Conformal prediction beyond exchangeability

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Abstract

Conformal prediction is a popular, modern technique for providing valid predictive inference for arbitrary machine learning models. Its validity relies on the assumptions of exchangeability of the data, and symmetry of the given model fitting algorithm as a function of the data. However, exchangeability is often violated when predictive models are deployed in practice. For example, if the data distribution drifts over time, then the data points are no longer exchangeable; moreover, in such settings, we might want to use an algorithm that treats recent observations as more relevant, which would violate the assumption that data points are treated symmetrically. This paper proposes new methodology to deal with both aspects: we use weighted quantiles to introduce robustness against distribution drift, and design a new technique to allow for algorithms that do not treat data points symmetrically. Our algorithms are provably robust, with substantially less loss of coverage when exchangeability is violated due to distribution drift or other challenging features of real data, while also achieving the same coverage guarantees as existing conformal prediction methods if the data points are in fact exchangeable. Finally, we demonstrate the practical utility of these new tools with simulations and real-data experiments.

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1 Introduction

The field of conformal prediction solves a challenging modern problem: given a "black box" algorithm that fits a predictive model to available training data, how can we calibrate prediction intervals around the output of the model, which are guaranteed to achieve some desired coverage level?

As an example, consider a holdout set method. Suppose we are given a pre-fitted model $\widehat{\mu}$ mapping features X to a predicted value of Y (e.g., the output of some machine learning algorithm trained on a prior data set), and a fresh holdout set of data $(X_1, Y_1), \ldots, (X_n, Y_n)$ not used for training. We can then use the empirical quantiles of the errors $|Y_i - \widehat{\mu}(X_i)|$ on the holdout set, to compute a prediction interval around our new prediction $\widehat{\mu}(X_{n+1})$ that aims to cover the unseen response Y_{n+1} . Split conformal prediction [Vovk et al., 2005] formalizes this method, with guaranteed predictive coverage when the data points (X_i, Y_i) are drawn i.i.d. from any distribution (see Section 2). However, the validity of this method relies heavily on the assumption that the data points are drawn from the same distribution, or more generally, that $(X_1, Y_1), \ldots, (X_{n+1}, Y_{n+1})$ are exchangeable.

In many applied domains, however, this assumption is often substantially violated—for example, due to distribution drift, correlations between data points, or other challenges. As an example, Figure 1 shows results from an experiment on a real data set monitoring electricity usage in Australia (the ELEC2 data set [Harries, 1999], which we will return to in Section 6.2).

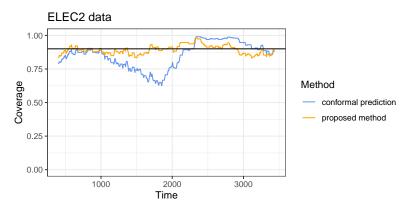


Figure 1: Experiment results from a real data set (details will be given in Section 6.2).

We see that over a substantial stretch of time, the prediction intervals constructed via conformal prediction lose coverage, decreasing far below the target 90% coverage level, while our proposed method, non-exchangeable conformal prediction, is able to maintain approximately the desired coverage level. In this paper, we will see how to quantify the loss of coverage due to violations of exchangeability, and how we can modify the conformal prediction methodology to regain predictive coverage even in the presence of distribution drift or other violations of exchangeability.

1.1 Beyond exchangeability

In Section 2, we will review three important classes of methods for distribution-free prediction: split conformal, full conformal, and the jackknife+. These methods all rely on exchangeability in two different ways:

- The data $Z_i = (X_i, Y_i)$ are assumed to be exchangeable (for example, i.i.d.).
- The algorithm \mathcal{A} , mapping data sets to fitted models $\widehat{\mu}$, is assumed to treat the data points symmetrically, to ensure that exchangeability of the Z_i 's still holds even after we observe the fitted model(s).

In this paper, we aim to provide distribution-free prediction guarantees in settings where we cannot rely on either of these assumptions:

- We may have data points Z_i that are not exchangeable—for instance, they may be independent but non-identically distributed (e.g., due to distribution drift), or there may be dependence among them that creates non-exchangeability (e.g., correlation over time).
- We may wish to use an algorithm \mathcal{A} that does not treat input data points symmetrically—for example, if we would like to predict Y_{n+1} at time n+1 based on past data $(X_1, Y_1), \ldots, (X_n, Y_n)$ that was gathered at times $i = 1, \ldots, n$, we may prefer to fit a model $\widehat{\mu}$ that places higher weights on more recent data points, and lower weights on data points in the distant past.

1.2 Our contributions

In this work, we modify the split conformal, full conformal, and jackknife+ methods to allow for both of these sources of non-exchangeability. Our goal will be to provide coverage guarantees that are identical to existing guarantees if the data points are in fact exchangeable, and only slightly lower under deviations from exchangeability. Specifically, we will bound the *coverage gap*, which is the loss in coverage compared to what one could achieve under exchangeability—for example, for split conformal prediction,

Coverage gap =
$$(1 - \alpha) - \mathbb{P}\left\{Y_{n+1} \in \widehat{C}_n(X_{n+1})\right\}$$

since, under exchangeability, the method guarantees coverage with probability $1 - \alpha$. To give an informal preview of our results, write

$$Z = ((X_1, Y_1), \dots, (X_{n+1}, Y_{n+1}))$$
(1)

to denote the full (training and test) data set, and let Z^i denote this same data set after swapping the test point (X_{n+1}, Y_{n+1}) with the *i*-th training point (X_i, Y_i) :

$$Z^{i} = ((X_{1}, Y_{1}), \dots, (X_{i-1}, Y_{i-1}), (X_{n+1}, Y_{n+1}), (X_{i+1}, Y_{i+1}), \dots, (X_{n}, Y_{n}), (X_{i}, Y_{i})).$$
(2)

To enable robustness, our methods will use weights $w_i \in [0,1]$, where w_i is a prespecified weight placed on data point i (with higher weights indicating greater "trust" that data point (X_i, Y_i) is drawn from the same or approximately the same distribution as the test point (X_{n+1}, Y_{n+1}) . We will see that the coverage gap can be bounded as

Coverage gap
$$\leq \frac{\sum_{i=1}^{n} w_i \cdot \mathsf{d}_{\mathsf{TV}}(Z, Z^i)}{1 + \sum_{i=1}^{n} w_i}$$
. (3)

Note that the above result does not make any assumption on the joint distribution of the n+1 points—but, of course, the result will be meaningful only if this upper bound is small.

Several further remarks are in order. First, $w_i \equiv 1$ reduces to the usual unweighted definitions of the corresponding methods. Thus, the above result also quantifies the degradation in performance of standard conformal methods in non-exchangeable settings. Second, this result also has new implications in exchangeable settings: if the data points are in fact exchangeable (including i.i.d. as a special case), then $Z \stackrel{d}{=} Z^i$ and the coverage gap bound (3) is equal to zero. Thus, our use of a weighted residual distribution does not hurt coverage if the data are exchangeable. Finally, the result provides insights on why one might prefer to use our new weighted procedures in (possibly) non-exchangeable settings: it can provide robustness in the case of distribution shift. To elaborate, consider a setting where the data points $Z_i = (X_i, Y_i)$ are independent, but are not identically distributed due to distribution drift. The following result relates $d_{TV}(Z, Z^i)$ to the distributions of the individual data points:

Lemma 1. If Z_1, \ldots, Z_{n+1} are independent, then

$$\mathsf{d_{TV}}(Z,Z^i) \leq 2\mathsf{d_{TV}}(Z_i,Z_{n+1}) - \mathsf{d_{TV}}(Z_i,Z_{n+1})^2 \leq 2\mathsf{d_{TV}}(Z_i,Z_{n+1}).$$

Combining this lemma with the bound (3), we can see that if we place small weights w_i on any data points Z_i with large total variation distance $d_{TV}(Z_i, Z_{n+1})$, then the coverage gap will be low. For example, under distribution drift, we might have $d_{TV}(Z_i, Z_{n+1})$ decreasing with i; we can achieve a low coverage gap by using, say, weights $w_i = \rho^{n+1-i}$ for some $\rho < 1$. We will return to this example in Section 5.2.

We will also see that the result given in (3) actually stems from a stronger result:

Coverage gap
$$\leq \frac{\sum_{i=1}^{n} w_i \cdot \mathsf{d}_{\mathsf{TV}}(R(Z), R(Z^i))}{1 + \sum_{i=1}^{n} w_i}.$$
 (4)

Here R(Z) denotes residuals: for split conformal prediction, this is the vector with entries $R(Z)_i = |Y_i - \widehat{\mu}(X_i)|$, where $\widehat{\mu}$ is the pre-fitted model, while for full conformal the entries are again given by $R(Z)_i = |Y_i - \widehat{\mu}(X_i)|$ but now $\widehat{\mu}$ is the model obtained by running \mathcal{A} on the entire data set Z. $R(Z^i)$ is simply the same function applied to the swapped data set Z^i instead of Z—that is, the residuals are computed after swapping data points i and i and i and i are the data set. (The definition of i are jackknife+ is more technical and so we will return to this later.)

Clearly, this upper bound is strictly stronger than (3), since the total variation distance between any function applied to both Z and Z^i , cannot be larger than $d_{\text{TV}}(Z, Z^i)$ itself—and in practice, this new bound (4) may be substantially tighter. For example, if the data is high dimensional, with $Z_i = (X_i, Y_i) \in \mathbb{R}^p \times \mathbb{R}$ for large p, then the distance $d_{\text{TV}}(Z, Z^i)$ may be extremely large since Z and Z^i each contain p+1 dimensions of information about each data point. On the other hand, if we only observe the residuals (e.g., $R_i = |Y_i - \widehat{\mu}(X_i)|$ for each i), then this reveals only a one-dimensional summary of each data point, thus greatly reducing the distance between the two distributions, especially if the distribution drift occurs in features that happen to be irrelevant for prediction and are thus ignored by $\widehat{\mu}$. In Section 5.2, we will see a specific example demonstrating the potentially large gap between these two upper bounds.

2 Background and related work

We briefly review several distribution-free prediction algorithms that offer guarantees under an exchangeability assumption on the data. We also set up notation that will be useful later in the paper.

Split conformal prediction. Split conformal prediction [Vovk et al., 2005] (also called "inductive conformal prediction") is a holdout method for constructing prediction intervals around a pre-trained model. Specifically, given a model $\hat{\mu}: \mathcal{X} \to \mathbb{R}$ that was fitted on an initial training data set, and given n additional data points $(X_1, Y_1), \ldots, (X_n, Y_n)$ (the holdout set), we define residuals

$$R_i = |Y_i - \widehat{\mu}(X_i)|, \ i = 1, \dots, n,$$

and then compute the prediction interval at the new feature vector X_{n+1} as

$$\widehat{C}_n(X_{n+1}) = \widehat{\mu}(X_{n+1}) \pm (\text{the } \lceil (1-\alpha)(n+1) \rceil \text{-st smallest value of } R_1, \dots, R_n).$$

Equivalently, we can write

$$\widehat{C}_n(X_{n+1}) = \widehat{\mu}(X_{n+1}) \pm Q_{1-\alpha} \left(\sum_{i=1}^n \frac{1}{n+1} \cdot \delta_{R_i} + \frac{1}{n+1} \cdot \delta_{+\infty} \right), \tag{5}$$

where $Q_{\tau}(\cdot)$ denotes the τ -quantile of a distribution, and δ_x denotes the point mass at x. This method is well known to guarantee distribution-free predictive coverage at the target level $1 - \alpha$, as we recall below.

Theorem 1a (Split conformal prediction [Vovk et al., 2005]). If the data points $(X_1, Y_1), \ldots, (X_n, Y_n), (X_{n+1}, Y_{n+1})$ are i.i.d. (or more generally, exchangeable), then the split conformal prediction interval defined in (5) satisfies

$$\mathbb{P}\left\{Y_{n+1} \in \widehat{C}_n(X_{n+1})\right\} \ge 1 - \alpha.$$

One drawback of the split conformal method is the loss of accuracy due to sample splitting—in practice, if only n labeled data points are available in total, we might use n/2 data points for training $\hat{\mu}$, and then the procedure defined in (5) above would actually be run with a holdout set of size n/2 in place of n. (In this paper, however, we will continue to write n to denote the holdout set size for the split conformal method, in order to allow for universal notation across different methods.)

Full conformal prediction. To avoid the cost of data splitting, an alternative is the full conformal method [Vovk et al., 2005] (also referred to as "transductive conformal prediction"). Fix any regression algorithm

$$\mathcal{A}: \cup_{n>0} (\mathcal{X} \times \mathbb{R})^n \to \{\text{Measurable functions } \widehat{\mu}: \mathcal{X} \to \mathbb{R} \},$$

which maps a data set containing any number of pairs (X_i, Y_i) , to a fitted regression function $\widehat{\mu}$. \mathcal{A} is required to treat data points symmetrically, i.e.,¹

$$\mathcal{A}((x_{\pi(1)}, y_{\pi(1)}), \dots, (x_{\pi(n)}, y_{\pi(n)})) = \mathcal{A}((x_1, y_1), \dots, (x_n, y_n))$$
(6)

for all $n \geq 1$, all permutations π on $[n] := \{1, \ldots, n\}$, and all $\{(x_i, y_i)\}_{i=1,\ldots,n}$. Next, for each $y \in \mathbb{R}$, let

$$\widehat{\mu}^y = \mathcal{A}((X_1, Y_1), \dots, (X_n, Y_n), (X_{n+1}, y))$$

denote the trained model, fitted to the training data together with a hypothesized test point (X_{n+1}, y) , and let

$$R_i^y = \begin{cases} |Y_i - \widehat{\mu}^y(X_i)|, & i = 1, \dots, n, \\ |y - \widehat{\mu}^y(X_{n+1})|, & i = n + 1. \end{cases}$$
 (7)

The prediction set (which might or might not be an interval) for feature vector X_{n+1} is then defined as

$$\widehat{C}_n(X_{n+1}) = \left\{ y \in \mathbb{R} : R_{n+1}^y \le Q_{1-\alpha} \left(\sum_{i=1}^{n+1} \frac{1}{n+1} \cdot \delta_{R_i^y} \right) \right\}.$$
 (8)

The full conformal method is again well known to guarantee distribution-free predictive coverage at the target level $1 - \alpha$, as summarized below.

Theorem 1b (Full conformal prediction [Vovk et al., 2005]). If the data points $(X_1, Y_1), \ldots, (X_n, Y_n), (X_{n+1}, Y_{n+1})$ are i.i.d. (or more generally, exchangeable), and the algorithm \mathcal{A} treats the input data points symmetrically as in (6), then the full conformal prediction set defined in (8) satisfies

$$\mathbb{P}\left\{Y_{n+1} \in \widehat{C}_n(X_{n+1})\right\} \ge 1 - \alpha.$$

 $[\]overline{{}^{1}\text{If }\mathcal{A}}$ is a randomized algorithm, then this equality is only required to hold in distribution.

By avoiding data splitting, full conformal sometimes (but not always) yields more precise prediction intervals than split conformal. This potential benefit comes at a steep computational cost, since in order to compute the prediction set (8) we need to re-run the model training algorithm \mathcal{A} for each $y \in \mathbb{R}$ (or in practice, for each y in a very fine grid), aside from certain special cases such as linear regression, ridge regression [Burnaev and Vovk, 2014], or the Lasso [Lei, 2019], where the prediction set (8) can be computed more efficiently.

The jackknife+. The jackknife+ [Barber et al., 2021] (closely related to "cross-conformal prediction" [Vovk, 2015]) is an alternative method that offers a compromise between the computational and statistical costs of the previous two methods. For each i = 1, ..., n, define the *i*-th leave-one-out model as

$$\widehat{\mu}_{-i} = \mathcal{A}((X_1, Y_1), \dots, (X_{i-1}, Y_{i-1}), (X_{i+1}, Y_{i+1}), \dots, (X_n, Y_n)), \tag{9}$$

fitted to the training data with *i*-th point removed. Define also the *i*-th leave-one-out residual $R_i^{\text{LOO}} = |Y_i - \widehat{\mu}_{-i}(X_i)|$, which avoids overfitting since data point (X_i, Y_i) is not used for training $\widehat{\mu}_{-i}$. The jackknife+ prediction interval is then given by

$$\left[Q_{\alpha} \left(\sum_{i=1}^{n} \frac{1}{n+1} \cdot \delta_{\widehat{\mu}_{-i}(X_{n+1}) - R_{i}^{\text{LOO}}} + \frac{1}{n+1} \cdot \delta_{-\infty} \right), \right. \\
\left. Q_{1-\alpha} \left(\sum_{i=1}^{n} \frac{1}{n+1} \cdot \delta_{\widehat{\mu}_{-i}(X_{n+1}) + R_{i}^{\text{LOO}}} + \frac{1}{n+1} \cdot \delta_{+\infty} \right) \right]. \quad (10)$$

While in practice the jackknife+ generally provides coverage close to the target level $1 - \alpha$ (and provably so under a stability assumption on \mathcal{A}), its theoretical guarantee only ensures $1 - 2\alpha$ probability of coverage in the worst case:

Theorem 1c (Jackknife+ [Barber et al., 2021]). If $(X_1, Y_1), \ldots, (X_n, Y_n), (X_{n+1}, Y_{n+1})$ are i.i.d. (or more generally, exchangeable), and the algorithm \mathcal{A} treats the input data points symmetrically as in (6), then the jackknife+ prediction interval defined in (10) satisfies

$$\mathbb{P}\left\{Y_{n+1} \in \widehat{C}_n(X_{n+1})\right\} \ge 1 - 2\alpha.$$

While jackknife+ is generally much more computationally efficient than full conformal, fitting n leave-one-out models may still be infeasible for large n. An alternative is the CV+ method [Barber et al., 2021], which uses a K-fold cross-validation scheme in place of leave-one-out. For simplicity, we will not discuss CV+ in this present work, but we remark that our results can be fairly directly applied to CV+ as well.

For completeness, and to set up our proof strategy used in for the proofs of our new results, we provide succinct proofs of the above three theorems in Section 7.1 (for split conformal and full conformal) and Appendix D (for jackknife+).

General nonconformity scores. In the exchangeable setting, conformal prediction (both split and full) was initially proposed more generally in terms of "nonconformity scores" $\widehat{S}(X_i, Y_i)$, where \widehat{S} is a fitted function that measure the extent to which a data point (X_i, Y_i) is unusual relative to a training data set [Vovk et al., 2005]. For simplicity, so far we have only presented the most commonly used nonconformity score, which is the residual from the fitted model:

$$\widehat{S}(X_i, Y_i) := |Y_i - \widehat{\mu}(X_i)| \text{ where } \widehat{\mu} = \mathcal{A}((X_j, Y_j) : j \in [n]),$$

and will also define our new methods with this particular choice of score. In many settings, other nonconformity scores are more effective—for example, Romano et al. [2019], Kivaranovic et al. [2020] propose scores based on quantile regression. Our proposed non-exchangeable conformal prediction procedures can also be extended to allow for general nonconformity scores—we will return to this generalization in Appendix B.

Additional related work. Conformal prediction was pioneered by Vladimir Vovk and various collaborators in the early 2000s; the book by Vovk et al. [2005] details their advances and remains a critical resource. The recent spurt of interest in these ideas in the field of statistics was catalyzed by Jing Lei, Larry Wasserman, and colleagues (see, e.g., Lei et al. [2013], Lei and Wasserman [2014], Lei et al. [2018]). For a gentle introduction and more history, we refer to the tutorials by Shafer and Vovk [2008] and Angelopoulos and Bates [2021].

Tibshirani et al. [2019] also extended conformal prediction to a setting with non-exchangeable data. This work leverages a new concept called "weighted exchangeability" in order to handle covariate shift. Here is a simplified version of the setup: consider i.i.d. training data from one distribution and i.i.d. test data from a different distribution, where the training and test distributions differ in a structured manner — their marginal covariate distributions differ, but the conditional distributions of the responses given covariates is unchanged. By reweighting the data points to account for this change in distribution, coverage can be guaranteed via an argument based on weighted exchangeability. This assumes full knowledge of the change in distribution, in order to define the weights appropriately—for example, if X is distributed continuously under both the training and test distributions, then training data point (X_i, Y_i) is reweighted by $w_i = w(X_i) = \frac{f_{\text{test}}(X_i)}{f_{\text{train}}(X_i)}$, where f_{train} and f_{test} are the marginal densities of X under the training and test distributions, respectively. (In practice, of course, the ratio $\frac{f_{\text{test}}}{f_{\text{train}}}$ is not known exactly but instead must be estimated.)

The current work differs from Tibshirani et al. [2019] in many fundamental ways, such that neither work subsumes the other in its methodology or theory. In their work, the change in distribution must be known exactly, and the weights on the data points are then calculated as a function of the data point (X_i, Y_i) to compensate

for the known distribution shift; the difference in training and test distributions can be arbitrarily large, as long as we have oracle knowledge (or in practice, a good estimate) of $\frac{f_{\text{test}}}{f_{\text{train}}}$. In our present work, on the other hand, the weights are required to be fixed rather than data-dependent (although we will discuss some extensions later on in Section 5.3), and can compensate for unknown violations of the exchangeability assumption, as long as the violations are small (to ensure a low coverage gap). Moreover, our theory can handle non-symmetric algorithms that treat different datapoints differently, and in particular, can depend on their order. Our results can be interpreted in two ways: they propose a broader class of algorithms and weighting schemes to handle non-exchangeable data with explicit quantification of the potential loss of coverage due to this non-exchangeability, but they also imply a natural robustness of standard conformal methods to mild deviations from exchangeability.

Since its publication, the ideas and techniques from Tibshirani et al. [2019] have been applied and extended in several ways. For example, Podkopaev and Ramdas [2021] demonstrate that reweighting can also deal with *label shift* (the marginal label distribution changes from training to test, but the conditional distribution of the covariates given the labels is unchanged). Lei and Candès [2021a] show how reweighting can be extended to causal inference setups for predictive inference on individual treatment effects, and Candès et al. [2021] show how to apply these ideas in the context of observing censored outcomes in survival analysis. A recent preprint by Fannjiang et al. [2022] applies reweighting to a setup where the test covariate distribution is in the statistician's control. Each of these works also contribute new ideas to problem-specific challenges, but we omit the details for brevity.

Conformal methods have also be used to design sequential tests for exchangeability of the underlying data [Vovk, 2021], and these sequential tests can form the basis of sequential algorithms for changepoint detection [Volkhonskiy et al., 2017] or outlier detection [Bates et al., 2021]. This line of work is quite different from ours in that they employ conformal prediction for detecting non-exchangeability, but do not provide algorithms or guarantees for the use of conformal methods for predictive inference on non-exchangeable data. Several other recent works propose conformal inference type methods for time series [Xu and Xie, 2021, Stankeviciute et al., 2021], but these results require either distributional assumptions or exchangeability assumptions, while in our present work we aim to avoid these conditions.

The recent work of Gibbs and Candès [2021] takes a different approach towards handling distribution drift in an online manner. Informally, they compare the empirically attained coverage to the target $(1 - \alpha)$ level, and if the former is bigger (or smaller) than the latter, then they iteratively increase (or decrease) the error level α_t to employ for the next prediction. Their algorithm can be viewed as an online rule for adjusting the levels $(\alpha_t)_{t\geq 1}$ using a stochastic approximation or gradient descent style algorithm. An alternative approach is that of Cauchois et al. [2020], where

robustness is introduced under the assumption that the test point's distribution is bounded in f-divergence from the distribution of the training data points.

For data that is instead drawn from a *spatial* domain, the recent work of Mao et al. [2020] uses weighted conformal prediction with higher weights assigned to data points drawn at spatial locations near that of the test point (or, as a special case, giving a weight of 1 to the nearest neighbors of the test point, and weight 0 to all other points), but theoretical guarantees require distributional assumptions.

Finally, we return full circle to the book of Vovk et al. [2005], which has chapters that discuss moving beyond exchangeability, for example using Mondrian conformal prediction (and its generalization, online compression models). Mondrian methods informally divide the observations into groups, and assume that the observations within each group are still exchangeable (e.g., class-conditional conformal classification). We also note the work of Dunn et al. [2022] that studies the case of two-layer hierarchical models (like random effect models) that shares strength across groups. These works involve very different ideas from those presented in the current paper.

3 Robust inference through weighted quantiles

As described above, our new methodology moves beyond the exchangeable setting by allowing both for non-exchangeable data, and for non-symmetric algorithms. In this section, for simplicity, we consider only the first extension—the data points $Z_i = (X_i, Y_i)$ are no longer required to be exchangeable, but the model fitting algorithm \mathcal{A} will still be assumed to be symmetric for now. In Section 4 below, we will generalize the method to allow non-symmetric algorithms as well.

For our non-exchangeable conformal methods, we choose weights $w_1, \ldots, w_n \in [0,1]$, with the intuition that a higher weight w_i should be assigned to a data point Z_i that is "trusted", i.e., that we believe comes from (nearly) the same distribution as the test point Z_{n+1} . We assume the weights w_i are fixed (see Section 5.3 for further discussion). For instance if data point Z_i occurs at time i, and we are concerned about distribution drift, we might choose weights $w_1 \leq \cdots \leq w_n$ so that our prediction interval relies mostly on recent data points and places little weight on data from the distant past.

We now modify the three predictive inference methods to use weighted quantiles, with weights given by the w_i 's, rather than the original definitions where all data points are implicitly given equal weight. In order to simplify notation, in what follows, given $w_1, \ldots, w_n \in [0, 1]$ we will define normalized weights

$$\tilde{w}_i = \frac{w_i}{w_1 + \dots + w_n + 1}, \ i = 1, \dots, n, \text{ and } \tilde{w}_{n+1} = \frac{1}{w_1 + \dots + w_n + 1}.$$
 (11)

Non-exchangeable split conformal. The prediction interval is given by

$$\widehat{C}_n(X_{n+1}) = \widehat{\mu}(X_{n+1}) \pm \mathsf{Q}_{1-\alpha} \left(\sum_{i=1}^n \widetilde{w}_i \cdot \delta_{R_i} + \widetilde{w}_{n+1} \cdot \delta_{+\infty} \right),\tag{12}$$

where $R_i = |Y_i - \widehat{\mu}(X_i)|$ for the pre-trained model $\widehat{\mu}$, as before.

Non-exchangeable full conformal. The prediction set is given by

$$\widehat{C}_n(X_{n+1}) = \left\{ y : R_{n+1}^y \le Q_{1-\alpha} \left(\sum_{i=1}^{n+1} \widetilde{w}_i \cdot \delta_{R_i^y} \right) \right\}, \tag{13}$$

where as before, we define $\widehat{\mu}^y = \mathcal{A}((X_1, Y_1), \dots, (X_n, Y_n), (X_{n+1}, y))$ by running the algorithm \mathcal{A} on the training data together with the hypothesized test point (X_{n+1}, y) , and define R_i^y as in (7) from before.

Non-exchangeable jackknife+. The prediction interval is given by

$$\left[Q_{\alpha} \left(\sum_{i=1}^{n} \tilde{w}_{i} \cdot \delta_{\widehat{\mu}_{-i}(X_{n+1}) - R_{i}^{\text{LOO}}} + \tilde{w}_{n+1} \cdot \delta_{-\infty} \right), \right. \\
\left. Q_{1-\alpha} \left(\sum_{i=1}^{n} \tilde{w}_{i} \cdot \delta_{\widehat{\mu}_{-i}(X_{n+1}) + R_{i}^{\text{LOO}}} + \tilde{w}_{n+1} \cdot \delta_{+\infty} \right) \right], \quad (14)$$

where $\widehat{\mu}_{-i}$ is defined as in (9), and $R_i^{\text{LOO}} = |Y_i - \widehat{\mu}_{-i}(X_i)|$ as before.

We note that for all three methods, their original (unweighted) versions are recovered by choosing weights $w_1 = \cdots = w_n = 1$.

The theoretical results for this section, which we previewed in (3) and (4), will follow as a corollary of more general results that can also handle non-symmetric algorithms (introduced next); we avoid restating the results here for brevity. In addition, the interested reader may already jump forward to Appendix A to examine a different style of result on the robustness of weighted (and unweighted) conformal methods—using symmetric algorithms—under a Huber-style adversarial contamination model.

4 Allowing for non-symmetric algorithms

Now, we will allow the algorithm \mathcal{A} to be an arbitrary function of the data points, entirely removing the requirement of a symmetric algorithm. This generalization will require only a small modification to the previous split conformal, full conformal, and

jackknife+ methods to ensure validity, and can result in more accurate predictors and boost efficiency of the resulting prediction intervals conformal sets, as demonstrated in the experiments (Section 6).

To begin, let us give some examples of algorithms that do not treat data points symmetrically, to see what types of settings we want to handle:

• Weighted regression. The algorithm \mathcal{A} might fit a model $\widehat{\mu}(x) = x^{\top}\widehat{\beta}$ where the parameter vector $\widehat{\beta}$ is fitted via a weighted regression. Specifically, for nonnegative weights t_i , consider solving

$$\widehat{\beta} = \arg\min_{\beta \in \mathbb{R}^p} \left\{ \sum_{i} t_i \cdot \ell(X_i^{\top} \beta, Y_i) + R(\beta) \right\}.$$
 (15)

for some loss function ℓ and regularization function R. For example, weighted least squares would be obtained by taking the loss function $\ell(t,y) = (t-y)^2$.

• Regression with drift. If each data point (X_i, Y_i) is gathered at time i, we might instead include a drift term in our regression model. For example, using a least-squares loss, we might solve

$$(\widehat{\beta}, \widehat{\gamma}) = \arg \min_{(\beta, \gamma) \in \mathbb{R}^p \times \mathbb{R}} \left\{ \sum_{i} \left(Y_i - (X_i^{\top} \beta + \gamma \cdot i) \right)^2 \right\}, \tag{16}$$

and our prediction for the test point at time n+1 will be given by $\widehat{\mu}(x) = x^{\top}\widehat{\beta} + \widehat{\gamma} \cdot (n+1)$. In this example, the data points are no longer weighted, but the order in which they are given to the algorithm \mathcal{A} matters—data point (X_i, Y_i) is associated with its index i, and thus running \mathcal{A} on a permuted version of the same data set would likely result in a different fitted model.

• Autoregressive models. Suppose that the response Y_{n+1} is best predicted by combining information from the features X_{n+1} together with response values $Y_n, Y_{n-1}, \ldots, Y_{n-k+1}$ from the recent past—for example, we might solve the minimization problem

$$(\widehat{\beta}, \widehat{\gamma}) = \arg \min_{(\beta, \gamma) \in \mathbb{R}^p \times \mathbb{R}^k} \left\{ \sum_i \left(Y_i - (X_i^\top \beta + (Y_{i-1}, \dots, Y_{i-k})^\top \gamma)^2 \right) \right\}.$$
 (17)

In this case, for the task of predicting Y_{n+1} given features X_{n+1} , our algorithm \mathcal{A} can return the fitted function

$$\widehat{\mu}(x) := x^{\top} \widehat{\beta} + (Y_n, Y_{n-1}, \dots, Y_{n-k+1})^{\top} \widehat{\gamma}.$$

To accommodate these settings and many other possibilities, we will now define \mathcal{A} as

$$\mathcal{A}: \cup_{n>0} (\mathcal{X} \times \mathbb{R} \times \mathcal{T})^n \to \{\text{Measurable functions } \widehat{\mu}: \mathcal{X} \to \mathbb{R} \},$$
 (18)

mapping a data set containing any number of "tagged" data points $(X_i, Y_i, t_i) \in \mathcal{X} \times \mathbb{R} \times \mathcal{T}$, to a fitted regression function $\widehat{\mu}$. The tag t_i associated with data point (X_i, Y_i) can play a variety of different roles, depending on the application:

- t_i can provide the weight for data point i in a weighted regression;
- t_i can indicate the time or spatial location at which data point i is sampled;
- t_i can simply indicate the order of the data points (i.e., setting $t_i = i$ for each i), so that \mathcal{A} is "aware" that data point (X_i, Y_i) is the i-th data point.

In particular, the algorithm \mathcal{A} is no longer required to treat the (X_i, Y_i) pairs symmetrically, since if we swap (X_i, Y_i) with (X_j, Y_j) (and thus, the algorithm receives tagged data points (X_j, Y_j, t_i) and (X_i, Y_i, t_j)), the fitted model may indeed change.² As for the weights w_i , we require the tags t_1, \ldots, t_{n+1} to be fixed (see Section 5.3 for further discussion of this).

With the added flexibility of a non-symmetric regression algorithm, we will need a key modification to the methods defined earlier in Section 3 to maintain predictive coverage. Our modification requires that, before applying the model fitting algorithm \mathcal{A} , we first randomly swap the tags of two of the data points in the ordering. First, draw a random index $K \in [n+1]$ from the multinomial distribution that takes the value i with probability \tilde{w}_i :

$$K \sim \sum_{i=1}^{n+1} \tilde{w}_i \cdot \delta_i, \tag{19}$$

where the normalized weights \tilde{w}_i are defined as in (11). Note that K is drawn independently from the data. We will apply our conformal methods to the data set Z^K in place of Z. In particular, the tagged data points are now (X_{n+1}, Y_{n+1}, t_K) and (X_K, Y_K, t_{n+1}) , i.e., these two data points have swapped tags. For each of the three non-exchangeable predictive inference methods, this modification is carried out as follows:

Non-exchangeable split conformal. For split conformal, the model $\widehat{\mu}$ is prefitted on separate data, and does not depend on the data points (X_i, Y_i) of the holdout set—in other words, $\widehat{\mu}$ is trivially a symmetric function of the (X_i, Y_i) 's. Therefore, no modification is needed, and our prediction interval (12) remains unaltered.

²For many common examples, the algorithm \mathcal{A} will instead be symmetric as a function of the tagged data points (X_i, Y_i, t_i) , but we do not require this assumption in this work.

Non-exchangeable full conformal. First, for any $y \in \mathbb{R}$ and any $k \in [n+1]$, define

 $\widehat{\mu}^{y,k} = \mathcal{A}\left((X_{\pi_k(i)}, Y^y_{\pi_k(i)}, t_i) : i \in [n+1]\right),$

where π_k is the permutation on [n+1] swapping indices k and n+1 (and π_{n+1} is the identity permutation), and where we define

$$Y_i^y = \begin{cases} Y_i, & i \in [n], \\ y, & i = n+1. \end{cases}$$

In other words, $\widehat{\mu}^{y,k}$ is fitted by applying the algorithm \mathcal{A} to the training data $(X_1, Y_1), \ldots, (X_n, Y_n)$ together with the hypothesized test point (X_{n+1}, y) , but with the k-th and (n+1)-st data points swapped (note that the tags t_k and t_{n+1} are now assigned to data points (X_{n+1}, y) and (X_k, Y_k) , respectively, after this swap).

Define the residuals from this model,

$$R_i^{y,k} = |Y_i - \widehat{\mu}^{y,k}(X_i)|, i = 1, \dots, n, \text{ and } R_{n+1}^{y,k} = |y - \widehat{\mu}^{y,k}(X_{n+1})|.$$

Then, after drawing a random index K as in (19), the prediction set is given by

$$\widehat{C}_n(X_{n+1}) = \left\{ y : R_{n+1}^{y,K} \le Q_{1-\alpha} \left(\sum_{i=1}^{n+1} \widetilde{w}_i \cdot \delta_{R_i^{y,K}} \right) \right\}.$$
 (20)

Non-exchangeable jackknife+. For any $k \in [n+1]$ and any $i \in [n]$, define the model $\widehat{\mu}_{-i}^k$ as

$$\widehat{\mu}_{-i}^{k} = \mathcal{A}\left((X_{\pi_{k}(j)}, Y_{\pi_{k}(j)}, t_{j}) : j \in [n+1], \pi_{k}(j) \notin \{i, n+1\} \right),$$

or equivalently,

$$\widehat{\mu}_{-i}^k = \begin{cases} \mathcal{A}\Big((X_j, Y_j, t_j) : j \in [n] \setminus \{i, k\}, (X_k, Y_k, t_{n+1})\Big), & \text{if } k \in [n] \text{ and } k \neq i, \\ \mathcal{A}\left((X_j, Y_j, t_j) : j \in [n] \setminus \{i\}\right), & \text{if } k = n+1 \text{ or } k = i. \end{cases}$$

As before, π_k is the permutation on [n+1] that swaps indices k and n+1 (or, the identity permutation in the case k=n+1). In other words, this model is fitted on the training data $(X_1, Y_1), \ldots, (X_n, Y_n)$ but with the i-th point removed, and furthermore the data point (X_k, Y_k) is given the tag t_{n+1} rather than t_k . (Note that computing the fitted model $\widehat{\mu}_{-i}^k$ does not require knowledge of the test point (X_{n+1}, Y_{n+1}) , since $\pi_k(j) = n+1$ is excluded from the data set when running \mathcal{A} .)

For the model $\widehat{\mu}_{-i}^k$, we define its corresponding leave-one-out residuals as

$$R_i^{k,\text{LOO}} = |Y_i - \widehat{\mu}_{-i}^k(X_i)|.$$

Then, after drawing a random index K as in (19), the prediction interval is given by

$$\left[Q_{\alpha} \left(\sum_{i=1}^{n} \tilde{w}_{i} \cdot \delta_{\widehat{\mu}_{-i}^{K}(X_{n+1}) - R_{i}^{K,\text{LOO}}} + \tilde{w}_{n+1} \cdot \delta_{-\infty} \right), \right.$$

$$\left. Q_{1-\alpha} \left(\sum_{i=1}^{n} \tilde{w}_{i} \cdot \delta_{\widehat{\mu}_{-i}^{K}(X_{n+1}) + R_{i}^{K,\text{LOO}}} + \tilde{w}_{n+1} \cdot \delta_{+\infty} \right) \right]. \quad (21)$$

We note that, for many practical settings, we would not expect the random swap to have a large impact on the output of the method, since many algorithms \mathcal{A} fitted on a large number of data points are often not very sensitive to this type of small perturbation in the training set. However, our theoretical results do not rely on any stability conditions or any assumptions of this type. For comparison, if we were to instead permute the data at random before applying the algorithm \mathcal{A} —i.e., use a permutation π chosen uniformly at random, rather than the single swap permutation π_K —then this would restore the symmetric algorithm assumption, but could potentially result in a highly inaccurate model. For instance, in the linear drift example (16), the drift term $\gamma \cdot i$ would be assigned to a random data point $(X_{\pi(i)}, Y_{\pi(i)})$ for every i, leading to a meaningless estimate of this drift coefficient γ .

Symmetric algorithms as a special case. The symmetric setting, discussed in Section 3, is actually a special case of the broader setting defined here. Specifically, for any symmetric algorithm \mathcal{A} that acts on (untagged) data points (x_i, y_i) , we can trivially regard it as an algorithm \mathcal{A}' acting on tagged data points (x_i, y_i, t_i) by simply ignoring the tags. For this reason, we will only give theoretical results for the general forms of the methods given in this section, but our theorems apply also to the symmetric setting considered in Section 3.

Extending to general nonconformity scores. As mentioned earlier, our methods (and theoretical results) for split conformal and full conformal can be extended to general nonconformity scores—we defer the details to Appendix B.

5 Theoretical guarantees

As described informally in Section 1.1 earlier, we will now establish a bound on the coverage gap for our proposed methods. For each of the three methods, we first need to define how we map a data set $z = (z_1, \ldots, z_{n+1}) \in (\mathcal{X} \times \mathbb{R})^{n+1}$ with entries $z_i = (x_i, y_i)$, to the residuals R(z) (recall our bound previewed in (4)).

Non-exchangeable split conformal. Given a data set z and a pre-fitted model $\widehat{\mu}$, we define the residual vector $R_{\text{splitCP}}(z) \in \mathbb{R}^{n+1}$ with entries

$$(R_{\text{splitCP}}(z))_i = |y_i - \widehat{\mu}(x_i)|.$$

Non-exchangeable full conformal. Given a data set z, we first define the model

$$\widehat{\mu} = \mathcal{A}((x_i, y_i, t_i) : i \in [n+1]).$$

Then define the residual vector $R_{\text{fullCP}}(z) \in \mathbb{R}^{n+1}$ with entries

$$(R_{\text{fullCP}}(z))_i = |y_i - \widehat{\mu}(x_i)|.$$

Non-exchangeable jackknife+. Given a data set z, we define $\binom{n+1}{2}$ many leave-two-out models: for each $i, j \in [n+1]$ with $i \neq j$, let

$$\widehat{\mu}_{-ij} = \widehat{\mu}_{-ji} = \mathcal{A}((x_k, y_k, t_k) : k \in [n+1] \setminus \{i, j\}).$$

Then define the matrix of residuals $R_{\text{jack+}}(z) \in \mathbb{R}^{(n+1)\times(n+1)}$ with entries

$$(R_{\text{jack+}}(z))_{ij} = |y_i - \widehat{\mu}_{-ij}(x_i)|$$

for all $i \neq j$, and zeros on the diagonal.

Now, as before, we let $Z=(Z_1,\ldots,Z_{n+1})$ denote the full data set, where $Z_i=(X_i,Y_i)$, and let

$$Z^{i} = (Z_{1}, \dots, Z_{i-1}, Z_{n+1}, Z_{i+1}, \dots, Z_{n}, Z_{i})$$

denote the same data set after swapping the test point Z_{n+1} with the *i*-th training point Z_i (or, for the case i = n + 1, we define $Z^{n+1} = Z$). We now state our theoretical results for each of the three methods.

Theorem 2a (Non-exchangeable split conformal prediction). Let $\widehat{\mu}$ be any pre-fitted model. Then the non-exchangeable split conformal method defined in (12) satisfies

$$\mathbb{P}\left\{Y_{n+1} \in \widehat{C}_n(X_{n+1})\right\} \ge 1 - \alpha - \sum_{i=1}^n \widetilde{w}_i \cdot \mathsf{d}_{\mathsf{TV}}\left(R_{\mathsf{splitCP}}(Z), R_{\mathsf{splitCP}}(Z^i)\right).$$

Theorem 2b (Non-exchangeable full conformal prediction). Let A be an algorithm mapping a data set of triples (X_i, Y_i, t_i) to a fitted function as in (18). Then the non-exchangeable full conformal method defined in (20) satisfies

$$\mathbb{P}\left\{Y_{n+1} \in \widehat{C}_n(X_{n+1})\right\} \ge 1 - \alpha - \sum_{i=1}^n \widetilde{w}_i \cdot \mathsf{d}_{\mathsf{TV}}\big(R_{\mathsf{fullCP}}(Z), R_{\mathsf{fullCP}}(Z^i)\big).$$

Theorem 2c (Non-exchangeable jackknife+). Let A be an algorithm mapping a data set of triples (X_i, Y_i, t_i) to a fitted function as in (18). Then the non-exchangeable jackknife+ defined in (21) satisfies

$$\mathbb{P}\left\{Y_{n+1} \in \widehat{C}_n(X_{n+1})\right\} \ge 1 - 2\alpha - \sum_{i=1}^n \widetilde{w}_i \cdot \mathsf{d}_{\mathsf{TV}}\left(R_{\mathsf{jack}+}(Z), R_{\mathsf{jack}+}(Z^i)\right).$$

To summarize, for each method, we see that the coverage gap is bounded by $\sum_{i=1}^{n} \tilde{w}_i \cdot \mathsf{d}_{\mathsf{TV}} (R(Z), R(Z^i))$, where $R(\cdot)$ should be interpreted as $R_{\mathsf{splitCP}}(\cdot)$, $R_{\mathsf{fullCP}}(\cdot)$, or $R_{\mathsf{jack+}}(\cdot)$ as appropriate for the method. Since it trivially holds that

$$d_{\mathsf{TV}}(R(Z), R(Z^i)) \le d_{\mathsf{TV}}(Z, Z^i)$$

for each of the three methods and for each i, we therefore also see that

Coverage gap
$$\leq \sum_{i} \tilde{w}_{i} \cdot \mathsf{d}_{\mathsf{TV}}(Z, Z^{i})$$

for all three of the methods. This last bound is arguably more interpretable, but could also be significantly more loose, and we consider it an important point that the coverage gap depends on the TV between swapped residual vectors, and not the swapped raw data vectors. Finally, recalling Lemma 1, we see that in the case of independent data points, we have

Coverage gap
$$\leq 2 \sum_{i} \tilde{w}_i \cdot \mathsf{d}_{\mathsf{TV}} \big((X_i, Y_i), (X_{n+1}, Y_{n+1}) \big)$$

for all three methods.

To complement these lower bounds on coverage, it is also possible to verify, for the nonexchangeable split and full conformal methods, the procedures do not substantially overcover—that is, the coverage probability is not much larger than $1 - \alpha$. We address this in Appendix C.

5.1 Remarks on the theorems

A few comments are in order to help us further understand the implications of these theoretical results.

New results in the exchangeable setting. We point out that when the data happen to be exchangeable, that is, $d_{TV}(Z, Z^i) = 0$ for all i, then the above results are new and cannot be inferred from the existing conformal literature. In particular, existing conformal methods are not able to handle non-symmetric algorithms, which limits their applicability in many practical settings (e.g., streaming data, as described above). In addition, our results show that, under exchangeability, there is no coverage

lost by introducing fixed weights w_i into the quantile calculations used for constructing the prediction interval; this means that we are free to use these weights to help ensure robustness against non-exchangeability without sacrificing any guarantees if indeed exchangeability happens to hold.

Robustness results for the original algorithms. Another interesting implication of these new bounds is that they yield robustness results for the original algorithms. Specifically, the original split conformal (5), full conformal (8), and jackknife+ (10) algorithms presented in Section 2 can be viewed as special cases of our proposed non-exchangeable methods (12), (20), and (21), respectively, by taking weights $w_1 = \cdots = w_n = 1$ and using a symmetric \mathcal{A} (i.e., no tags). In this setting, our theorems establish a new robustness result,

Coverage gap
$$\leq \frac{\sum_{i=1}^{n} \mathsf{d}_{\mathsf{TV}}(R(Z), R(Z^i))}{n+1} \leq \frac{\sum_{i=1}^{n} \mathsf{d}_{\mathsf{TV}}(Z, Z^i)}{n+1}.$$

For example, in the case of independent data points, applying Lemma 1 we obtain

Coverage gap
$$\leq \frac{2\sum_{i=1}^{n} \mathsf{d}_{\mathsf{TV}} \big((X_i, Y_i), (X_{n+1}, Y_{n+1}) \big) \big)}{n+1}.$$

These new bounds ensure robustness of existing methods against mild violations of the exchangeability (or i.i.d.) assumption, and thus help explain the success of these methods on real data, where the exchangeability assumption may not hold.

Choosing the weights. Our theoretical results confirm the intuition that we should give higher weights w_i to data points (X_i, Y_i) that we believe are drawn from a similar distribution as (X_{n+1}, Y_{n+1}) , and lower weights to data points that are less reliable. In particular, the coverage gap bounds in our theorems above might suggest that it is beneficial to choose weights that are very low for many points, to reduce the loss of coverage. However, as is always the case with inference methods, we are faced with a tradeoff: if the weights w_i are chosen to be quite low, then this reduces the effective sample size of the method (e.g., for split conformal prediction, we are reducing the effective sample size for estimating the empirical quantile of the residual distribution). Thus, overly low weights will often lead to wider prediction intervals—at the extreme, if we choose $w_1 = \cdots = w_n = 0$, this yields a coverage gap of zero but results in $C_n(X_{n+1}) \equiv \mathbb{R}$, a completely uninformative prediction interval. Empirically, we find that simple choices often work well—for example, weights that decay exponentially over time, although an overly aggressive decay could lead to a low effective sample size and thus overly conservative sets. How to choose weights optimally (and, how to quantify what it means for weights to be optimal) is an interesting and important question that we leave for future work.

Are these results assuming the data is approximately exchangeable? Finally, we point out that these coverage gap bounds are very different in flavor than simply assuming that Z is "nearly exchangeable". In particular, in a setting where $\mathsf{d}_{\mathsf{TV}}(Z,\tilde{Z})$ is small for some exchangeable \tilde{Z} , it follows immediately that the coverage gap is bounded by $\mathsf{d}_{\mathsf{TV}}(Z,\tilde{Z})$ for (unweighted) split or full conformal or the (unweighted) jackknife+, since these methods are guaranteed to have coverage $1-\alpha$ or $1-2\alpha$, respectively, with data \tilde{Z} . However, our coverage gap bound $\sum_i \tilde{w}_i \cdot \mathsf{d}_{\mathsf{TV}}(Z,Z^i)$ is substantially stronger.

To take an example, consider a distribution where the X_i 's are i.i.d., and where $Y_i \sim \text{Bernoulli}(0.5 + (-1)^i \cdot \epsilon)$ for some small constant $\epsilon > 0$. Suppose we run conformal prediction without weights, i.e., $w_i \equiv 1$. Then we have $\mathsf{d}_{\mathsf{TV}}(Z_i, Z_{n+1}) \leq 2\epsilon$ for all i, and thus our coverage gap bound ensures that conformal prediction has coverage $\geq 1 - \alpha - 2\epsilon$. On the other hand, we have

$$d_{TV}(Z, \tilde{Z}) \approx 1$$
 for any exchangeable \tilde{Z} ,

which we can verify since, under the distribution of Z, we have

$$\sum_{i=1}^{\lfloor \frac{n+1}{2} \rfloor} \mathbb{1} \left\{ Y_{2i-1} < Y_{2i} \right\} + \frac{1}{2} \mathbb{1} \left\{ Y_{2i-1} = Y_{2i} \right\} \sim \text{Binomial} \left(\lfloor \frac{n+1}{2} \rfloor, 0.5 + \epsilon \right),$$

while under any exchangeable distribution, this same sum is distributed as Binomial $(\lfloor \frac{n+1}{2} \rfloor, 0.5)$ (and these two Binomial distributions have total variation distance ≈ 1 , for large n). Thus, in this example, our coverage gap is low even though it is not the case that Z is "nearly exchangeable".

5.2 Examples

Before turning to our empirical results, we pause to give several examples of settings where the coverage gap bound is favorable.

Bounded distribution drift. First consider a setting where the data points (X_i, Y_i) are independent, but experience distribution drift over time. In this type of setting, we would want to choose weights w_i that decay as we move into the distant past, for example, $w_i = \rho^{n+1-i}$ for some decay parameter $\rho \in (0,1)$. If we assume that the distribution drift is bounded with a Lipschitz-type condition,

$$d_{\mathsf{TV}}(Z_i, Z_{n+1}) \le \epsilon \cdot (n+1-i), \ i = 1, \dots, n+1$$

for some $\epsilon > 0$, then the coverage gap for all three methods is bounded as

Coverage gap
$$\leq \sum_{i} \tilde{w}_{i} \cdot \mathsf{d}_{\mathsf{TV}}(Z, Z^{i}) \leq \sum_{i} \tilde{w}_{i} \cdot 2\mathsf{d}_{\mathsf{TV}}(Z_{i}, Z_{n+1})$$

$$\leq \sum_{i=1}^{n} \frac{\rho^{n+1-i}}{1 + \sum_{j=1}^{n} \rho^{n+1-j}} \cdot 2\epsilon \cdot (n+1-i) \leq \frac{2\epsilon}{1-\rho},$$

which is small as long as the distribution drift parameter ϵ is sufficiently small.

Changepoints. In other settings with independent data points (X_i, Y_i) , we might have periodic large changes in the distribution rather than the gradual drift studied above—that is, we may be faced with a changepoint. Suppose that the most recent changepoint occurred k time steps ago, so that $d_{\text{TV}}(Z_i, Z_{n+1}) = 0$ for i > n - k (but, before that time, the distribution might be arbitrarily different from the test point, so we might even have $d_{\text{TV}}(Z_i, Z_{n+1}) = 1$ for $i \le n - k$). In this setting, again taking weights $w_i = \rho^{n+1-i}$ that decay as we move into the past, we have

Coverage gap
$$\leq \frac{\sum_{i=1}^{n} w_i \cdot \mathsf{d}_{\mathsf{TV}}(Z, Z^i)}{1 + \sum_{i=1}^{n} w_i} \leq \frac{\sum_{i=1}^{n-k} \rho^{n+1-i}}{1 + \sum_{i=1}^{n} \rho^{n+1-i}} \leq \rho^k.$$

This yields a small coverage gap as long as k is large, i.e., as long as we have a substantial amount of data gathered after the most recent changepoint.

Covariate time series. Next, to highlight the distinction between $d_{\mathsf{TV}}(Z, Z^i)$ and $d_{\mathsf{TV}}(R(Z), R(Z^i))$, we will consider a setting where the data points (X_i, Y_i) are no longer independent. Suppose $Y_i = X_i^{\mathsf{T}} \beta + \epsilon_i$ where $\epsilon_i \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)$ but where the X_i 's are not i.i.d.—for example, the X_i 's may be dependent due to a time series structure, or the X_i 's might be independent but not identically distributed. Writing $X \in \mathbb{R}^{n \times p}$ to denote the matrix with rows X_i , we will assume that $\text{vec}(X) \sim \mathcal{N}(0, \Sigma)$ for some $\Sigma \in \mathbb{R}^{(n+1)p \times (n+1)p}$, which allows for both non-independent and/or non-identically distributed X. Now consider running full conformal prediction with least squares as the base algorithm, so that we have residuals

$$R_{\text{fullCP}}(Z) = Y - (X^{\top}X)^{-1}X^{\top}Y = \mathcal{P}_X^{\perp}(Y) = \mathcal{P}_X^{\perp}(\epsilon),$$

where \mathcal{P}_X^{\perp} denotes projection to the orthogonal complement of the column span of X. In Appendix E.5 below we will prove that

$$\mathsf{d}_{\mathsf{TV}}(R_{\mathsf{fullCP}}(Z), R_{\mathsf{fullCP}}(Z^i)) \le \kappa_{\Sigma} \sqrt{8} \cdot \frac{p}{\sqrt{n+1-p}},\tag{22}$$

where κ_{Σ} is the condition number of Σ ; if $n \gg p^2$ then this total variation distance is extremely small. On the other hand, it is likely that $\mathsf{d}_{\mathsf{TV}}(Z,Z^i)$ is very large (it may

even be close to the largest possible value of 1), unless the X_i 's are essentially i.i.d. (or exchangeable). For example, in dimension p = 1, under the auto-regressive model $X_i = \gamma \cdot X_{i-1} + \mathcal{N}(0, 1 - \gamma^2)$ (with $X_1 \sim \mathcal{N}(0, 1)$ so that the X_i 's are identically distributed), we have

$$d_{\mathsf{TV}}(Z, Z^i) \ge d_{\mathsf{TV}}(X_i - \gamma X_{i-1}, X_{n+1} - \gamma X_{i-1})$$

$$= d_{\mathsf{TV}}(\mathcal{N}(0, 1 - \gamma^2), \mathcal{N}(0, 1 + \gamma^2 - 2\gamma^{n+3-i})),$$

which is proportional to γ^2 . This shows that $\mathsf{d}_{\mathsf{TV}}(R_{\mathsf{fullCP}}(Z), R_{\mathsf{fullCP}}(Z^i))$ can be vanishingly small even when $\mathsf{d}_{\mathsf{TV}}(Z, Z^i)$ is bounded away from zero.

5.3 Extensions

We now briefly describe several extensions of our general framework.

Additive versus multiplicative bounds. In each of our results above, the reduction in coverage is additive—that is, the probability $\mathbb{P}\{Y_{n+1} \notin \widehat{C}_n(X_{n+1})\}$ has the form $\alpha + ...$ or $2\alpha + ...$, where the additional term reflects the extent to which the exchangeability assumption is violated (as measured by total variation distance). If the target non-coverage level α is extremely low, then this additive bound may represent a substantial increase in the probability of error. In Appendix A, we give an alternative bound under a Huber contamination model, which is multiplicative rather than additive, but holds only for the symmetric algorithm case.

Fixed versus data-dependent weights. Throughout our work, we have assumed that the weights w_i on the training data points, as well as the tags t_i used in model fitting in the non-symmetric case, are fixed ahead of time. In contrast, when weighted conformal prediction is used for addressing problems such as covariate shift [Tibshirani et al., 2019] or data censoring [Candès et al., 2021], the weights are data-dependent, e.g., $w_i = w(X_i)$ for both of these settings. We pause here to comment on this distinction. In our work, while the theoretical results assume that the w_i 's and t_i 's are fixed, in practice it may be the case that the weights w_i and/or the tags t_i are somehow random as well—for example, if the data is gathered at random timepoints, we might have triples (X_i, Y_i, T_i) (i.e., data (X_i, Y_i) observed at time T_i), and the weight w_i and tag t_i might then need to depend on T_i . In this type of setting, our results will still apply if the terms $d_{\mathsf{TV}}(Z, Z^i)$ appearing in our bounds on the coverage gap are replaced with conditional total variation distance, i.e.,

Coverage gap
$$\leq \mathbb{E}\left[\sum_{i=1}^{n} \tilde{w}_{i} \cdot \mathsf{d}_{\mathsf{TV}}(Z, Z_{i} \mid w_{1}, \dots, w_{n}, t_{1}, \dots, t_{n+1})\right],$$

where now the *i*-th term on the right-hand side is the total variation distance between the *conditional* distributions of Z and Z^i , after conditioning on the weights and tags.

	Setting 1 (i.i.d. data)		Setting 2 (changepoints)		Setting 3 (drift)	
	Coverage	Width	Coverage	Width	Coverage	Width
CP+LS	0.900	3.310	0.835	5.990	0.838	3.732
nex-CP+LS	0.907	3.388	0.884	6.825	0.888	4.287
nex-CP+WLS	0.907	3.415	0.906	4.125	0.907	3.450

Table 1: Simulation results showing mean prediction interval coverage and width, averaged over all time points and over 200 trials. See Section 6.1 for details.

To better understand the types of settings where the conditional form of this result might or might not be meaningful, we compare two different hypothetical scenarios. Suppose data point i is observed at a random time T_i , and the weight w_i is a function of the time elapsed between the i-th training point and the test point, e.g., $w_i = \rho^{|T_i - T_{n+1}|}$ for some $\rho \in (0, 1)$.

- If the time T_i is included in the feature vector X_i (i.e., $X_i = (T_i, ...)$, containing both the time T_i and some additional features), then we will generally have $\mathsf{d}_{\mathsf{TV}}(Z, Z^i \mid w_1, \ldots, w_n, t_1, \ldots, t_{n+1}) = 1$, since knowing the weights w_1, \ldots, w_n fully determines all pairwise differences $|T_i T_j|$ for the times.
- If instead the data point (X_i, Y_i) is only weakly dependent on T_i (e.g., a distribution drift setting, where the distribution of $(X_i, Y_i) \mid T_i = t$ varies slowly with t), then we might have a very small $\mathsf{d}_{\mathsf{TV}}(Z, Z^i \mid w_1, \ldots, w_n, t_1, \ldots, t_{n+1})$, as in the distribution drift settings described above.

We leave a detailed investigation of the pros and cons of data dependent weights as an open question for future work.

6 Experiments

In this section, we will examine the empirical performance of non-exchangeable full conformal prediction, adding the new weights and allowing for a non-symmetric algorithm, against the original full conformal method.³ We will see that adding weights enables robustness against changes in the data distribution (i.e., better coverage), while allowing for a non-symmetric algorithm enables shorter prediction intervals.

6.1 Simulations

We consider three simulated data distributions:

³Code for reproducing all experiments is available at https://rinafb.github.io/code/nonexchangeable_conformal.zip.

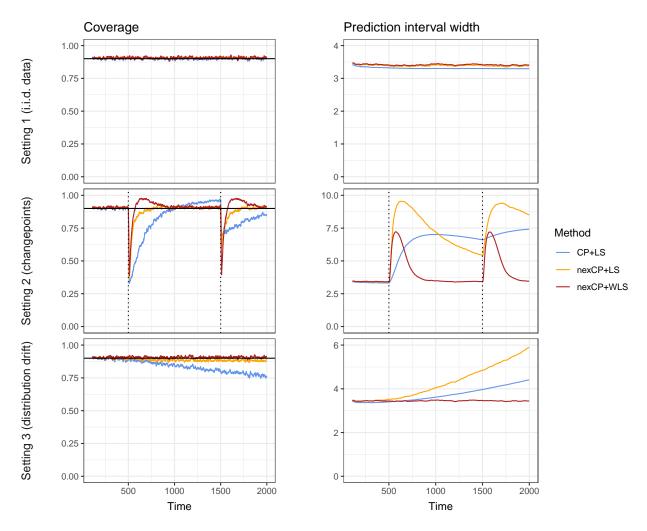


Figure 2: Simulation results showing mean prediction interval coverage and width, averaged over 200 independent trials. The displayed plots are smoothed by taking a rolling average with a window of 10 time points. See Section 6.1 for details.

- Setting 1: i.i.d. data. We generate N = 2000 i.i.d. data points (X_i, Y_i) , with $X_i \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \mathbf{I}_4)$ and $Y_i = X_i^{\top} \beta + \mathcal{N}(0, 1)$ for a coefficient vector $\beta = (2, 1, 0, 0)$.
- Setting 2: changepoints. We generate N=2000 data points (X_i, Y_i) , with $X_i \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \mathbf{I}_4)$ and $Y_i = X_i^{\top} \beta^{(i)} + \mathcal{N}(0, 1)$. Here $\beta^{(i)}$ is the coefficient vector at time i, and changes two times over the duration of data collection: we have $\beta^{(1)} = \cdots = \beta^{(500)} = (2, 1, 0, 0), \ \beta^{(501)} = \cdots = \beta^{(1500)} = (0, -2, -1, 0), \ \text{and} \ \beta^{(1501)} = \cdots = \beta^{(2000)} = (0, 0, 2, 1).$
- Setting 3: distribution drift. We generate N = 2000 data points (X_i, Y_i) , with $X_i \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \mathbf{I}_4)$ and $Y_i = X_i^{\top} \beta^{(i)} + \mathcal{N}(0, 1)$. Here $\beta^{(i)}$ is the coefficient vector at time i—we set $\beta^{(1)} = (2, 1, 0, 0)$ and $\beta^{(N)} = (0, 0, 2, 1)$, and then compute each intermediate $\beta^{(i)}$ by linear interpolation.

For each task, we implement the following three methods, with target coverage level $1 - \alpha = 0.9$:

• Full conformal prediction with least squares (CP+LS). First, we consider the original definition of full conformal prediction (8), with $\widehat{\mu}$ defined via least squares regression: for any data set $(x_1, y_1), \ldots, (x_n, y_n)$, we set $\widehat{\mu} = \mathcal{A}((x_1, y_1), \ldots, (x_n, y_n))$ as

$$\widehat{\mu}(x) = x^{\top} \widehat{\beta}$$
, where $\widehat{\beta} = \arg\min_{\beta \in \mathbb{R}^p} \sum_{i=1}^n (y_i - x_i^{\top} \beta)^2$.

- Non-exchangeable full conformal prediction with least squares (nex-CP+LS). Next, we run non-exchangeable full conformal prediction (13) with weights $w_i = 0.99^{n+1-i}$, and with the same algorithm \mathcal{A} (i.e., least squares).
- Non-exchangeable full conformal prediction with weighted least squares (nex-CP+WLS). Finally, we run non-exchangeable full conformal prediction with a non-symmetric algorithm (13), weighted least squares. Specifically, given tagged data points (x_i, y_i, t_i) , the fitted function $\widehat{\mu} = \mathcal{A}((x_1, y_1, t_1), \dots, (x_n, y_n, t_n))$ is defined as

$$\widehat{\mu}(x) = x^{\top} \widehat{\beta}$$
, where $\widehat{\beta} = \arg\min_{\beta \in \mathbb{R}^p} \sum_{i=1}^n t_i \cdot (y_i - x_i^{\top} \beta)^2$.

Here the tags t_i are used as weights for computing the fitted coefficients $\widehat{\beta}$. We implement the algorithm with $t_i = 0.99^{n+1-i}$, and again use weights $w_i = 0.99^{n+1-i}$.

After a burn-in period of the first 100 time points, at each time n = 100, ..., N-1 we run the methods with training data i = 1, ..., n and test point n + 1. The results shown are averaged over 200 independent replications of the simulation.

Our results are shown in Figure 2, and are summarized in Table 1. In terms of coverage, we see that all three methods have coverage $\approx 90\%$ across the time range of the experiment for the i.i.d. data setting (Setting 1), while for the changepoint (Setting 2) and distribution drift (Setting 3) experiments, the two proposed methods achieve approximately the desired coverage level, but the original full conformal method CP+LS undercovers. In particular, as expected, in Setting 2 CP+LS shows steep drops in coverage after changepoints, while in Setting 3 the coverage for CP+LS declines gradually over time as the distribution drift grows. The nex-CP+LS and nex-CP+WLS methods are better able to maintain coverage in these settings. (In fact, in Setting 2, we see that nex-CP+WLS overcovers for a period of time after each changepoint—this is because, a short period of time after the changepoint, the fitted weighted least squares model is already quite accurate for the new data distribution, but the weights \tilde{w}_i are still placing some weight on data points from before the changepoint, leading briefly to an overestimate of our model error.)

Turning to the prediction interval width, for the i.i.d. data setting (Setting 1), the three methods show similar mean widths, although the widths for nex-CP+LS and nex-CP+WLS are very slightly higher than for CP+LS; in addition, variability is higher for nex-CP+LS and nex-CP+WLS than for CP+LS, which is to be expected since using decaying weights w_i for computing the prediction intervals leads to a lower effective sample size. For the changepoint (Setting 2) and distribution drift (Setting 3) experiments, we see that nex-CP+LS leads to wider prediction intervals than the original method CP+LS, which is to be expected since nex-CP+LS is using the same model fitting algorithm but avoiding the undercoverage issue of CP+LS. More importantly, nex-CP+WLS is able to construct narrower prediction intervals than CP+LS, while avoiding undercoverage. This is due to the fact that weighted least squares leads to more accurate fitted models. This highlights the utility of non-symmetric algorithms for settings where exchangeability of the data cannot be assumed.

6.2 Electricity data set

Next, we compare the three methods on real data. The ELEC2 data set⁴ [Harries, 1999] tracks electricity usage and pricing in the states of New South Wales and Victoria in Australia, every 30 minutes over a 2.5 year period in 1996–1999. (This data set was previously analyzed by Vovk et al. [2021] in the context of conformal prediction, finding distribution drift that violated exchangeability.)

For our experiment, we use four covariates: nswprice and vicprice, the price

⁴Data was obtained from https://www.kaggle.com/yashsharan/the-elec2-dataset.

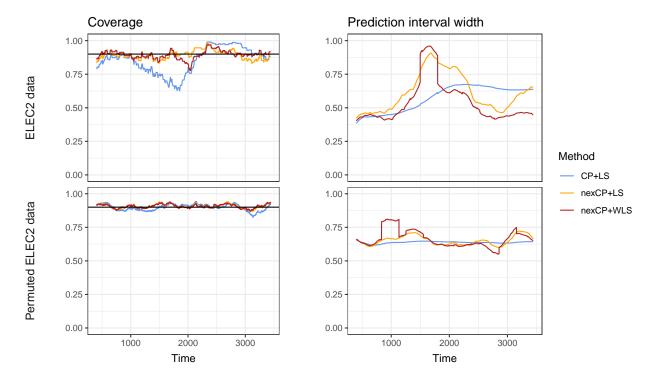


Figure 3: Experiment results showing coverage and prediction interval width on the ELEC2 data and the permuted ELEC2 data. The displayed plots are smoothed by taking a rolling average with a window of 300 time points. See Section 6.2 for details of the experiments.

of electricity in each of the two states, and nswdemand and vicdemand, the usage demand in each of the two states. Our response variable is transfer, the quantity of electricity transferred between the two states. We work with a subset of the data, keeping only those observations in the time range 9:00am-12:00pm (aiming to remove daily fluctuation effects), and discarding an initial stretch of time during which the value transfer is constant. After these steps, we have N=3444 time points. We then implement the same three methods as in the simulations (CP+LS, nex-CP+LS, and nex-CP+WLS), using the exact same definitions and settings as before.

Our goal is to examine how distribution drift over the duration of this 2.5 year period will affect each of the three methods. As a sort of "control group", we also perform the experiment with a permuted version of this same data set—we draw a permutation π on [N] uniformly at random, and then repeat the same experiment on the permuted data set $(X_{\pi(1)}, Y_{\pi(1)}), \ldots, (X_{\pi(N)}, Y_{\pi(N)})$. The random permutation ensures that the distribution of this data set now satisfies exchangeability.

Our results are shown in Figure 3, and are summarized in Table 2. On the original data set, we see that the unweighted method CP+LS shows some undercoverage, while both nex-CP+LS and nex-CP+WLS achieve nearly the desired 90% coverage level. In particular, CP+LS shows undercoverage during a long range of time around

	ELEC2 data		Permuted ELEC2 data		
	Coverage	Width	Coverage	Width	
CP+LS	0.852	0.565	0.899	0.639	
nex-CP+LS	0.890	0.606	0.908	0.652	
nex-CP+WLS	0.893	0.527	0.908	0.663	

Table 2: Experiment results showing coverage and prediction interval width on the ELEC2 data and the permuted ELEC2 data, averaged over all time points. See Section 6.2 for details of the experiments.

the middle of the duration of the experiment, and then recovers, showing the effects of distribution drift in this data set—it may be the case that the response transfer is more noisy during the middle of the time range, and becomes less variable towards the end. On the permuted data set, on the other hand, all three methods show coverage that is close to 90% throughout the time range, which is expected since the permuted data set is exchangeable.

Turning now to prediction interval width, on the original data set we see that the width for CP+LS increases gradually over time, showing the drawbacks of using a symmetric algorithm (which by definition, must give high weight to data in the distant past). In contrast, nex-CP+WLS shows larger prediction interval width during the middle of the time range (when, perhaps, the response is more noisy), but returns to narrower width towards the end. The behavior of the prediction interval width for nex-CP+LS is somewhere in between the other two. For the permuted data set, on the other hand, due to exchangeability the width of the prediction interval is approximately constant across the time range for all three methods, although nex-CP+LS and nex-CP+WLS show higher variability; this is likely due to the lower effective sample size that is introduced by weighting the data points.

7 Proofs

In this section, we will prove the theorems relating to split conformal and full conformal. Proofs for the jackknife+ are deferred to Appendix D.

7.1 Background: proofs of Theorems 1a and 1b

To help build intuition for the tools we will use later on in this work, we reformulate Vovk et al. [2005]'s proofs of these results with unified notation, and will then explain some of the challenges in extending these existing results to our new setting. Since split conformal is actually a special case of full conformal (i.e., we can choose the model fitting algorithm \mathcal{A} that simply returns the fixed pre-fitted model $\widehat{\mu}$), the same proof holds for both of these methods.

Let $R_i = R_i^{Y_{n+1}}$ denote the *i*-th residual, at the hypothesized value $y = Y_{n+1}$. By our assumptions, the data points $(X_1, Y_1), \ldots, (X_{n+1}, Y_{n+1})$ are i.i.d. (or exchangeable), and the fitted model $\widehat{\mu} = \widehat{\mu}^{Y_{n+1}} = \mathcal{A}((X_1, Y_1), \ldots, (X_{n+1}, Y_{n+1}))$ is constructed via an algorithm \mathcal{A} that treats these n+1 data points symmetrically. The residuals $R_i = |Y_i - \widehat{\mu}(X_i)|$ are thus exchangeable.

Now define the set of "strange" points

$$S(R) = \left\{ i \in [n+1] : R_i > Q_{1-\alpha} \left(\sum_{j=1}^{n+1} \frac{1}{n+1} \cdot \delta_{R_j} \right) \right\}.$$

That is, index *i* corresponds to a "strange" point if its residual R_i is one of the $\lfloor \alpha(n+1) \rfloor$ largest elements of the list R_1, \ldots, R_{n+1} . By definition, this can include at most $\alpha(n+1)$ entries of the list, i.e.,

$$|\mathcal{S}(R)| \le \alpha(n+1).$$

Next, by definition of the full conformal prediction set, we see that $Y_{n+1} \notin \widehat{C}_n(X_{n+1})$ (i.e., coverage fails) if and only if $R_{n+1} > Q_{1-\alpha}\left(\sum_{i=1}^{n+1} \frac{1}{n+1} \cdot \delta_{R_i}\right)$, or equivalently, if and only if the test point n+1 is "strange", i.e., $n+1 \in \mathcal{S}(R)$. Therefore, we have

$$\mathbb{P}\left\{Y_{n+1} \notin \widehat{C}_n(X_{n+1})\right\} = \mathbb{P}\left\{n+1 \in \mathcal{S}(R)\right\} = \frac{1}{n+1} \sum_{i=1}^{n+1} \mathbb{P}\left\{i \in \mathcal{S}(R)\right\}$$
$$= \frac{1}{n+1} \mathbb{E}\left[\sum_{i=1}^{n+1} \mathbb{1}\left\{i \in \mathcal{S}(R)\right\}\right] = \frac{1}{n+1} \mathbb{E}\left[|\mathcal{S}(R)|\right] \leq \frac{1}{n+1} \cdot \alpha(n+1) = \alpha,$$

where the second equality holds due to the exchangeability of R_1, \ldots, R_{n+1} .

Challenges for the new algorithms. Even if the data points (X_i, Y_i) are exchangeable, the above proofs fail in several ways. First, suppose that \mathcal{A} is symmetric (i.e., we do not use tags t_i). For the original (unweighted) full conformal prediction method, in the proof of Theorem 1b, exchangeability of the data points is used to verify that $\mathbb{P}\{n+1\in\mathcal{S}(R)\}=\mathbb{P}\{i\in\mathcal{S}(R)\}$ for each $i\in[n]$, or equivalently,

$$\mathbb{P}\left\{R_{n+1} > \mathsf{Q}_{1-\alpha}\left(\sum_{j=1}^{n+1} \frac{1}{n+1} \cdot \delta_{R_j}\right)\right\} = \mathbb{P}\left\{R_i > \mathsf{Q}_{1-\alpha}\left(\sum_{j=1}^{n+1} \frac{1}{n+1} \cdot \delta_{R_j}\right)\right\}.$$

This equality holds since the R_i 's are exchangeable (by assumption on the data) and since $Q_{1-\alpha}\left(\sum_{j=1}^{n+1} \frac{1}{n+1} \cdot \delta_{R_j}\right)$ is a symmetric function of R_1, \ldots, R_{n+1} . For the non-exchangeable full conformal algorithm proposed in (13), on the other hand, we would need to check whether

$$\mathbb{P}\left\{R_{n+1} > \mathsf{Q}_{1-\alpha}\left(\sum_{j=1}^{n+1} \tilde{w}_j \cdot \delta_{R_j}\right)\right\} \stackrel{?}{=} \mathbb{P}\left\{R_i > \mathsf{Q}_{1-\alpha}\left(\sum_{j=1}^{n+1} \tilde{w}_j \cdot \delta_{R_j}\right)\right\}.$$

Even though the R_i 's are exchangeable (if the data points are), the weighted quantile $Q_{1-\alpha}\left(\sum_{j=1}^{n+1} \tilde{w}_j \cdot \delta_{R_j}\right)$ is no longer a symmetric function of R_1, \ldots, R_{n+1} if the weights \tilde{w}_j take varying values, and therefore, the equality will no longer be true in general.

Next, if we use non-symmetric algorithms that take tagged data points (X_i, Y_i, t_i) as input, the situation becomes even more complex—even if the data points (X_i, Y_i) are exchangeable, the residuals R_1, \ldots, R_{n+1} may no longer be exchangeable since they depend on a fitted model $\hat{\mu}$ that treats the training data points non-symmetrically.

Finally, in this paper we are of course primarily interested in the setting where the data points are no longer exchangeable, and in bounding the resulting coverage gap. This leads to additional challenges, which we address in the proofs below.

7.2 Proofs of Theorem 2a and 2b

Since split conformal is simply a special case of full conformal as mentioned before, Theorem 2a follows immediately from Theorem 2b, and so we only prove Theorem 2b here.

For each $k \in [n+1]$, define

$$\widehat{\mu}^k = \widehat{\mu}^{Y_{n+1},k} = \mathcal{A}\Big((X_{\pi_k(1)}, Y_{\pi_k(1)}, t_1), \dots, (X_{\pi_k(n+1)}, Y_{\pi_k(n+1)}, t_{n+1})\Big),$$

where for any $k \in [n]$, as before π_k denotes the permutation on [n+1] that swaps indices k and n+1, while π_{n+1} is the identity permutation. Then, for any $k \in [n+1]$, we can calculate

$$(R_{\text{fullCP}}(Z^k))_i = |Y_{\pi_k(i)} - \widehat{\mu}^k(X_{\pi_k(i)})|,$$

and therefore, for each $k \in [n+1]$,

$$\pi_k(R_{\text{fullCP}}(Z^k)) = (|Y_1 - \widehat{\mu}^k(X_1)|, \dots, |Y_{n+1} - \widehat{\mu}^k(X_{n+1})|).$$

We can therefore write

$$\pi_K(R_{\text{fullCP}}(Z^K)) = (|Y_1 - \widehat{\mu}^K(X_1)|, \dots, |Y_{n+1} - \widehat{\mu}^K(X_{n+1})|) = (R_1^{K, Y_{n+1}}, \dots, R_{n+1}^{K, Y_{n+1}}).$$
(23)

The construction of the non-exchangeable full conformal prediction set (20) shows us that

$$Y_{n+1} \notin \widehat{C}_n(X_{n+1}) \iff R_{n+1}^{K,Y_{n+1}} > Q_{1-\alpha} \left(\sum_{i=1}^{n+1} \widetilde{w}_i \cdot \delta_{R_i^{K,Y_{n+1}}} \right),$$

and we can equivalently write this as

$$Y_{n+1} \notin \widehat{C}_n(X_{n+1}) \quad \Leftrightarrow \quad R_{n+1}^{K,Y_{n+1}} > \mathsf{Q}_{1-\alpha} \left(\sum_{i=1}^n \widetilde{w}_i \cdot \delta_{R_i^{K,Y_{n+1}}} + \widetilde{w}_{n+1} \cdot \delta_{+\infty} \right). \tag{24}$$

Next, we verify that deterministically, (23) implies

$$Q_{1-\alpha}\left(\sum_{i=1}^{n} \tilde{w}_{i} \cdot \delta_{R_{i}^{K,Y_{n+1}}} + \tilde{w}_{n+1} \cdot \delta_{+\infty}\right) \geq Q_{1-\alpha}\left(\sum_{i=1}^{n+1} \tilde{w}_{i} \cdot \delta_{(R_{\text{fullCP}}(Z^{K}))_{i}}\right). \tag{25}$$

Indeed, if K = n + 1, then $R_{\text{fullCP}}(Z^K) = R^{K,Y_{n+1}}$ by (23), and the bound holds trivially. If instead $K \leq n$, then the distribution on the left-hand side of (25) equals

$$\sum_{i=1}^{n} \tilde{w}_{i} \cdot \delta_{R_{i}^{K,Y_{n+1}}} + \tilde{w}_{n+1} \cdot \delta_{+\infty} = \sum_{i=1,\dots,n; i \neq K} \tilde{w}_{i} \cdot \delta_{R_{i}^{K,Y_{n+1}}} + \tilde{w}_{K} (\delta_{R_{K}^{K,Y_{n+1}}} + \delta_{+\infty}) + (\tilde{w}_{n+1} - \tilde{w}_{K}) \delta_{+\infty},$$

while the distribution on the right-hand side of (25) can be rewritten as

$$\begin{split} \sum_{i=1}^{n+1} \tilde{w}_i \cdot \delta_{(R_{\text{fullCP}}(Z^K))_i} &= \sum_{i=1,\dots,n; i \neq K} \tilde{w}_i \cdot \delta_{R_i^{K,Y_{n+1}}} + \tilde{w}_K \delta_{R_{n+1}^{K,Y_{n+1}}} + \tilde{w}_{n+1} \delta_{R_K^{K,Y_{n+1}}} \\ &= \sum_{i=1,\dots,n: i \neq K} \tilde{w}_i \cdot \delta_{R_i^{K,Y_{n+1}}} + \tilde{w}_K (\delta_{R_K^{K,Y_{n+1}}} + \delta_{R_{n+1}^{K,Y_{n+1}}}) + (\tilde{w}_{n+1} - \tilde{w}_K) \delta_{R_K^{K,Y_{n+1}}}, \end{split}$$

by again applying (23). Since $w_K \in [0,1]$ by assumption and therefore $\tilde{w}_{n+1} \geq \tilde{w}_K$, this verifies that (25) must hold. Combining (24) and (25), we have

$$Y_{n+1} \not\in \widehat{C}_n(X_{n+1}) \Rightarrow R_{n+1}^{K,Y_{n+1}} > \mathsf{Q}_{1-\alpha} \left(\sum_{i=1}^{n+1} \widetilde{w}_i \cdot \delta_{(R_{\mathrm{fullCP}}(Z^K))_i} \right),$$

or equivalently by (23),

$$Y_{n+1} \notin \widehat{C}_n(X_{n+1}) \Rightarrow (R_{\text{fullCP}}(Z^K))_K > \mathsf{Q}_{1-\alpha} \left(\sum_{i=1}^{n+1} \widetilde{w}_i \cdot \delta_{(R_{\text{fullCP}}(Z^K))_i} \right). \tag{26}$$

Next define a function S from \mathbb{R}^{n+1} to subsets of [n+1], as follows: for any $r \in \mathbb{R}^{n+1}$,

$$S(r) = \left\{ i \in [n+1] : r_i > Q_{1-\alpha} \left(\sum_{j=1}^{n+1} \tilde{w}_j \cdot \delta_{r_j} \right) \right\}. \tag{27}$$

These are the "strange" points—indices i for which r_i is unusually large, relative to the (weighted) empirical distribution of r_1, \ldots, r_{n+1} . By definition, we see that

$$\sum_{i \in \mathcal{S}(r)} \tilde{w}_i \le \alpha \text{ for all } r \in \mathbb{R}^{n+1}, \tag{28}$$

that is, the (weighted) fraction of "strange" points cannot exceed α . From (26), we have that miscoverage of Y_{n+1} implies strangeness of point K:

$$Y_{n+1} \notin \widehat{C}_n(X_{n+1}) \Rightarrow K \in \mathcal{S}(R_{\text{fullCP}}(Z^K)).$$
 (29)

Finally,

$$\mathbb{P}\left\{K \in \mathcal{S}\left(R_{\text{fullCP}}(Z^{K})\right)\right\} = \sum_{i=1}^{n+1} \mathbb{P}\left\{K = i \text{ and } i \in \mathcal{S}\left(R_{\text{fullCP}}(Z^{i})\right)\right\} \\
= \sum_{i=1}^{n+1} \tilde{w}_{i} \cdot \mathbb{P}\left\{i \in \mathcal{S}\left(R_{\text{fullCP}}(Z^{i})\right)\right\} \\
\leq \sum_{i=1}^{n+1} \tilde{w}_{i} \cdot \left(\mathbb{P}\left\{i \in \mathcal{S}\left(R_{\text{fullCP}}(Z)\right)\right\} + \mathsf{d}_{\mathsf{TV}}\left(R_{\text{fullCP}}(Z), R_{\text{fullCP}}(Z^{i})\right)\right) \\
= \mathbb{E}\left[\sum_{i \in \mathcal{S}\left(R_{\text{fullCP}}(Z)\right)} \tilde{w}_{i}\right] + \sum_{i=1}^{n} \tilde{w}_{i} \cdot \mathsf{d}_{\mathsf{TV}}\left(R_{\text{fullCP}}(Z), R_{\text{fullCP}}(Z^{i})\right) \\
\leq \alpha + \sum_{i=1}^{n} \tilde{w}_{i} \cdot \mathsf{d}_{\mathsf{TV}}\left(R_{\text{fullCP}}(Z), R_{\text{fullCP}}(Z^{i})\right).$$
(30)

where the last step holds by (28), while step (30) holds because $K \perp \!\!\! \perp Z$ while $Z^i = \pi_i(Z)$ is a function of the data Z, and therefore, $K \perp \!\!\! \perp Z^i$.

8 Discussion

Our primary contribution was to demonstrate how conformal predictive inference, which has crucially relied on exchangeability, can be modified to handle non-symmetric regression (or classification) algorithms, and utilize weighted residual distributions in order to provide robustness against deviations from exchangeability. With no assumptions whatsoever on either the algorithm or on the underlying joint distribution of the data, it is possible to give a coverage guarantee for both existing conformal methods and our new proposed non-exchangeable conformal procedures. The coverage gap, expressing the extent to which the guaranteed coverage level is lower than what would be guaranteed under exchangeability, is bounded by a weighted sum of total variation distances between the residual vectors obtained by swapping the i-th point with the (n+1)-st point.

Our work opens the door to applying conformal prediction in applications where the data is globally likely far from exchangeable but locally deviates gently from exchangeability. Tags and weights can be prudently used to downweight "faraway" points during both training and calibration, and obtain reasonable coverage in practice, while being robust to even adversarial corruptions; smart tag/weight designs will improve efficiency and robustness. The main strength of conformal prediction has been the ability to provide valid inference without any knowledge of the underlying stochastic model, and that strength is only amplified by relaxing the last remaining assumption: exchangeability.

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A Huber-robustness of conformal prediction

In this section, we consider an alternative form of robustness, which requires stricter assumptions on the distribution drift but will yield a stronger predictive coverage guarantee. First, consider a version of the classic Huber contamination model from robust statistics, where most of the data is i.i.d. from the target distribution $\mathcal{D}_{\text{target}}$, but some fraction ϵ of the data is arbitrarily corrupted. For simplicity (to start), consider observing training data point (X_i, Y_i) from the mixture model

$$\mathcal{D}_i = (1 - \epsilon)\mathcal{D}_{\text{target}} + \epsilon \mathcal{D}_i', \tag{31}$$

where \mathcal{D}'_i represents an arbitrary adversarial distribution that could potentially corrupt the *i*th training data point. However, we want to ensure coverage with respect to the target distribution $\mathcal{D}_{\text{target}}$ —that is, the test point (X_{n+1}, Y_{n+1}) will be drawn from $\mathcal{D}_{\text{target}}$. Standard conformal prediction assumes $\epsilon = 0$. But, one may ask: how badly can such adversarial corruptions hurt coverage? Here, we will answer that question, but do so in a slightly more general manner. First, define a new measure of distance between distributions,

$$\mathsf{d}_{\mathrm{mix}}(\mathcal{D}, \mathcal{D}') = \inf \left\{ t \geq 0 : \mathcal{D} = (1 - t) \cdot \mathcal{D}' + t \cdot \mathcal{D}'' \text{ for any distribution } \mathcal{D}'' \right\}.$$

Abusing notation, we will write $d_{\text{mix}}(Z, Z') = d_{\text{mix}}(\mathcal{D}, \mathcal{D}')$ if $Z \sim \mathcal{D}$ and $Z' \sim \mathcal{D}'$.

This "distance" can be thought of as measuring the contamination of \mathcal{D}' , in the Huber sense. Indeed, if the data did indeed come from the mixture model (31), then we would have $\mathsf{d}_{\mathrm{mix}}(Z,Z') \leq \epsilon$. (We note that $\mathsf{d}_{\mathrm{mix}}$ is not a metric, and in particular, is not symmetric in its two arguments.)

We now state our results for our weighted version of full conformal and jackknife+, in the setting where the data points are independent and the algorithm is symmetric. Define

$$\bar{w}_i = \frac{w_i}{w_1 + \dots + w_n}, \ i = 1, \dots, n.$$

Theorem 3 (Multiplicative bound). Suppose Z_1, \ldots, Z_{n+1} are independent. For any pre-fitted function $\widehat{\mu}$, the non-exchangeable split conformal method (12) satisfies

$$\mathbb{P}\left\{Y_{n+1} \notin \widehat{C}_n(X_{n+1})\right\} \le \frac{\alpha}{1 - \sum_{i=1}^n \bar{w}_i \mathsf{d}_{\text{mix}}(Z_i, Z_{n+1})}.$$

Further, for any symmetric algorithm A, the non-exchangeable full conformal method (13) satisfies

 $\mathbb{P}\left\{Y_{n+1} \notin \widehat{C}_n(X_{n+1})\right\} \le \frac{\alpha}{1 - \sum_{i=1}^n \bar{w}_i \mathsf{d}_{\min}(Z_i, Z_{n+1})},$

and the non-exchangeable jackknife+ method (14) satisfies

$$\mathbb{P}\left\{Y_{n+1} \notin \widehat{C}_n(X_{n+1})\right\} \le \frac{2\alpha}{1 - \sum_{i=1}^n \bar{w}_i \mathsf{d}_{\text{mix}}(Z_i, Z_{n+1})}.$$

In particular, if each Z_i follows an ϵ -Huber contamination model relative to Z_{n+1} as in (31), then the bound on the miscoverage rate for both unweighted and weighted conformal methods inflates by a factor of at most $1/(1-\epsilon)$.

To compare this result to our other theorems, consider the case when the multiplicative factor $\sum_{i=1}^{n} \bar{w}_{i} \mathsf{d}_{\text{mix}}(Z_{i}, Z_{n+1})$ is small. Then $(1 - \sum_{i=1}^{n} \bar{w}_{i} \mathsf{d}_{\text{mix}}(Z_{i}, Z_{n+1}))^{-1} \approx 1 + \sum_{i=1}^{n} \bar{w}_{i} \mathsf{d}_{\text{mix}}(Z_{i}, Z_{n+1})$, and so our coverage gap is bounded as

$$pprox lpha \cdot \sum_{i=1}^n \bar{w}_i \mathsf{d}_{\mathrm{mix}}(Z_i, Z_{n+1})$$

for split or full conformal, or as $\approx 2\alpha \cdot \sum_{i=1}^{n} \bar{w}_{i} d_{\text{mix}}(Z_{i}, Z_{n+1})$ for the jackknife+. If the target error level α is very low, this multiplicative bound may offer much tighter error control, as compared to the additive bounds in our earlier theorems. For example, if $\alpha = 0.05$ and the Huber contamination model (31) is true with $\epsilon = 0.1$, then for split or full conformal, the above bounds yield a miscoverage of 0.055, while our additive bounds yield a miscoverage of 0.15.

On the other hand, if the Huber contamination model is false, since it always holds that $d_{\text{mix}}(Z_i, Z_{n+1}) \ge d_{\text{TV}}(Z_i, Z_{n+1})$, it is possible to have $d_{\text{mix}}(Z_i, Z_{n+1}) = 1$ even with $d_{\text{TV}}(Z_i, Z_{n+1})$ arbitrarily small, and in such settings the original additive bounds may give tighter results. Of course, an additional restriction is that the multiplicative bound holds only for independent data and for symmetric algorithms, while the earlier theorems have no such assumptions.

B Extension to general nonconformity scores

In this section, we extend our new methods for split and full conformal to the setting of general nonconformity scores. For this setting, the response variables Y_i are no longer required to be real-valued, so we will consider the general setting of data points $(X_i, Y_i) \in \mathcal{X} \times \mathcal{Y}$.

We now define these generalized methods. For split conformal, we assume that the nonconformity score function $S: \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ is pre-fitted. The non-exchangeable

split conformal set is then given by

$$\widehat{C}_n(X_{n+1}) = \left\{ y \in \mathcal{Y} : S(X_{n+1}, y) \le Q_{1-\alpha} \left(\sum_{i=1}^n \frac{1}{n+1} \cdot \delta_{S(X_i, Y_i)} + \frac{1}{n+1} \cdot \delta_{+\infty} \right) \right\}.$$
(32)

For the special case $S(x,y) = |y - \widehat{\mu}(x)|$ (where $\widehat{\mu}$ is a pre-fitted function), this reduces to the previous definition (12) from before.

For full conformal, we now consider algorithms \mathcal{A} of the form

$$\mathcal{A}: \cup_{n\geq 0} \left(\mathcal{X} \times \mathcal{Y} \times \mathcal{T}\right)^n \rightarrow \left\{ \text{Measurable functions } \widehat{S}: \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R} \right\}.$$
 (33)

(As before, the symmetric algorithm setting, with no tags t_i , is simply a special case of this general formulation.) First, for any $y \in \mathbb{R}$ and any $k \in [n+1]$, define

$$\widehat{S}^{y,k} = \mathcal{A}\left((X_{\pi_k(i)}, Y^y_{\pi_k(i)}, t_i) : i \in [n+1]\right),$$

where the permutation π_k is defined as before, and where

$$Y_i^y = \begin{cases} Y_i, & i \in [n], \\ y, & i = n+1 \end{cases}$$

as before. Define the scores from this model,

$$S_i^{y,k} = \widehat{S}^{y,k}(X_i, Y_i), i = 1, \dots, n, \text{ and } S_{n+1}^{y,k} = \widehat{S}^{y,k}(X_{n+1}, y).$$

Then, after drawing a random index K as in (19), the prediction set is given by

$$\widehat{C}_n(X_{n+1}) = \left\{ y \in \mathcal{Y} : S_{n+1}^{y,K} \le \mathsf{Q}_{1-\alpha} \left(\sum_{i=1}^{n+1} \widetilde{w}_i \cdot \delta_{S_i^{y,K}} \right) \right\}. \tag{34}$$

For the special case $\widehat{S}(x,y) = |y - \widehat{\mu}(x)|$ (where $\widehat{\mu}$ is fitted on the same data), this reduces to the previous definition (20) from before.

The same theoretical results hold for these more general methods as well (i.e., Theorem 2a for split conformal, and Theorem 2b for full conformal). Since the necessary modifications of the proofs are very straightforward, we omit them here.

Finally, it is nontrivial to modify the jackknife+ directly to handle general non-conformity scores, but jackknife+ is closely related to the cross-conformal prediction method of Vovk [2015], Vovk et al. [2018] (see Barber et al. [2021] for details on the connection between these methods). Cross-conformal prediction can indeed be modified in a similar fashion to above, to allow for general nonconformity scores, but we omit the details for brevity.

C Upper bounds on coverage

In this section, we will establish an upper bound the coverage of nonexchangeable conformal prediction (for either split or full conformal), under a mild additional condition. This results verifies that these methods are not overly conservative. For the exchangeable setting, Lei et al. [2018, Theorem 2.1] shows that, in a setting where the residuals R_i (for split conformal) or R_i^y (for full conformal) are distinct with probability 1, conformal prediction satisfies

$$1 - \alpha \le \mathbb{P}\left\{Y_{n+1} \in \widehat{C}_n(X_{n+1})\right\} < 1 - \alpha + \frac{1}{n+1}.$$

That is, coverage is essentially equal to $1 - \alpha$, rather than lower bounded by $1 - \alpha$, ensuring that the prediction sets are not constructed in an overly conservative way. Here we give the analogous results for our nonexchangeable methods.

Theorem 4 (Upper bound on coverage). For any pre-fitted function $\widehat{\mu}$, if it holds that $R_1, \ldots, R_n, R_{n+1}$ are distinct with probability 1, then the non-exchangeable split conformal method (12) satisfies

$$\mathbb{P}\left\{Y_{n+1} \in \widehat{C}_n(X_{n+1})\right\} < 1 - \alpha + \tilde{w}_{n+1} + \sum_{i=1}^n \tilde{w}_i \cdot \mathsf{d}_{\mathsf{TV}}\left(R_{\mathsf{fullCP}}(Z), R_{\mathsf{fullCP}}(Z^i)\right).$$

Further, for any algorithm \mathcal{A} mapping a data set of triples (X_i, Y_i, t_i) to a fitted function as in (18), if it holds that $R_1^{Y_{n+1},K}, \ldots, R_n^{Y_{n+1},K}, R_{n+1}^{Y_{n+1},K}$ are distinct with probability 1, then the non-exchangeable full conformal method (20) satisfies

$$\mathbb{P}\left\{Y_{n+1} \in \widehat{C}_n(X_{n+1})\right\} < 1 - \alpha + \tilde{w}_{n+1} + \sum_{i=1}^n \tilde{w}_i \cdot \mathsf{d}_{\mathsf{TV}}\left(R_{\mathsf{fullCP}}(Z), R_{\mathsf{fullCP}}(Z^i)\right).$$

From this result, we see that if the weight

$$\tilde{w}_{n+1} = \frac{1}{w_1 + \dots + w_n + 1}$$

is small (which essentially corresponds to the effective sample size of our weighted method being large), then in the exchangeable setting where $\mathsf{d}_{\mathsf{TV}}\big(R_{\mathsf{fullCP}}(Z), R_{\mathsf{fullCP}}(Z^i)\big) = \mathsf{d}_{\mathsf{TV}}(Z, Z^i) = 0$ for all i, the coverage of the conformal methods cannot be much higher than $1 - \alpha$. On the other hand, if there is substantial violation of exchangeability, then the term $\sum_{i=1}^n \tilde{w}_i \cdot \mathsf{d}_{\mathsf{TV}}\big(R_{\mathsf{fullCP}}(Z), R_{\mathsf{fullCP}}(Z^i)\big)$ can either decrease coverage (as bounded by our earlier guarantees, Theorems 2a and 2b, controlling undercoverage) or increase coverage (as bounded by this new Theorem 4 that controls the overcoverage).

D Proofs for the jackknife+

D.1 Background: proof of Theorem 1c

Before proving our new results for jackknife+, we first recall the proof of Theorem 1c from Barber et al. [2021], for the exchangeable case. Let $\widehat{\mu}_{-ij}$ denote the model fitted by running the symmetric algorithm \mathcal{A} on the n-1 data points $\{(X_k, Y_k) : k \in [n+1] \setminus \{i,j\}\}$. Let $R \in \mathbb{R}^{(n+1)\times(n+1)}$ be the matrix with entries

$$R_{ij} = |Y_i - \widehat{\mu}_{-ij}(X_i)|$$

for each $i \neq j$, and zeros on the diagonal. By exchangeability of the n+1 data points, the matrix R also satisfies an exchangeability property, namely, $\Pi \cdot R \cdot \Pi^{\top} \stackrel{d}{=} R$ for any fixed permutation matrix Π . Moreover, for each $i \in [n]$, $\widehat{\mu}_{-i,(n+1)} = \widehat{\mu}_{-(n+1),i} = \widehat{\mu}_{-i}$, where $\widehat{\mu}_{-i}$ is the usual leave-one-out model defined earlier, and so

$$R_{i,n+1} = |Y_{n+1} - \widehat{\mu}_{-i}(X_{n+1})|$$
 and $R_{n+1,i} = R_i^{\text{LOO}} = |Y_i - \widehat{\mu}_{-i}(X_i)|, i = 1, \dots, n.$

Next, define the set of "strange" points

$$S(R) = \left\{ i \in [n+1] : \sum_{j=1}^{n+1} \mathbb{1} \left\{ R_{ij} > R_{ji} \right\} \ge (1-\alpha)(n+1) \right\}.$$

In [Barber et al., 2021, Proof of Theorem 1] it is shown that the bound

$$|\mathcal{S}(R)| \le 2\alpha(n+1)$$

must hold deterministically as a consequence of Landau's theorem for tournaments [Landau, 1953]. Furthermore, by definition of the jackknife+ prediction interval, Barber et al. [2021, Proof of Theorem 1] verify that failure of coverage, i.e., $Y_{n+1} \notin \widehat{C}_n(X_{n+1})$, implies that $n+1 \in \mathcal{S}(R)$. Thus, we have

$$\mathbb{P}\left\{Y_{n+1} \notin \widehat{C}_n(X_{n+1})\right\} \le \mathbb{P}\left\{n+1 \in \mathcal{S}(R)\right\} = \frac{1}{n+1} \sum_{i=1}^{n+1} \mathbb{P}\left\{i \in \mathcal{S}(R)\right\} \le 2\alpha,$$

where the second equality holds due to the exchangeability property of the matrix R, while the last step follows the same calculations as in the proof of Theorem 1b for full conformal.

D.2 Proof of Theorem 2c

For each $k \in [n]$, let Π_k be the permutation matrix swapping indices k and n + 1, and let Π_{n+1} denote the identity matrix. Then we can observe that, for each $i \in [n]$,

$$\left(\Pi_K \cdot R_{\text{jack+}}(Z^K) \cdot \Pi_K\right)_{i,n+1} = |Y_i - \widehat{\mu}_{-i}^K(X_i)| = R_i^{K,\text{LOO}},$$

and

$$(\Pi_K \cdot R_{\text{jack+}}(Z^K) \cdot \Pi_K)_{n+1,i} = |Y_{n+1} - \widehat{\mu}_{-i}^K(X_{n+1})|.$$

Therefore, for each $i \in [n]$,

$$\begin{split} \mathbb{1}\left\{|Y_{n+1} - \widehat{\mu}_{-i}^K(X_{n+1})| &> R_i^{K,\text{LOO}}\right\} \\ &= \mathbb{1}\left\{\left(\Pi_K \cdot R_{\text{jack+}}(Z^K) \cdot \Pi_K\right)_{n+1,i} > \left(\Pi_K \cdot R_{\text{jack+}}(Z^K) \cdot \Pi_K\right)_{i,n+1}\right\} \\ &= \mathbb{1}\left\{\left(R_{\text{jack+}}(Z^K)\right)_{K,\pi_K(i)} > \left(R_{\text{jack+}}(Z^K)\right)_{\pi_K(i),K}\right\}, \end{split}$$

where π_K is the permutation swapping indices K and n+1 as before. Therefore,

$$\begin{split} & \sum_{i=1}^{n} \tilde{w}_{i} \cdot \mathbb{1} \left\{ |Y_{n+1} - \hat{\mu}_{-i}^{K}(X_{n+1})| > R_{i}^{\text{LOO}} \right\} \\ & = \sum_{i=1}^{n} \tilde{w}_{i} \cdot \mathbb{1} \left\{ \left(R_{\text{jack}+}(Z^{K}) \right)_{K,\pi_{K}(i)} > \left(R_{\text{jack}+}(Z^{K}) \right)_{\pi_{K}(i),K} \right\} \\ & = \sum_{i \in [n+1] \setminus \{n+1\}} \tilde{w}_{i} \cdot \mathbb{1} \left\{ \left(R_{\text{jack}+}(Z^{K}) \right)_{K,\pi_{K}(i)} > \left(R_{\text{jack}+}(Z^{K}) \right)_{\pi_{K}(i),K} \right\} \\ & = \sum_{i \in [n+1] \setminus \{K\}} \tilde{w}_{\pi_{K}(i)} \cdot \mathbb{1} \left\{ \left(R_{\text{jack}+}(Z^{K}) \right)_{Ki} > \left(R_{\text{jack}+}(Z^{K}) \right)_{iK} \right\} \text{ by replacing } i \text{ with } \pi_{K}(i) \\ & \leq \sum_{i \in [n+1] \setminus \{K\}} \tilde{w}_{i} \cdot \mathbb{1} \left\{ \left(R_{\text{jack}+}(Z^{K}) \right)_{Ki} > \left(R_{\text{jack}+}(Z^{K}) \right)_{iK} \right\} \\ & = \sum_{i=1}^{n+1} \tilde{w}_{i} \cdot \mathbb{1} \left\{ \left(R_{\text{jack}+}(Z^{K}) \right)_{Ki} > \left(R_{\text{jack}+}(Z^{K}) \right)_{iK} \right\}, \end{split}$$

where the inequality holds since $\tilde{w}_{\pi_K(i)} \leq \tilde{w}_i$ for all $i \in [n+1] \setminus \{K\}$ (since we either have $i = \pi_K(i)$, or i = n+1 in which case we have $\tilde{w}_{\pi_K(n+1)} = \tilde{w}_K \leq \tilde{w}_{n+1}$, since $w_K \in [0,1]$ by assumption).

Next, analogously to the proof of Theorem 1c, we can verify that the non-coverage event can be recharacterized as

$$Y_{n+1} \notin \widehat{C}_n(X_{n+1}) \implies \sum_{i=1}^{n+1} \widetilde{w}_i \cdot \mathbb{1}\left\{ |Y_{n+1} - \widehat{\mu}_{-i}^K(X_{n+1})| > R_i^{\text{LOO}} \right\} \ge 1 - \alpha.$$

Combined with the above, this gives

$$Y_{n+1} \notin \widehat{C}_n(X_{n+1}) \quad \Rightarrow \quad \sum_{i=1}^{n+1} \widetilde{w}_i \cdot \mathbb{1}\left\{ \left(R_{\text{jack}+}(Z^K) \right)_{Ki} > \left(R_{\text{jack}+}(Z^K) \right)_{iK} \right\} \ge 1 - \alpha.$$

$$(35)$$

Next for any $r \in \mathbb{R}^{(n+1)\times(n+1)}$, define

$$S(r) = \left\{ i \in [n+1] : \sum_{j=1}^{n+1} \tilde{w}_j \cdot \mathbb{1} \left\{ r_{ij} > r_{ji} \right\} \ge 1 - \alpha \right\}.$$
 (36)

These are the "strange" points—indices i for which $r_{ij} > r_{ji}$ holds for most indices j. The following lemma verifies that $\sum_{i \in \mathcal{S}(r)} \tilde{w}_i \leq 2\alpha$ for any r:

Lemma 2 (Lei and Candès [2021b]). Fix any $\tilde{w}_1, \ldots, \tilde{w}_{n+1}$ with $\sum_{i=1}^{n+1} \tilde{w}_{n+1} = 1$. Let S(r) be defined as in (36). Then

$$\sum_{i \in \mathcal{S}(r)} \tilde{w}_i \le 2\alpha \text{ for all } r \in \mathbb{R}^{(n+1)\times (n+1)}.$$

Lemma 2 is proved in Appendix E.2 for completeness. In words, it states that the (weighted) fraction of "strange" points cannot exceed 2α . From (35), we have that miscoverage of Y_{n+1} implies strangeness of point K:

$$Y_{n+1} \notin \widehat{C}_n(X_{n+1}) \Rightarrow K \in \mathcal{S}(R_{\text{jack}+}(Z^K)).$$
 (37)

Finally, following the exact same steps as in the proof of Theorem 2b, we have

$$\mathbb{P}\left\{K \in \mathcal{S}\left(R_{\text{jack+}}(Z^K)\right)\right\} \le 2\alpha + \sum_{i=1}^n \tilde{w}_i \cdot \mathsf{d}_{\mathsf{TV}}\left(R_{\text{jack+}}(Z), R_{\text{jack+}}(Z^i)\right),$$

which completes the proof.

E Additional proofs and calculations

E.1 Proof of Lemma 1

First, by the maximal coupling theorem (e.g., [Ross and Peköz, 2007, Proposition 2.7]), there exists a distribution \mathcal{D} on (Z'_i, Z'_{n+1}) such that, marginally, $Z'_i \stackrel{\mathrm{d}}{=} Z_i$ and $Z'_{n+1} \stackrel{\mathrm{d}}{=} Z_{n+1}$, and such that $\mathbb{P}\left\{Z'_i = Z'_{n+1}\right\} = 1 - \mathsf{d}_{\mathsf{TV}}(Z_i, Z_{n+1})$. Now draw Z_j independently for each $j \in [n+1]$, and draw $(Z'_i, Z'_{n+1}), (Z''_i, Z''_{n+1}) \stackrel{\mathrm{iid}}{\sim} \mathcal{D}$. Define

$$Z' = (Z_1, \dots, Z_{i-1}, Z'_i, Z_{i+1}, \dots, Z_n, Z''_{n+1})$$

and

$$Z'' = (Z_1, \dots, Z_{i-1}, Z_i'', Z_{i+1}, \dots, Z_n, Z_{n+1}').$$

Then clearly, $Z' \stackrel{\text{d}}{=} Z'' \stackrel{\text{d}}{=} Z$. In particular, recalling the swapped indices notation (2), this implies that $(Z'')^i \stackrel{\text{d}}{=} Z^i$, and so

$$\mathsf{d}_{\mathsf{TV}}(Z,Z^i) = \mathsf{d}_{\mathsf{TV}}(Z',(Z'')^i).$$

Again applying the maximal coupling theorem, we have

$$d_{\mathsf{TV}}(Z', (Z'')^i) \le 1 - \mathbb{P} \left\{ Z' = (Z'')^i \right\}$$

$$= 1 - \mathbb{P} \left\{ Z'_i = Z'_{n+1}, Z''_i = Z''_{n+1} \right\}$$

$$= 1 - \mathbb{P} \left\{ Z'_i = Z'_{n+1} \right\} \cdot \mathbb{P} \left\{ Z''_i = Z''_{n+1} \right\}$$

$$= 1 - (1 - \mathsf{d}_{\mathsf{TV}}(Z_i, Z_{n+1}))^2$$

$$= 2\mathsf{d}_{\mathsf{TV}}(Z_i, Z_{n+1}) - \mathsf{d}_{\mathsf{TV}}(Z_i, Z_{n+1})^2,$$

completing the proof.

E.2 Proof of Lemma 2

Lemma 2 is stated and proved in Lei and Candès [2021b]; we reproduce the proof here for completeness since that paper is currently an unpublished manuscript. For each $i \in \mathcal{S}$, by definition of \mathcal{S} , we have

$$1 - \alpha \leq \sum_{j=1}^{n+1} \tilde{w}_{j} \mathbb{1} \left\{ r_{ij} > r_{ji} \right\} \leq \sum_{j \in \mathcal{S}(r)} \tilde{w}_{j} \mathbb{1} \left\{ r_{ij} > r_{ji} \right\} + \sum_{j \in [n+1] \setminus \mathcal{S}(r)} \tilde{w}_{j}$$
$$= \sum_{j \in \mathcal{S}(r)} \tilde{w}_{j} \mathbb{1} \left\{ r_{ij} > r_{ji} \right\} + 1 - \sum_{j \in \mathcal{S}(r)} \tilde{w}_{j},$$

where the last step holds since $\sum_{i=1}^{n+1} \tilde{w}_i = 1$ by definition. Therefore, taking a weighted sum over $i \in \mathcal{S}(r)$,

$$(1 - \alpha) \sum_{i \in \mathcal{S}(r)} \tilde{w}_i \le \sum_{i \in \mathcal{S}(r)} \tilde{w}_i \cdot \left[\sum_{j \in \mathcal{S}(r)} \tilde{w}_j \mathbb{1} \left\{ r_{ij} > r_{ji} \right\} + 1 - \sum_{j \in \mathcal{S}(r)} \tilde{w}_j \right].$$

Rearranging terms, we have

$$\left(\sum_{i \in \mathcal{S}(r)} \tilde{w}_i\right)^2 \leq \sum_{i,j \in \mathcal{S}(r)} \tilde{w}_i \tilde{w}_j \mathbb{1} \left\{r_{ij} > r_{ji}\right\} + \alpha \sum_{i \in \mathcal{S}(r)} \tilde{w}_i$$

$$= \frac{1}{2} \sum_{i,j \in \mathcal{S}(r)} \tilde{w}_i \tilde{w}_j \left(\mathbb{1} \left\{r_{ij} > r_{ji}\right\} + \mathbb{1} \left\{r_{ji} > r_{ij}\right\}\right) + \alpha \sum_{i \in \mathcal{S}(r)} \tilde{w}_i$$

$$\leq \frac{1}{2} \sum_{i,j \in \mathcal{S}(r)} \tilde{w}_i \tilde{w}_j + \alpha \sum_{i \in \mathcal{S}(r)} \tilde{w}_i$$

$$= \frac{1}{2} \left(\sum_{i \in \mathcal{S}(r)} \tilde{w}_i\right)^2 + \alpha \sum_{i \in \mathcal{S}(r)} \tilde{w}_i.$$

Rearranging terms again we have

$$\frac{1}{2} \left(\sum_{i \in \mathcal{S}(r)} \tilde{w}_i \right)^2 \le \alpha \left(\sum_{i \in \mathcal{S}(r)} \tilde{w}_i \right) \quad \Rightarrow \quad \sum_{i \in \mathcal{S}(r)} \tilde{w}_i \le 2\alpha,$$

which proves the lemma.

E.3 Proof of Theorem 3

In order to prove the theorem, we first need a lemma about weighted sums of Bernoulli random variables.

Lemma 3. Fix any $p_1, \ldots, p_n, a_1, \ldots, a_n \in [0, 1]$. Let B_1, \ldots, B_n be independent, with $B_i \sim \text{Bernoulli}(p_i)$. Then

$$\frac{a_1 + \dots + a_n + 1}{a_1 p_1 + \dots + a_n p_n + 1} \le \mathbb{E}\left[\frac{a_1 + \dots + a_n + 1}{a_1 B_1 + \dots + a_n B_n + 1}\right] \le \frac{a_1 + \dots + a_n}{a_1 p_1 + \dots + a_n p_n}.$$

The lower bound clearly holds by Jensen's inequality, but the upper bound is more challenging to prove. Several special cases of this upper bound are well known in the multiple testing literature. For example, the case where $a_1 = \cdots = a_n = 1$ and $p_1 = \cdots = p_n$ is proved in [Storey et al., 2004, Theorem 3] and used for proving FDR control of Storey [2002]'s modification of the Benjamini–Hochberg procedure [Benjamini and Hochberg, 1995]. The case where $p_1 = \cdots = p_n$ (but the a_i 's are arbitrary) is proved in [Ramdas et al., 2019, Lemma 3] and used for proving FDR control for a hierarchical multiple testing procedure (the p-filter).

We are now ready to prove the theorem. By definition of d_{mix} , the data Z_1, \ldots, Z_{n+1} can equivalently be generated as follows:

- Draw C_1, \ldots, C_n independently, with $C_i \sim \text{Bernoulli}(\mathsf{d}_{\text{mix}}(Z_i, Z_{n+1}))$.
- For each $i \in [n]$ with $C_i = 0$, as well as i = n + 1, draw Z_i i.i.d. from the distribution of Z_{n+1} .
- For each $i \in [n]$ with $C_i = 1$, draw Z_i from the corresponding contamination distribution.

Below, we will show that for non-exchangeable split conformal and full conformal,

$$\mathbb{P}\left\{Y_{n+1} \notin \widehat{C}_n(X_{n+1}) \mid C_1, \dots, C_n\right\} \ge 1 - \frac{\alpha}{\sum_{i=1}^n \widetilde{w}_i \mathbb{1}\left\{C_i = 0\right\} + \widetilde{w}_{n+1}}, \quad (38)$$

while for non-exchangeable jackknife+,

$$\mathbb{P}\left\{Y_{n+1} \notin \widehat{C}_n(X_{n+1}) \mid C_1, \dots, C_n\right\} \ge 1 - \frac{2\alpha}{\sum_{i=1}^n \widetilde{w}_i \mathbb{1}\left\{C_i = 0\right\} + \widetilde{w}_{n+1}}.$$
 (39)

Finally,

$$\mathbb{E}\left[\frac{1}{\sum_{i=1}^{n} \tilde{w}_{i} \mathbb{1}\left\{C_{i}=0\right\} + \tilde{w}_{n+1}}\right] = \mathbb{E}\left[\frac{\sum_{i=1}^{n} w_{i} + 1}{\sum_{i=1}^{n} w_{i} \mathbb{1}\left\{C_{i}=0\right\} + 1}\right]$$

$$\leq \frac{\sum_{i=1}^{n} w_{i}}{\sum_{i=1}^{n} w_{i} (1 - \mathsf{d}_{\text{mix}}(Z_{i}, Z_{n+1}))} = \frac{1}{\sum_{i=1}^{n} \bar{w}_{i} (1 - \mathsf{d}_{\text{mix}}(Z_{i}, Z_{n+1}))}$$

$$= \frac{1}{1 - \sum_{i=1}^{n} \bar{w}_{i} \mathsf{d}_{\text{mix}}(Z_{i}, Z_{n+1})},$$

where the inequality holds by Lemma 3. This implies that

$$\mathbb{P}\left\{Y_{n+1} \notin \widehat{C}_n(X_{n+1})\right\} = \mathbb{E}\left[\mathbb{P}\left\{Y_{n+1} \notin \widehat{C}_n(X_{n+1}) \mid C_1, \dots, C_n\right\}\right]$$

$$\geq 1 - \frac{\alpha}{1 - \sum_{i=1}^n \bar{w}_i \mathsf{d}_{\mathrm{mix}}(Z_i, Z_{n+1})}$$

for non-exchangeable split and full conformal prediction, and

$$\mathbb{P}\left\{Y_{n+1} \notin \widehat{C}_n(X_{n+1})\right\} = \mathbb{E}\left[\mathbb{P}\left\{Y_{n+1} \notin \widehat{C}_n(X_{n+1}) \mid C_1, \dots, C_n\right\}\right]$$

$$\geq 1 - \frac{2\alpha}{1 - \sum_{i=1}^n \bar{w}_i \mathsf{d}_{\mathrm{mix}}(Z_i, Z_{n+1})}$$

for non-exchangeable jackknife+, as desired.

To complete the proof, we now need to verify the bounds (38) and (39). For the bound (38) for conformal prediction, we have

$$\begin{split} Y_{n+1} \not\in \widehat{C}_n(X_{n+1}) &\Leftrightarrow R_{n+1}^{K,Y_{n+1}} > \mathsf{Q}_{1-\alpha} \left(\sum_{i=1}^{n+1} \widetilde{w}_i \delta_{R_i^{K,Y_{n+1}}} \right) \\ &\Leftrightarrow \sum_{i=1}^{n+1} \widetilde{w}_i \mathbb{1} \left\{ R_{n+1}^{K,Y_{n+1}} \le R_i^{K,Y_{n+1}} \right\} \le \alpha. \end{split}$$

Now let $w_i' = w_i \mathbb{1} \{C_i = 0\}$ and let

$$\tilde{w}'_i = \frac{w'_i}{w'_1 + \dots + w'_n + 1}, \ i = 1, \dots, n; \ \tilde{w}'_{n+1} = \frac{1}{w'_1 + \dots + w'_n + 1}.$$

Then, deterministically,

$$\sum_{i=1}^{n+1} \tilde{w}_i \mathbb{1}\left\{R_{n+1}^{K,Y_{n+1}} \le R_i^{K,Y_{n+1}}\right\} \ge \sum_{i=1}^{n+1} \tilde{w}_i \cdot \mathbb{1}\left\{C_i = 0\right\} \cdot \mathbb{1}\left\{R_{n+1}^{K,Y_{n+1}} \le R_i^{K,Y_{n+1}}\right\},$$

and so we can write

$$Y_{n+1} \notin \widehat{C}_n(X_{n+1}) \implies \sum_{i=1}^{n+1} \widetilde{w}_i' \mathbb{1} \left\{ R_{n+1}^{K, Y_{n+1}} \le R_i^{K, Y_{n+1}} \right\} \le \alpha \cdot \frac{w_1 + \dots + w_n + 1}{w_1' + \dots + w_n' + 1}.$$

Now suppose we had instead conditioned on C_1, \ldots, C_n , and had run non-exchangeable full conformal on the same data set Z but with weights w'_i in place of w_i , and with $\alpha \cdot \frac{w_1+\cdots+w_n+1}{w'_1+\cdots+w'_n+1}$ in place of α . Let $\widehat{C}'_n(X_{n+1})$ denote the resulting prediction interval. Then by the same arguments as before, we have

$$Y_{n+1} \not\in \widehat{C}'_n(X_{n+1}) \iff \sum_{i=1}^{n+1} \widetilde{w}'_i \mathbb{1} \left\{ R_{n+1}^{K, Y_{n+1}} \le R_i^{K, Y_{n+1}} \right\} \le \alpha \cdot \frac{w_1 + \dots + w_n + 1}{w'_1 + \dots + w'_n + 1}.$$

Moreover, Theorem 2b ensures that

$$\mathbb{P}\left\{Y_{n+1} \notin \widehat{C}'_{n}(X_{n+1}) \mid C_{1}, \dots, C_{n}\right\} \leq \alpha \cdot \frac{w_{1} + \dots + w_{n} + 1}{w'_{1} + \dots + w'_{n} + 1} + \sum_{i=1}^{n} \widetilde{w}'_{i} \cdot \mathsf{d}_{\mathsf{TV}}(Z^{i}, Z \mid C_{1}, \dots, C_{n}).$$

Furthermore, we can see that $d_{\mathsf{TV}}(Z^i, Z \mid C_1, \dots, C_n) = 0$ for all $i \in [n]$ with $C_i = 0$. Since \tilde{w}'_i is nonzero only for i with $C_i = 0$, we therefore have

$$\mathbb{P}\left\{Y_{n+1} \notin \widehat{C}'_n(X_{n+1}) \mid C_1, \dots, C_n\right\} \le \alpha \cdot \frac{w_1 + \dots + w_n + 1}{w'_1 + \dots + w'_n + 1}.$$

Therefore, we have

$$\mathbb{P}\left\{Y_{n+1} \notin \widehat{C}_n(X_{n+1})\right\} = \mathbb{E}\left[\mathbb{P}\left\{Y_{n+1} \notin \widehat{C}_n(X_{n+1}) \mid C_1, \dots, C_n\right\}\right]$$

$$\leq \mathbb{E}\left[\mathbb{P}\left\{Y_{n+1} \notin \widehat{C}'_n(X_{n+1}) \mid C_1, \dots, C_n\right\}\right] \leq \alpha \cdot \frac{w_1 + \dots + w_n + 1}{w'_1 + \dots + w'_n + 1},$$

which verifies (38).

Next, the proof of the bound (39) for the jackknife+ is nearly identical. As calculated before, we have

$$Y_{n+1} \notin \widehat{C}_n(X_{n+1}) \Rightarrow \sum_{i=1}^n \widetilde{w}_i \mathbb{1}\left\{ |Y_{n+1} - \widehat{\mu}_{-i}(X_{n+1})| > R_i^{\text{LOO}} \right\} \ge 1 - \alpha$$

$$\Leftrightarrow \sum_{i=1}^n \widetilde{w}_i \mathbb{1}\left\{ |Y_{n+1} - \widehat{\mu}_{-i}(X_{n+1})| \le R_i^{\text{LOO}} \right\} \le \alpha.$$

Define w'_i and \tilde{w}'_i as above. Then, deterministically,

$$\sum_{i=1}^{n} \tilde{w}_{i} \mathbb{1}\left\{ |Y_{n+1} - \widehat{\mu}_{-i}(X_{n+1})| \le R_{i}^{\text{LOO}} \right\} \ge \sum_{i=1}^{n} \tilde{w}_{i} \cdot \mathbb{1}\left\{ |C_{i} = 0 \right\} \cdot \mathbb{1}\left\{ |Y_{n+1} - \widehat{\mu}_{-i}(X_{n+1})| \le R_{i}^{\text{LOO}} \right\},$$

and so we can write

$$Y_{n+1} \notin \widehat{C}_n(X_{n+1}) \Rightarrow \sum_{i=1}^{n+1} \widetilde{w}_i' \mathbb{1} \left\{ |Y_{n+1} - \widehat{\mu}_{-i}(X_{n+1})| \le R_i^{\text{LOO}} \right\} \le \alpha \cdot \frac{w_1 + \dots + w_n + 1}{w_1' + \dots + w_n' + 1}.$$

Now suppose we had instead conditioned on C_1, \ldots, C_n , and had run non-exchangeable jackknife+ on the same data set Z but with weights w'_i in place of w_i , and with $\alpha \cdot \frac{w_1 + \cdots + w_n + 1}{w'_1 + \cdots + w'_n + 1}$ in place of α . Then by the same arguments as in the proof of Theorem 2c, we have

$$\mathbb{P}\left\{\sum_{i=1}^{n+1} \tilde{w}_{i}' \mathbb{1}\left\{|Y_{n+1} - \hat{\mu}_{-i}(X_{n+1})| \leq R_{i}^{\text{LOO}}\right\} \leq \alpha \cdot \frac{w_{1} + \dots + w_{n} + 1}{w'_{1} + \dots + w'_{n} + 1} \mid C_{1}, \dots, C_{n}\right\} \\
\leq 2\alpha \cdot \frac{w_{1} + \dots + w_{n} + 1}{w'_{1} + \dots + w'_{n} + 1} + \sum_{i=1}^{n} \tilde{w}_{i}' \cdot \mathsf{d}_{\mathsf{TV}}(Z^{i}, Z \mid C_{1}, \dots, C_{n}) = 2\alpha \cdot \frac{w_{1} + \dots + w_{n} + 1}{w'_{1} + \dots + w'_{n} + 1},$$

where the last step is shown exactly as for full conformal. Therefore, we have

$$\mathbb{P}\left\{Y_{n+1} \notin \widehat{C}_n(X_{n+1})\right\} = \mathbb{E}\left[\mathbb{P}\left\{Y_{n+1} \notin \widehat{C}_n(X_{n+1}) \mid C_1, \dots, C_n\right\}\right]$$

$$\leq \mathbb{E}\left[\mathbb{P}\left\{\sum_{i=1}^{n+1} \widetilde{w}_i' \mathbb{1}\left\{|Y_{n+1} - \widehat{\mu}_{-i}(X_{n+1})| \leq R_i^{\text{LOO}}\right\} \leq \alpha \cdot \frac{w_1 + \dots + w_n + 1}{w_1' + \dots + w_n' + 1} \mid C_1, \dots, C_n\right\}\right]$$

$$\leq 2\alpha \cdot \frac{w_1 + \dots + w_n + 1}{w_1' + \dots + w_n' + 1},$$

which verifies (38).

E.3.1 Proof of Lemma 3

The lower bound holds by Jensen's inequality. For the upper bound, we will instead prove the claim

$$\mathbb{E}\left[\frac{a_1 + \dots + a_n + 1 + c}{a_1 B_1 + \dots + a_n B_n + 1 + c}\right] \le \frac{a_1 + \dots + a_n + c}{a_1 p_1 + \dots + a_n p_n + c},\tag{40}$$

for any $p_1, \ldots, p_n, a_1, \ldots, a_n \in [0, 1]$ and $c \geq 0$ (where as before, the expectation is taken with respect to independent Bernoulli random variables $B_i \sim \text{Bernoulli}(p_i)$). Initially this appears stronger than the claim in the lemma (i.e., the lemma claims this bound only for the case c = 0), but in fact these claims are equivalent. To see why, suppose that the lemma holds and now we want to prove (41) for some $p, a \in [0, 1]^n$ and some c > 0. Let $m \geq c$ be any integer, and let $\tilde{p}, \tilde{a} \in [0, 1]^{n+m}$ be defined as

$$\tilde{p} = (p_1, \dots, p_n, 1 \dots, 1), \quad \tilde{a} = (a_1, \dots, a_n, c/m, \dots, c/m).$$

Then the claim (41) is equivalent to $\mathbb{E}_{B_i \stackrel{\mathbb{L}}{\sim} \text{Bernoulli}(\tilde{p}_i)} \left[\frac{\tilde{a}^{\top} \mathbf{1} + 1}{\tilde{a}^{\top} B + 1} \right] \leq \frac{1}{\tilde{p}_{\tilde{a}}}$, which holds by applying the lemma with $\tilde{p}, \tilde{a}, n + m$ in place of p, a, n.

Step 1: unit weights and equal p_i 's. Suppose $a_1 = \cdots = a_n = 1$ and $p_1 = \cdots = p_n$. We will prove that (41) holds in this case, which is equivalent to proving that

$$\mathbb{E}_{A \sim \text{Binomial}(n, p_1)} \left[\frac{n+c+1}{A+c+1} \right] \le \frac{n+c}{np_1+c}. \tag{41}$$

In particular, if c = 0, then this is the well-known bound $\mathbb{E}_{A \sim \text{Binomial}(n, p_1)} \left[\frac{n+1}{A+1} \right] \leq \frac{1}{p_1}$ (e.g., [Storey et al., 2004, Theorem 3]), while if $p_1 = 0$ then the result is trivial. If instead c > 0 and $p_1 > 0$, then we calculate

$$\begin{split} \mathbb{E}\left[\frac{n+c+1}{A+c+1}\right] &= 1 + \mathbb{E}\left[\frac{n-A}{A+c+1}\right] \\ &= 1 + \sum_{k=0}^{n-1} \mathbb{P}\left\{A = k\right\} \cdot \frac{n-k}{k+c+1} \\ &= 1 + \sum_{k=0}^{n-1} \frac{n!}{k!(n-k)!} p_1^k (1-p_1)^{n-k} \cdot \frac{n-k}{k+c+1} \\ &= 1 + \sum_{k=0}^{n-1} \frac{n!}{(k+1)!(n-k-1)!} p_1^k (1-p_1)^{n-k} \cdot \frac{k+1}{k+c+1} \\ &= 1 + \frac{1-p_1}{p_1} \cdot \sum_{k=0}^{n-1} \mathbb{P}\left\{A = k+1\right\} \cdot \frac{k+1}{k+c+1} \\ &= 1 + \frac{1-p_1}{p_1} \cdot \mathbb{E}\left[\frac{A}{A+c}\right] \\ &\leq 1 + \frac{1-p_1}{p_1} \cdot \frac{\mathbb{E}\left[A\right]}{\mathbb{E}\left[A\right]+c} \text{ by Jensen's inequality} \\ &= \frac{n+c}{np_1+c}. \end{split}$$

Step 2: arbitrary weights and equal p_i 's. Suppose $p_1 = \cdots = p_n$. We will prove that (41) holds in this case, which is equivalent to proving that

$$\mathbb{E}\left[\frac{a^{\top}\mathbf{1} + c + 1}{a^{\top}B + c + 1}\right] \leq \frac{a^{\top}\mathbf{1} + c}{a^{\top}\mathbf{1} \cdot p_1 + c}$$

where $B = (B_1, \ldots, B_n)$ for $B_i \stackrel{\text{iid}}{\sim} \text{Bernoulli}(p_1)$. (For the special case c = 0, this result is shown in [Ramdas et al., 2019, Lemma 3].)

Let $A_i \stackrel{\perp}{\sim} \text{Bernoulli}(a_i)$. Then

$$\frac{a^{\top}\mathbf{1} + c + 1}{a^{\top}B + c + 1} = 1 + \frac{a^{\top}(\mathbf{1} - B)}{a^{\top}B + c + 1} = 1 + \frac{\mathbb{E}\left[A^{\top}(\mathbf{1} - B) \mid B\right]}{\mathbb{E}\left[A^{\top}B \mid B\right] + c + 1}.$$

Note that, conditional on B, it holds that $A^{\top}B \perp A^{\top}(\mathbf{1} - B)$. Therefore,

$$\frac{\mathbb{E}\left[A^{\top}(\mathbf{1}-B) \mid B\right]}{\mathbb{E}\left[A^{\top}B \mid B\right] + c + 1} = \mathbb{E}\left[\frac{A^{\top}(\mathbf{1}-B)}{\mathbb{E}\left[A^{\top}B \mid B\right] + c + 1} \mid B\right] \text{ by linearity}$$

$$= \mathbb{E}\left[\frac{A^{\top}(\mathbf{1}-B)}{\mathbb{E}\left[A^{\top}B \mid B, A^{\top}(\mathbf{1}-B)\right] + c + 1} \mid B\right] \text{ since } A^{\top}B \perp A^{\top}(\mathbf{1}-B) \mid B$$

$$= \mathbb{E}\left[\mathbb{E}\left[\frac{A^{\top}(\mathbf{1}-B)}{\mathbb{E}\left[A^{\top}B \mid B, A^{\top}(\mathbf{1}-B)\right] + c + 1} \mid B, A^{\top}(\mathbf{1}-B)\right] \mid B\right]$$

$$\leq \mathbb{E}\left[\mathbb{E}\left[\frac{A^{\top}(\mathbf{1}-B)}{A^{\top}B + c + 1} \mid B, A^{\top}(\mathbf{1}-B)\right] \mid B\right] \text{ by Jensen's inequality}$$

$$= \mathbb{E}\left[\frac{A^{\top}(\mathbf{1}-B)}{A^{\top}B + c + 1} \mid B\right].$$

Therefore,

$$\mathbb{E}\left[\frac{a^{\top}\mathbf{1}+c+1}{a^{\top}B+c+1}\right] \leq 1 + \mathbb{E}\left[\frac{A^{\top}(\mathbf{1}-B)}{A^{\top}B+c+1}\right] = \mathbb{E}\left[\frac{A^{\top}\mathbf{1}+c+1}{A^{\top}B+c+1}\right].$$

Next, writing $S = A^{\top} \mathbf{1}$, we see that $A^{\top} B$ follows a Binomial (S, p_1) distribution conditional on S, and therefore,

$$\mathbb{E}\left[\frac{A^{\top}\mathbf{1}+c+1}{A^{\top}B+c+1} \mid S\right] = \mathbb{E}\left[\frac{S+c+1}{\text{Binomial}(S,p_1)+c+1} \mid S\right] \leq \frac{S+c}{Sp_1+c},$$

where the last step holds by Step 1. We can also observe that $s \mapsto \frac{s+c}{sp_1+c}$ is a concave function, and so

$$\mathbb{E}\left[\frac{A^{\top}\mathbf{1} + c + 1}{A^{\top}B + c + 1}\right] = \mathbb{E}\left[\mathbb{E}\left[\frac{A^{\top}\mathbf{1} + c + 1}{A^{\top}B + c + 1} \mid S\right]\right]$$

$$\leq \mathbb{E}\left[\frac{S + c}{Sp_1 + c}\right] \leq \frac{\mathbb{E}\left[S\right] + c}{\mathbb{E}\left[S\right] \cdot p_1 + c} = \frac{a^{\top}\mathbf{1} + c}{a^{\top}\mathbf{1} \cdot p_1 + c}.$$

This proves the claim for the case that the p_i 's are equal.

Step 3: arbitrary weights and arbitrary p_i 's. We will proceed by induction. For n = 1, we have

$$\mathbb{E}_{B_1 \sim \text{Bernoulli}(p_1)} \left[\frac{a_1 + c + 1}{a_1 B_1 + c + 1} \right] = p_1 \cdot \frac{a_1 + c + 1}{a_1 + c + 1} + (1 - p_1) \cdot \frac{a_1 + c + 1}{c + 1}$$

$$= 1 + (1 - p_1) \cdot \frac{a_1}{c + 1}$$

$$\leq 1 + (1 - p_1) \cdot \frac{a_1}{a_1 p_1 + c} \text{ since } a_1 p_1 \leq 1$$

$$= \frac{a_1 + c}{a_1 p_1 + c},$$

proving the claim as desired.

Now suppose $n \geq 2$. Without loss of generality, assume $p_1 \leq \cdots \leq p_n$. If $p_n = 0$ then the claim is trivial. Otherwise, let $A_i \stackrel{\mathbb{I}}{\sim} \text{Bernoulli}(p_i/p_n)$ for $i = 1, \dots, n-1$, and let $C_i \stackrel{\text{iid}}{\sim} \text{Bernoulli}(p_n)$ for $i = 1, \dots, n$. Then $a_1B_1 + \cdots + a_nB_n$ is equal in distribution to $a_1A_1C_1 + \cdots + a_{n-1}A_{n-1}C_{n-1} + a_nC_n$.

Next define random weights $W = (W_1, \ldots, W_n)$ where $W_i = a_i A_i$ for $i = 1, \ldots, n-1$ and $W_n = a_n$. Then by Step 2, we have

$$\mathbb{E}\left[\frac{W_1 + \dots + W_n + c + 1}{W_1 C_1 + \dots + W_n C_n + c + 1} \mid W\right] \le \frac{W^\top \mathbf{1} + c}{W^\top \mathbf{1} \cdot p_n + c}.$$

Equivalently, we have shown that

$$\mathbb{E}\left[\frac{a_{-n}^{\top}A + a_n + c + 1}{a^{\top}B + c + 1} \mid A\right] \le \frac{a_{-n}^{\top}A + a_n + c}{(a_{-n}^{\top}A + a_n) \cdot p_n + c} = \frac{1}{p_n} - \frac{c\left(\frac{1}{p_n} - 1\right)}{(a_{-n}^{\top}A + a_n) \cdot p_n + c}.$$

Next,

$$\begin{split} \mathbb{E}\left[\frac{a^{\intercal}\mathbf{1}+c+1}{a^{\intercal}B+c+1}\right] &= \mathbb{E}\left[\frac{a^{\intercal}\mathbf{1}+c+1}{a_{-n}^{\intercal}A+a_{n}+c+1} \cdot \frac{a_{-n}^{\intercal}A+a_{n}+c+1}{a^{\intercal}B+c+1}\right] \\ &= \mathbb{E}\left[\frac{a^{\intercal}\mathbf{1}+c+1}{a_{-n}^{\intercal}A+a_{n}+c+1} \cdot \mathbb{E}\left[\frac{a_{-n}^{\intercal}A+a_{n}+c+1}{a^{\intercal}B+c+1} \mid A\right]\right] \\ &\leq \mathbb{E}\left[\frac{a^{\intercal}\mathbf{1}+c+1}{a_{-n}^{\intercal}A+a_{n}+c+1} \cdot \left(\frac{1}{p_{n}}-\frac{c\left(\frac{1}{p_{n}}-1\right)}{(a_{-n}^{\intercal}A+a_{n}) \cdot p_{n}+c}\right)\right] \\ &\leq \mathbb{E}\left[\frac{a^{\intercal}\mathbf{1}+c+1}{a_{-n}^{\intercal}A+a_{n}+c+1}\right] \cdot \mathbb{E}\left[\frac{1}{p_{n}}-\frac{c\left(\frac{1}{p_{n}}-1\right)}{(a_{-n}^{\intercal}A+a_{n}) \cdot p_{n}+c}\right], \end{split}$$

where the last step holds since the first quantity is a monotone decreasing function of $a_{-n}^{\top}A$, and the second quantity is a monotone increasing function of $a_{-n}^{\top}A$. By induction, we can apply (41) at size n-1 in place of n to see that the first expected value is bounded as

$$\mathbb{E}\left[\frac{a^{\top}\mathbf{1} + c + 1}{a_{-n}^{\top}A + a_n + c + 1}\right] \le \frac{a^{\top}\mathbf{1} + c}{a_{-n}^{\top}(p_n^{-1}p_{-n}) + a_n + c} = p_n \cdot \frac{a^{\top}\mathbf{1} + c}{a^{\top}p + cp_n},$$

and therefore we have shown so far that

$$\mathbb{E}\left[\frac{a^{\top}\mathbf{1} + c + 1}{a^{\top}B + c + 1}\right] \leq p_n \cdot \frac{a^{\top}\mathbf{1} + c}{a^{\top}p + cp_n} \cdot \mathbb{E}\left[\frac{1}{p_n} - \frac{c\left(\frac{1}{p_n} - 1\right)}{(a_{-n}^{\top}A + a_n) \cdot p_n + c}\right].$$

Next, applying Jensen's inequality, we calculate

$$\mathbb{E}\left[\frac{1}{p_n} - \frac{c\left(\frac{1}{p_n} - 1\right)}{(a_{-n}^\top A + a_n) \cdot p_n + c}\right] \le \left(\frac{1}{p_n} - \frac{c\left(\frac{1}{p_n} - 1\right)}{(a_{-n}^\top \mathbb{E}\left[A\right] + a_n) \cdot p_n + c}\right)$$

$$= \left(\frac{1}{p_n} - \frac{c\left(\frac{1}{p_n} - 1\right)}{(a_{-n}^\top (p_n^{-1} p_{-n}) + a_n) \cdot p_n + c}\right)$$

$$= \left(\frac{1}{p_n} - \frac{c\left(\frac{1}{p_n} - 1\right)}{a^\top p + c}\right)$$

$$= \frac{a^\top p + cp_n}{p_n(a^\top p + c)},$$

and so combining with the work above we have

$$\mathbb{E}\left[\frac{a^{\top}\mathbf{1} + c + 1}{a^{\top}B + c + 1}\right] \le p_n \cdot \frac{a^{\top}\mathbf{1} + c}{a^{\top}p + cp_n} \cdot \frac{a^{\top}p + cp_n}{p_n(a^{\top}p + c)} = \frac{a^{\top}\mathbf{1} + c}{a^{\top}p + c},$$

which proves that (41) holds as desired.

E.4 Proof of Theorem 4

Since nonexchangeable split conformal is simply a special case of nonexchangeable full conformal, we only need to prove the result for full conformal. We recall from the proof of Theorem 2b, found in Section 7.2, that for nonexchangeable full conformal, the coverage event can be characterized as

$$Y_{n+1} \in \widehat{C}_n(X_{n+1}) \iff R_{n+1}^{K,Y_{n+1}} \le Q_{1-\alpha} \left(\sum_{i=1}^{n+1} \widetilde{w}_i \cdot \delta_{R_i^{K,Y_{n+1}}} \right),$$

or equivalently,

$$Y_{n+1} \in \widehat{C}_n(X_{n+1}) \Leftrightarrow R_{\text{fullCP}}(Z^K)_K \leq \mathsf{Q}_{1-\alpha} \left(\sum_{i=1}^{n+1} \widetilde{w}_{\pi_K(i)} \cdot \delta_{R_{\text{fullCP}}(Z^K)_i} \right).$$

Therefore,

$$\begin{split} & \mathbb{P}\left\{Y_{n+1} \in \widehat{C}_n(X_{n+1})\right\} \\ & = \mathbb{P}\left\{R_{\text{fullCP}}(Z^K)_K \leq \mathsf{Q}_{1-\alpha}\left(\sum_{i=1}^{n+1} \tilde{w}_{\pi_K(i)} \cdot \delta_{R_{\text{fullCP}}(Z^K)_i}\right)\right\} \\ & = \sum_{k=1}^{n+1} \mathbb{P}\left\{K = k \text{ and } R_{\text{fullCP}}(Z^k)_k \leq \mathsf{Q}_{1-\alpha}\left(\sum_{i=1}^{n+1} \tilde{w}_{\pi_k(i)} \cdot \delta_{R_{\text{fullCP}}(Z^k)_i}\right)\right\} \\ & = \sum_{k=1}^{n+1} \tilde{w}_k \cdot \mathbb{P}\left\{R_{\text{fullCP}}(Z^k)_k \leq \mathsf{Q}_{1-\alpha}\left(\sum_{i=1}^{n+1} \tilde{w}_{\pi_k(i)} \cdot \delta_{R_{\text{fullCP}}(Z^k)_i}\right)\right\} \\ & \leq \sum_{k=1}^{n+1} \tilde{w}_k \cdot \mathbb{P}\left\{R_{\text{fullCP}}(Z)_k \leq \mathsf{Q}_{1-\alpha}\left(\sum_{i=1}^{n+1} \tilde{w}_{\pi_k(i)} \cdot \delta_{R_{\text{fullCP}}(Z)_i}\right)\right\} \\ & + \sum_{k=1}^{n+1} \tilde{w}_k \cdot \mathsf{d}_{\mathsf{TV}}(R_{\text{fullCP}}(Z), R_{\text{fullCP}}(Z^k)) \\ & = \mathbb{E}\left[\sum_{k=1}^{n+1} \tilde{w}_k \cdot \mathbb{I}\left\{R_{\text{fullCP}}(Z)_k \leq \mathsf{Q}_{1-\alpha}\left(\sum_{i=1}^{n+1} \tilde{w}_{\pi_k(i)} \cdot \delta_{R_{\text{fullCP}}(Z)_i}\right)\right\}\right] \\ & + \sum_{k=1}^{n+1} \tilde{w}_k \cdot \mathsf{d}_{\mathsf{TV}}(R_{\text{fullCP}}(Z), R_{\text{fullCP}}(Z^k)). \end{split}$$

Here, as in the proof of Theorem 2b, the third equality holds since K is drawn independently from Z. Below, we will show that, for any distinct and fixed $r_1, \ldots, r_{n+1} \in \mathbb{R}$, it holds that

$$\sum_{k=1}^{n+1} \tilde{w}_k \cdot \mathbb{1} \left\{ r_k \le \mathsf{Q}_{1-\alpha} \left(\sum_{i=1}^{n+1} \tilde{w}_{\pi_k(i)} \cdot \delta_{r_i} \right) \right\} < 1 - \alpha + \tilde{w}_{n+1}. \tag{42}$$

By applying this inequality with $r_i = R_{\text{fullCP}}(Z)_i$ (and recalling that, by assumption of the theorem, the values $R_{\text{fullCP}}(Z)_1, \ldots, R_{\text{fullCP}}(Z)_{n+1}$ are distinct with probability 1), we obtain

$$\mathbb{P}\left\{Y_{n+1} \in \widehat{C}_n(X_{n+1})\right\} \leq 1 - \alpha + \tilde{w}_{n+1} + \sum_{k=1}^{n+1} \tilde{w}_k \cdot \mathsf{d}_{\mathsf{TV}}(R_{\mathsf{fullCP}}(Z), R_{\mathsf{fullCP}}(Z^k)),$$

which completes the proof of the theorem.

Now we need to verify (42). Define

$$\mathcal{K} = \left\{ k \in [n+1] : r_k \le \mathsf{Q}_{1-\alpha} \left(\sum_{i=1}^{n+1} \tilde{w}_{\pi_k(i)} \cdot \delta_{r_i} \right) \right\},\,$$

so that proving (42) is equivalent to proving that $\sum_{k \in \mathcal{K}} \tilde{w}_k \leq 1 - \alpha + \tilde{w}_{n+1}$. Let

$$k_* = \arg\max_{k} \left\{ r_k : k \in \mathcal{K} \right\},$$

indexing the largest value r_k over indices $k \in \mathcal{K}$. Since $k_* \in \mathcal{K}$ by definition,

$$r_{k_*} \leq \mathsf{Q}_{1-\alpha} \left(\sum_{i=1}^{n+1} \tilde{w}_{\pi_{k_*}(i)} \cdot \delta_{r_i} \right) \quad \Rightarrow \quad \sum_{i=1}^{n+1} \tilde{w}_{\pi_{k_*}(i)} \cdot \mathbb{1} \left\{ r_i < r_{k_*} \right\} < 1 - \alpha.$$

And, since k_* is defined to attain the maximum, we also have $\mathcal{K} \subseteq \{k \in [n+1] : r_k \leq r_{k_*}\}$. Therefore,

$$\begin{split} \sum_{k \in \mathcal{K}} \tilde{w}_k & \leq \sum_{k=1}^{n+1} \tilde{w}_k \cdot \mathbbm{1} \left\{ r_k \leq r_{k_*} \right\} \\ & = \tilde{w}_{k_*} + \sum_{k=1}^{n+1} \tilde{w}_k \cdot \mathbbm{1} \left\{ r_k < r_{k_*} \right\} \quad \text{since the } r_k \text{'s are distinct} \\ & = \tilde{w}_{k_*} + \sum_{k=1}^{n+1} \left(\tilde{w}_k - \tilde{w}_{\pi_{k_*}(k)} \right) \cdot \mathbbm{1} \left\{ r_k < r_{k_*} \right\} + \sum_{k=1}^{n+1} \tilde{w}_{\pi_{k_*}(k)} \cdot \mathbbm{1} \left\{ r_k < r_{k_*} \right\} \\ & < \tilde{w}_{k_*} + \sum_{k=1}^{n+1} \left(\tilde{w}_k - \tilde{w}_{\pi_{k_*}(k)} \right) \cdot \mathbbm{1} \left\{ r_k < r_{k_*} \right\} + (1 - \alpha) \quad \text{by the calculations above.} \end{split}$$

Finally, consider the term $(\tilde{w}_k - \tilde{w}_{\pi_{k_*}(k)}) \cdot \mathbb{1} \{r_k < r_{k_*}\}$ in the remaining sum. If $k = k_*$, then $\mathbb{1} \{r_k < r_{k_*}\} = 0$. If k = n + 1, then

$$\left(\tilde{w}_{k} - \tilde{w}_{\pi_{k_{*}}(k)}\right) \cdot \mathbb{1}\left\{r_{k} < r_{k_{*}}\right\} = \left(\tilde{w}_{n+1} - \tilde{w}_{k_{*}}\right) \cdot \mathbb{1}\left\{r_{k} < r_{k_{*}}\right\} \leq \tilde{w}_{n+1} - \tilde{w}_{k_{*}}$$

If $k \notin \{k_*, n+1\}$, then $\pi_{k_*}(k) = k$ and so the term is again zero. Therefore, we have $\sum_{k=1}^{n+1} \left(\tilde{w}_k - \tilde{w}_{\pi_{k_*}(k)} \right) \cdot \mathbb{1} \left\{ r_k < r_{k_*} \right\} \leq \tilde{w}_{n+1} - \tilde{w}_{k_*}$, and combining this with the work above, we have shown that

$$\sum_{k \in \mathcal{K}} \tilde{w}_k < 1 - \alpha + \tilde{w}_{n+1}.$$

This completes the proof of (42), and thus we have proved the theorem.

E.5 Calculations for (22)

Define $U = \frac{\mathcal{P}_X^{\perp}(\epsilon)}{\|\mathcal{P}_X^{\perp}(\epsilon)\|_2}$ and $L = \|\mathcal{P}_X^{\perp}(\epsilon)\|_2$. Then $R = U \cdot L$, and (U, L) can be written as a function of R, and in particular we have

$$d_{\mathsf{TV}}(U, U^i) \le d_{\mathsf{TV}}((U, L), (U^i, L^i)) = d_{\mathsf{TV}}(R, R^i).$$

On the other hand, conditional on X, we know that $U \perp L$, with $L \sim \sigma \cdot \chi_{n+1-p}$. Therefore, $\mathsf{d}_{\mathsf{TV}}((U,L),(U^i,L^i)) = \mathsf{d}_{\mathsf{TV}}(U,U^i)$ and so we have shown

$$\mathsf{d}_{\mathsf{TV}}(R, R^i) = \mathsf{d}_{\mathsf{TV}}(U, U^i)$$

and now we only need to bound this last term.

Conditional on the subspace $\operatorname{span}(X)^{\perp}$, the unit vector U is drawn uniformly from this subspace intersected with the unit sphere, and therefore the joint density of (X, U) is given by

$$f(x, u) \propto \frac{1}{(2\pi)^{(n+1)p/2} |\Sigma|^{1/2}} e^{-\text{vec}(x)^{\top} \Sigma^{-1} \text{vec}(x)/2}$$

with respect to Lebesgue measure on the manifold $\{(x,u) \in \mathbb{R}^{(n+1)\times p} \times \mathbb{S}^n : x \perp u\}$. Therefore the marginal density of u is given by

$$g(u) \propto \int_{x \in \mathbb{R}^{(n+1) \times p}; x \perp u} \frac{1}{(2\pi)^{(n+1)p/2} |\Sigma|^{1/2}} e^{-\operatorname{vec}(x)^{\top} \Sigma^{-1} \operatorname{vec}(x)/2} \, \mathrm{d}x$$

where the integral is taken over the np-dimensional subspace of matrices x where all columns are orthogonal to u. Equivalently we can take x = Wy where $W \in \mathbb{R}^{(n+1)p \times np}$ is an orthonormal basis for the subspace orthogonal to u, and so

$$\begin{split} g(u) &\propto \int_{y \in \mathbb{R}^{n \times p}} \frac{1}{(2\pi)^{(n+1)p/2} |\Sigma|^{1/2}} e^{-(W \text{vec}(y))^\top \Sigma^{-1}(W \text{vec}(y))/2} \; \mathrm{d}y \\ &= \frac{(2\pi)^{np/2} |(W^\top \Sigma^{-1} W)^{-1}|^{1/2}}{(2\pi)^{(n+1)p/2} |\Sigma|^{1/2}} \cdot \int_{y \in \mathbb{R}^{n \times p}} \frac{1}{(2\pi)^{np/2} |(W^\top \Sigma^{-1} W)^{-1}|^{1/2}} e^{-(W \text{vec}(y))^\top \Sigma^{-1}(W \text{vec}(y))/2} \; \mathrm{d}y \\ &= \frac{(2\pi)^{np/2} |(W^\top \Sigma^{-1} W)^{-1}|^{1/2}}{(2\pi)^{(n+1)p/2} |\Sigma|^{1/2}} \propto |(W^\top \Sigma^{-1} W)^{-1}|^{1/2} = |W^\top \Sigma^{-1} W|^{-1/2}. \end{split}$$

Since $(W \mid u \otimes \mathbf{I}_p)$ is an orthogonal matrix, we can verify through matrix identities that

$$|W^{\top}\Sigma^{-1}W| = |(u \otimes \mathbf{I}_p)^{\top}\Sigma(u \otimes \mathbf{I}_p)| \cdot |\Sigma|^{-1},$$

and therefore,

$$g_U(u) = g(u) \propto \frac{1}{\sqrt{|(u \otimes \mathbf{I}_p)^{\top} \Sigma(u \otimes \mathbf{I}_p)|}}.$$

We can also calculate

$$g_{U^i}(u) = g(u^i) \propto \frac{1}{\sqrt{|(u^i \otimes \mathbf{I}_p)^\top \Sigma (u^i \otimes \mathbf{I}_p)|}},$$

and note that these two densities have the same normalizing constant, so we have

$$\frac{g_{U^i}(u)}{g_U(u)} = \frac{g(u^i)}{g(u)} = \sqrt{\frac{|(u \otimes \mathbf{I}_p)^\top \Sigma (u \otimes \mathbf{I}_p)|}{|(u^i \otimes \mathbf{I}_p)^\top \Sigma (u^i \otimes \mathbf{I}_p)|}}.$$

Next, the multiplicative property of the determinant yields

$$|(u^{i} \otimes \mathbf{I}_{p})^{\top} \Sigma(u^{i} \otimes \mathbf{I}_{p})| = |(u \otimes \mathbf{I}_{p})^{\top} \Sigma(u \otimes \mathbf{I}_{p})|$$

$$\cdot \left| \left((u \otimes \mathbf{I}_{p})^{\top} \Sigma(u \otimes \mathbf{I}_{p}) \right)^{-1/2} \cdot (u^{i} \otimes \mathbf{I}_{p})^{\top} \Sigma(u^{i} \otimes \mathbf{I}_{p}) \cdot \left((u \otimes \mathbf{I}_{p})^{\top} \Sigma(u \otimes \mathbf{I}_{p}) \right)^{-1/2} \right|,$$

and so

$$\frac{g_{U^i}(u)}{g_U(u)} = \frac{1}{\sqrt{\left| ((u \otimes \mathbf{I}_p)^\top \Sigma (u \otimes \mathbf{I}_p))^{-1/2} \cdot (u^i \otimes \mathbf{I}_p)^\top \Sigma (u^i \otimes \mathbf{I}_p) \cdot ((u \otimes \mathbf{I}_p)^\top \Sigma (u \otimes \mathbf{I}_p))^{-1/2} \right|}}$$

Next, for any positive definite matrices $A, B \in \mathbb{R}^{p \times p}$, we calculate

$$|A^{-1/2} \cdot B \cdot A^{-1/2}| \le ||A^{-1/2} \cdot B \cdot A^{-1/2}||^p = ||\mathbf{I}_p + A^{-1/2} \cdot (B - A) \cdot A^{-1/2}||^p \le (1 + ||A^{-1/2} \cdot (B - A) \cdot A^{-1/2}||)^p \le (1 + ||A^{-1}|| \cdot ||B - A||)^p,$$

and so applying this with $A = (u \otimes \mathbf{I}_p)^{\top} \Sigma(u \otimes \mathbf{I}_p)$ and $B = (u^i \otimes \mathbf{I}_p)^{\top} \Sigma(u^i \otimes \mathbf{I}_p)$, we have

$$\frac{g_{U^i}(u)}{g_U(u)} \ge \left(1 + \|\Sigma^{-1}\| \cdot \|(u^i \otimes \mathbf{I}_p)^\top \Sigma (u^i \otimes \mathbf{I}_p) - (u \otimes \mathbf{I}_p)^\top \Sigma (u \otimes \mathbf{I}_p) \|\right)^{-p/2}$$

Now we calculate the remaining matrix norm. Fix any unit vector $v \in \mathbb{R}^p$. We have

$$\begin{aligned} & \left| v^{\top} \left((u^{i} \otimes \mathbf{I}_{p})^{\top} \Sigma (u^{i} \otimes \mathbf{I}_{p}) - (u \otimes \mathbf{I}_{p})^{\top} \Sigma (u \otimes \mathbf{I}_{p}) \right) v \right| \\ &= \left| (u^{i} \otimes v)^{\top} \Sigma (u^{i} \otimes v) - (u \otimes v)^{\top} \Sigma (u \otimes v) \right| \\ &= \left| (u^{i} \otimes v)^{\top} \Sigma ((u^{i} - u) \otimes v) + ((u^{i} - u) \otimes v)^{\top} \Sigma (u \otimes v) \right| \\ &\leq \left\| \Sigma \right\| \cdot \left(\left\| u^{i} \otimes v \right\|_{2} \cdot \left\| (u^{i} - u) \otimes v \right\|_{2} + \left\| (u^{i} - u) \otimes v \right\|_{2} \cdot \left\| u \otimes v \right\|_{2} \right) \\ &= \left\| \Sigma \right\| \cdot \left(\left\| u^{i} \right\|_{2} \cdot \left\| v \right\|_{2} \cdot \left\| u^{i} - u \right\|_{2} \cdot \left\| v \right\|_{2} + \left\| u^{i} - u \right\|_{2} \cdot \left\| v \right\|_{2} \cdot \left\| v \right\|_{2} \cdot \left\| v \right\|_{2} \right) \\ &= 2 \left\| \Sigma \right\| \left\| u^{i} - u \right\|_{2} \\ &= \sqrt{8} \left\| \Sigma \right\| \left| u_{i} - u_{n+1} \right|. \end{aligned}$$

Combining everything so far, then, we have

$$\frac{g_{U^i}(u)}{g_U(u)} \ge \left(1 + \sqrt{8}\|\Sigma\|\|\Sigma^{-1}\||u_i - u_{n+1}|\right)^{-p/2} = \left(1 + \sqrt{8}\kappa_{\Sigma}|u_i - u_{n+1}|\right)^{-p/2}.$$

In particular, this implies that

$$1 - \frac{g_{U^i}(u)}{g_{U^i}(u)} \le 1 - \left(1 + \sqrt{8}\kappa_{\Sigma}|u_i - u_{n+1}|\right)^{-p/2} \le p\sqrt{2}\kappa_{\Sigma} \cdot |u_i - u_{n+1}|.$$

Next we have

$$\begin{split} \mathrm{d}_{\mathsf{TV}}(U,U^i) &= \int_{u \in \mathbb{S}^n} \left(g_U(u) - g_{U^i}(u) \right)_+ \, \mathrm{d}u \\ &= \int_{u \in \mathbb{S}^n} g_U(u) \left(1 - \frac{g_{U^i}(u)}{g_U(u)} \right)_+ \, \mathrm{d}u \\ &\leq \int_{u \in \mathbb{S}^n} g_U(u) \cdot p \sqrt{2} \kappa_\Sigma \cdot |u_i - u_{n+1}| \, \mathrm{d}u \\ &= \mathbb{E} \left[p \sqrt{2} \kappa_\Sigma \cdot |U_i - U_{n+1}| \right] \\ &\leq p \sqrt{2} \kappa_\Sigma \cdot (\mathbb{E} \left[|U_i| \right] + \mathbb{E} \left[|U_{n+1}| \right] \right). \end{split}$$

Now we need to bound $\mathbb{E}[|U_i|]$. Recall that $R = U \cdot L$, with $U \perp L \mid X$. We can therefore calculate

$$\mathbb{E}\left[R_i^2 \mid X\right] = \mathbb{E}\left[U_i^2 \cdot L^2 \mid X\right] = \mathbb{E}\left[U_i^2 \mid X\right] \cdot \mathbb{E}\left[L^2 \mid X\right] = \mathbb{E}\left[U_i^2 \mid X\right] \cdot \sigma^2(n+1-p),$$

since $L \mid X \sim \sigma \cdot \chi_{n+1-p}$. Therefore,

$$\mathbb{E}\left[U_i^2 \mid X\right] = \frac{\mathbb{E}\left[R_i^2 \mid X\right]}{\sigma^2(n+1-p)}.$$

We also have $R = \mathcal{P}_X^{\perp}(\epsilon)$, and so

$$R \mid X \sim \mathcal{N}(0, \sigma^2 \mathcal{P}_X^{\perp}),$$

and therefore,

$$\mathbb{E}\left[R_i^2 \mid X\right] = \sigma^2(\mathcal{P}_X^{\perp})_{ii} \le \sigma^2.$$

This proves

$$\mathbb{E}\left[U_i^2 \mid X\right] \le \frac{1}{n+1-n}$$

and therefore

$$\mathbb{E}\left[|U_i|\right] \le \sqrt{\mathbb{E}\left[U_i^2\right]} \le \frac{1}{\sqrt{n+1-p}}.$$

Since this also holds for U_{n+1} in place of U_i , we therefore have

$$\mathsf{d}_{\mathsf{TV}}(U, U^i) \le \kappa_{\Sigma} \sqrt{8} \cdot \frac{p}{\sqrt{n+1-p}}.$$