis but using $S(\cdot)$ trained on the first 1250 data points and $Q(\cdot)$ calibrated on the subsequent 1250 data points. We compare ACI local coverage rate, ACI α_t values, and fixed-α local coverage rate for each QS approach.

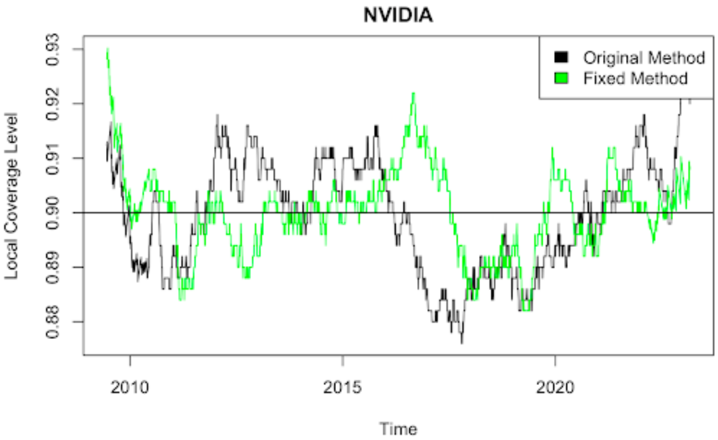
A quick caveat: While the authors provide some R code to replicate Figure 1, there are a few minor details about their implementation that are unclear from the code or the paper. Specifically, it is unclear if their starting $t = 1$ is the first day of 2005, or 1250 days before that (their initial training/calibration period), and it's not specified how they handle the calculation of local coverage within 250 time steps of the edges of their predictions. We chose to take $t = 1$ as 1250 days before 2005 (ie July 2, 2001) and padded errors with NaNs. Based on these choices, our results may differ slightly from the authors', but an inspection of our local coverage plots confirms that we largely replicate their output for both NVIDIA and Fannie Mae. (Note: Our for-comparison Bernoulli sequence does differ from the authors' for obvious reasons.)

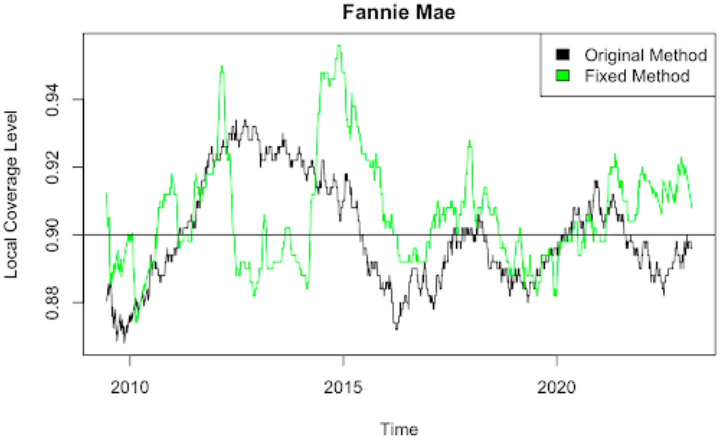
Using a non-adaptive approach (ie fixed α), varying-QS ("unadaptive online") seems to clearly outperform fixed-QS ("unadaptive fixed"). This supports the idea that re-training Q and S on recent data points partially accounts for distribution shift (and in this case, that effect outweighs possible overfitting effects).





Moving to ACI, varying-QS ("original method") performs similarly to fixed-QS ("fixed method") for the NVIDIA dataset, but shows significantly more variability in local coverage for Fannie Mae. This is related to the fact that Fannie Mae's fixed-QS α_t is much more variable than its varying-QS α_t. An interesting situation arises for Fannie Mae post-2015: α_t is significantly elevated in the fixed-QS method, but local coverage is similar for both methods. Both of these observations again point to the fact that varying Q and S dampen the need for variation in α_t, allowing α_t to remain near α over time with variation to help account for rapid shifts.


NVIDIA
■ Original Method
🟩 Fixed Method
Local Coverage Level
0.88
0.89
0.90
0.91
0.92
0.93
2010
2015
2020
Time


Fannie Mae
■ Original Method
🟩 Fixed Method
Local Coverage Level
0.88
0.90
0.92
0.94
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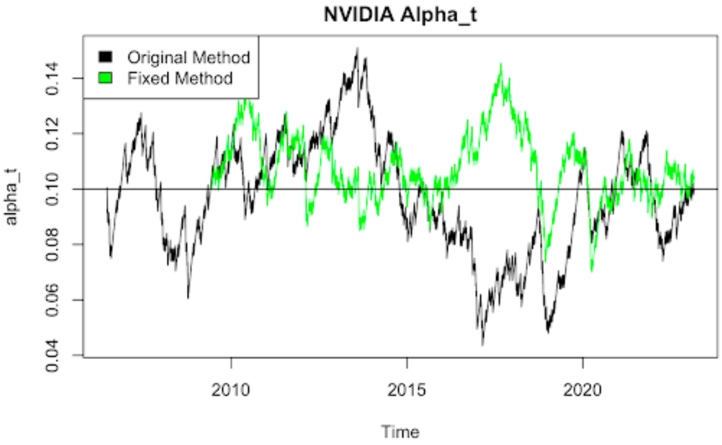
NVIDIA Alpha_t
■ Original Method
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alpha_t
0.04
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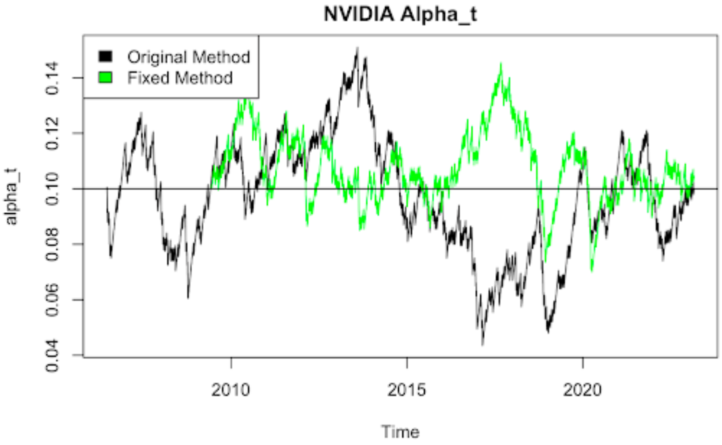
NVIDIA Alpha_t
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Of course, this experiment's external validity is very limited: it's possible that differences we observe are unique to these datasets. Still, these results do support the intuition that the performance guarantee for ACI under fixed-QS would hold under varying-QS. On the other hand, they don't provide any strong evidence for better performance. One hypothesis emerging from this experiment is that the local performance guarantee proof's setting (a smaller distribution shift with fixed-QS) may be equivalent to a larger-distribution-shift setting with varying-QS for the purposes of the proof, since retraining Q and S dampens the effective distribution shift faced by α_t.

Possible Other Extensions

We mention here but do not implement a number of other possible extensions to the paper:

- It would be useful to experiment, possibly via simulation, with the method's performance under different forms of nonstationarity. Similar to the fixed-QS analysis above, this could provide support for or against the broader applicability of the local performance guarantee.
- The weighted method proposed by the authors could be better analyzed, both theoretically and over a broad range of weights (extending to uniform weights). The authors say that they found it to be similar in performance to the unweighted method, but only mention testing it with a quite rapid decrease in weight going back in time.
- On a related note, it would be valuable to evaluate other methods of adding momentum to α_t updates. For example, if we have missed coverage quite a few times recently, we guess that we are in the midst of a distribution shift and so accelerate quantile widening by even more. Specifically, we could apply momentum implementations similar to those often used in gradient descent. This would make sense in light of the online-learning view of the α_t updates (although, unlike in many other gradient-descent settings, α_t optimization must be convex). The weighting proposed by the authors achieves this to a significant degree (in fact, they call the weighting "momentum" in their code!) but is not directly equivalent to several other momentum approaches.
- The authors apply ACI to prediction of the next time step, but it could be extended in a straightforward manner to prediction intervals for longer forecast horizons, which would be updated each time step as well.
- Finally, it would be interesting to explore the use of ACI in a setting where the prediction model is moving between different environments (as opposed to the environment changing over time).

Conclusion

As proposed by Gibbs and Candès, adaptive conformal inference is a powerful extension of conformal inference for the online setting; despite some limitations in its performance guarantees, it appears to perform quite well in practice. ACI provides a solid platform for additional experimentation and extension.

Code & Additional Figures

https://github.com/ajkeller10/multiple-testing-final-project (https://github.com/ajkeller10/multiple-testing-final-project)