T-SCI: A Two-Stage Conformal Inference Algorithm with Guaranteed Coverage for Cox-MLP

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Abstract
It is challenging to deal with censored data, where we only have access to the incomplete information of survival time instead of its exact value. Fortunately, under linear predictor assumption, people can obtain guaranteed coverage for the confidence band of survival time using methods like Cox Regression. However, when relaxing the linear assumption with neural networks (e.g., Cox-MLP (Katzman et al., 2018; Kvamme et al., 2019)), we lose the guaranteed coverage. To recover the guaranteed coverage without linear assumption, we propose two algorithms based on conformal inference. In the first algorithm WCCI, we revisit weighted conformal inference and introduce a new non-conformity score based on partial likelihood. We then propose a two-stage algorithm T-SCI, where we run WCCI in the first stage and apply quantile conformal inference to calibrate the results in the second stage. Theoretical analysis shows that T-SCI returns guaranteed coverage under milder assumptions than WCCI. We conduct extensive experiments on synthetic data and real data using different methods, which validate our analysis.

1. Introduction
In survival analysis, censoring indicates that the value of interest (survival time) is only partially known (e.g., the information can be \( t > 5 \) instead of \( t = 7 \)). It is common and inevitable in numerous fields, including medical care (Robins & Finkelstein, 2000; Klein & Moeschberger, 2006), astronomy (Feldmann, 2019), finance (Bellotti & Crook, 2009), etc. It is an annoying issue since ignoring or deleting censored data causes bias and inefficiency (Nakagawa & Freckleton, 2008), as illustrated in Figure 1.

Figure 1. Bias in censoring. Ignoring (middle) or deleting (bottom) censored data (light blue) causes bias compared to the ground truth (top) linear approximation (red line), where the linear approximation under censoring (black) does not overlap the ground truth (red).

When dealing with censored data, we usually focus on the confidence band of the survival time since confidence bands give a more conservative estimation than point estimation. Under linear assumptions on covariate effect (See Assumption 1), one can derive the survival time distribution using Cox regression by asymptotic normality of linear coefficient. It further leads to guaranteed coverage, meaning that survival time provably falls into the confidence band with high probability (larger than the given confidence level).

However, the linear assumption broadly harms its performances and restricts its applications. After all, the reality is not always entirely linear. To relax the linear assumption, Katzman et al. (2018); Kvamme et al. (2019) applies neural networks into Cox regression (Cox-MLP), yielding the best performance in terms of some metrics such as Brier score and binomial log-likelihood. Unfortunately, the confidence band in Cox-MLP has no guaranteed coverage since one cannot expect neural network converges to the expected function, not to mention the asymptotic normality.

In general, we can use conformal inference to recover the
confidence band with guaranteed coverage by splitting the dataset into training and calibration set (Vovk et al., 2005; Nouretdinov et al., 2011; Lei & Cand`es, 2020). One of its advantages is that conformal inference does not harm the model performance since it is post-hoc. Therefore, we propose to apply conformal inference into Cox-MLP.

When applying conformal inference into Cox-MLP, there are several problems to be solved. Firstly, Cox-regression does not return survival time explicitly, which requires a modification of the non-conformity score. Secondly, censoring causes covariate shift, meaning that the covariate distribution differs in censored and uncensored data. Therefore, we cannot apply conformal inference directly. Thirdly, we need to consider the estimation error and provide theoretical guarantees for the coverage.

In this paper, we propose a new non-conformity score based on the partial likelihood of Cox regression. This non-conformity score does not need an explicit estimation of the survival time. We then apply weighted conformal conformal inference (WCCI), a weighted conformal inference based on this non-conformity score inspired by Tibshirani & Foygel (2019) to deal with the covariate shift problem. Furthermore, inspired by Romano et al. (2019), we provide a two-stage conformal inference (T-SCI) which returns “nearly perfect” coverage, meaning that the coverage has not only guaranteed lower bound but also upper bound. Inspired by (Lei & Cand`es, 2020), we provide theoretical guarantees for both WCCI and T-SCI algorithms.

We summarize our contributions as follows:

- We provide coverage for Cox-MLP in WCCI based on weighted conformal inference frameworks by introducing a new non-conformity score.
- We further propose a T-SCI algorithm based on the quantile conformal inference framework. We show that T-SCI returns nearly perfect guaranteed coverage, namely, theoretical guarantees for coverage’s lower and upper bound.
- We conduct extensive experiments on both synthetic data and real-world data, showing that T-SCI based algorithm outperforms other approaches in terms of empirical coverage and interval length.

2. Related work

Censored data analysis. An early analysis of censored data can be dating back to the famous Kaplan–Meier estimator Kaplan & Meier (1958). However, this approach is valid only when all patients have the same survival function. Therefore, several individual-level analysis is proposed, such as proportional hazard model (Breslow, 1975) and accelerated failure time model (Wei, 1992).

On the other hand, researchers apply machine learning techniques to deal with censored data. For example, random survival forests (Ishwaran et al., 2008) train random forests using the log-rank test as the splitting criterion. Moreover, DeepHit (Lee et al., 2018) apply neural networks to estimate the probability mass function and introduce a ranking loss. This paper mainly focuses on the Cox-based model, one of the famous proportional hazard model branches.

Cox regression was first proposed in Cox (1972), which is a semi-parametric method focusing on estimating the hazard function. Among all its extensions, Akritas et al. (1995) first proposed using a one-hidden layer perceptron to replace the linear predictor of the coefficient. However, it generally failed mainly due to the low expressivity of the one-hidden layer perceptron (Xiang et al., 2000; Sargent, 2001). Therefore, Katzman et al. (2018) proposed to use the multi-layer perceptron instead of the one-layer perceptron (DeepSurv). Furthermore, (Kvamme et al., 2019) generalize the idea to the non-proportional hazard settings. In this paper, we unify their names as Cox-MLP when the context is clear. However, this line of work lacks a theoretical guarantee. This paper tries to fill this blank and propose the first guaranteed coverage of the survival time.

Conformal inference was pioneered by Vladimir Vovk and his collaborators [e.g., Vovk et al. (2005); Shafer & Vovk (2008); Nouretdinov et al. (2011)], focusing on the inference of response variables by splitting a training fold and a calibration fold. There are several variations of conformal inference. For example, weighted conformal inference (Tibshirani & Foygel, 2019) focus on dealing with the covariate shift phenomenon, and quantile conformal inference (Romano et al., 2019) returns coverage with not only an upper bound but also the lower bound guaranteed coverage. Conformal inference, as well as its variations, are widely studied and used in Lei et al. (2013); Lei & Wasserman (2014); Lei et al. (2018); Barber et al. (2019b); Sadinle et al. (2019); Romano et al. (2020).

Recently, Lei & Cand`es (2020) apply conformal inference under counterfactual settings and derive a double robust guarantee for their proposed methods. Our work is partially inspired by Lei & Cand`es (2020) but considers a different censoring setting. Furthermore, we propose a different algorithm and derive a “nearly perfect” guaranteed coverage.

There are some approaches to apply conformal inference under censoring settings. For example, Bostr et al. (2017); Boström et al. (2019) apply conformal inference into random survival forests, and Chen (2020) derive the confidence band for DeepHit. However, these approaches cannot be applied to Cox-based models since Cox-based models do not explicitly return a predicted survival time.
3. Preliminary

Denote $X \sim \mathcal{P}_X \subset \mathbb{R}^d$ as the covariate, $T \sim \mathcal{P}_T \subset \mathbb{R}$ as the survival time, and $C \sim \mathcal{P}_C \subset \mathbb{R}$ as the censoring time. Denote the joint distribution as $\mathcal{P}_{XTC}$, its marginal distribution as $\mathcal{P}_{TC}$, and its conditional distribution as $\mathcal{P}_{T|X}$. The survival time cannot be observed when it is larger than the censoring time. Therefore, observed time is the minimum of censoring time and survival time. Let $Y \in \mathbb{R}$ be the observed time with uncensoring indicator $\Delta \in \mathbb{R}$, then

$$Y = \min\{T, C\}, \quad \Delta = \mathbb{I}_{\{T \leq C\}}.$$  

Denote the dataset as $Z = \{X_i, Y_i, \Delta_i\}_{i \in \mathcal{I}}$ where we can only access the covariate, the observed time, and the censoring indicator. However, the value of interest is the survival time $T$. Therefore, the censored data is incomplete due to the information loss when $\Delta = 0$. We next introduce how censoring happens, namely, censoring mechanism.

Censoring Mechanism. In this paper, we consider the random censoring regimes, which assumes that $C$ is independent of $T$ given $X$, namely, $C \perp T \mid X$.

However, under random censoring regimes, there can be covariate shift, namely, the distributions of covariate $X$ under censoring and non-censoring are different

$$(X \mid \Delta = 1) \overset{d}{\neq} (X \mid \Delta = 0).$$

Why does covariate shift happen? The fundamental reason is that samples with larger survival time are more likely to be censored even under the random censoring regimes, leading to an implicit bias, namely, covariate shift. We refer to Figure 2 for an illustration.

Under the random censoring regimes, we estimate the distribution of the survival time via the dataset $\mathcal{D}$ by Cox regression. We denote $F_T(t)$ as the survival time’s CDF.

Cox Regression. In Cox regression, we focus on two important terms survival function $S_T(t)$ and cumulative hazard function $\Lambda_T(t)$, as defined in Equation 1. We emphasize that they are defined with respect to the survival time $T$ instead of the observed time $Y$.

$$S_T(t) \triangleq 1 - F_T(t), \quad \Lambda_T(t) \triangleq -\log S_T(t).$$  \hspace{1cm} (1)

When the context is clear, we omit the subscript $T$ and denote the above function as $F(t)$, $S(t)$, and $\Lambda(t)$, respectively. Cox-based models usually require proportional hazard assumption, formally stated in Assumption 1.

Assumption 1 (Proportional Hazard) For each individual $i$, we assume

$$\Lambda_i(t; X_i) = \Lambda_0(t) \exp(g(X_i))$$  \hspace{1cm} (2)

where $\Lambda_0(t)$ is the baseline cumulative hazard function, and $g(X_i)$ is the individual effect named as predictor.

Remark: There are several non-proportional hazard Cox models which replace $g(x_i)$ with $g(x_i, t)$ (e.g., Kvamme et al. (2019)). Although our proposed algorithm can be directly generalized to non-proportional settings, we only consider proportional hazard models for clarity in this paper.

Specifically, Cox regression solves the case when the predictor $g(\cdot)$ is linear by maximizing partial log-likelihood $l(g)$, defined in Equation 3.

$$l(g) \triangleq \sum_{j: \Delta_j = 1} \log \left( \sum_{k \in R(T_j)} \exp[g(X_k) - g(X_j)] \right),$$  \hspace{1cm} (3)

where $R(T_j)$ is the set of all individuals at risk at time $T_j$ (the observed time is no less than $T_j$), and $g(X_j) = X_j^\top \beta$ is the linear predictor.

For the case when $g(\cdot)$ is not linear, Lee et al. (2018) and Kvamme et al. (2019) propose Cox-MLP which uses neural networks to replace the linear predictor $g(X_i)$. Concretely, they use the negative partial log-likelihood as the training loss, with a penalty on the complexity of $g(\cdot)$.

Conformal inference. Conformal inference does post-hoc estimation based on the splitting of training and calibration fold. One trains a model $\mu$ using the training fold and then calculates the non-conformity score $V_i$ on the calibration fold. A commonly used non-conformity score is the absolute error $V_i = |T_i - \mu(X_i)|$ where $(X_i, T_i)$ is the $i$th calibration sample. When designing the non-conformity score, one of the most important characteristics is exchangeability.

Assumption 2 (Exchangeability) For $n \geq 1$ random variables $V_1, \ldots, V_n$, they satisfy exchangeability if

$$(V_1, \ldots, V_n) \overset{d}{=} (V_{\pi(1)}, \ldots, V_{\pi(n)}).$$

1The simulation dataset is from Kvamme et al. (2019)
for any permutation $\pi : [n] \to [n]$, where $d = \pi$ means they have the same distribution, and $[n] = \{1, 2, \ldots, n\}$.

Exchangeability is weaker than independence since independence implies exchangeability. Under the exchangeability assumption on the non-conformity score, we reach a theoretical guarantee of the confidence band. In this paper, we mainly focus on two varieties of conformal inference, weighted conformal inference (to deal with covariate shift, Lemma 1) and quantile conformal inference (to return a nearly perfectly guarantee, Lemma 2), respectively.

**Lemma 1 (WCI, Tibshirani & Foygel (2019) Theorem 2) (Informal.)** Assume that the data $(X_i, T_i), i \in [n + 1]$ are weighted exchangeable with weight $w_1, \ldots, w_{n+1}$, then the returned confidence band $\hat{C}_n$ has guaranteed coverage:

$$
\mathbb{P}(T_{n+1} \in \hat{C}_n(X_{n+1})) \geq 1 - \alpha.
$$

**Remark.** One may wonder why not use $S(t)$ to return the confidence band in Cox-MLP. People usually do so in practice, but the confidence band has no theoretical guarantee in Cox-MLP. To derive the theoretical guarantee under $S(t)$, one needs to show the convergence of the predictor $g(X_i)$. However, it cannot be proved unless the generalization guarantee of neural networks is obtained.

**4. Confidence band for the Survival Time**

In this section, we derive the confidence band for the survival time. We start by analyzing the basic properties and the critical ideas before proposing the algorithm.

**The non-conformity score.** In traditional conformal inference, the most commonly used non-conformity score is the absolute form $V_i = |T_i - \hat{T}_i|$. That is because we can directly derive the confidence band of $T_i$ based on the band of the non-conformity score $V_i$. Unfortunately, it is hard to compute $\hat{T}_i$ in Cox-based models since they output the survival hazard function instead of the survival time, which requires a modification of the non-conformity score.

Inspired by the standard Cox regression, we introduce a non-conformity score based on partial likelihood. Specifically, we use the sample partial log-likelihood as the non-conformity score (shown in Equation 4). Compared to the absolute non-conformity score, the newly proposed non-conformity score $V_i = \tilde{V}_g(X_i, T_i)$ do not need to calculate $\hat{T}_i$ explicitly. Figure 3 illustrates the distribution of the non-conformity score using a simulation dataset.

$$
V_i = \log \left( \sum_{k \in R(T_i)} \exp[g(X_k) - g(X_i)] \right). \quad (4)
$$

**The incomplete data.** Compared to the i.i.d. (independent and identically distributed) data, censored data is incomplete. Notice that we can only calculate the non-conformity scores of the uncensored data in Equation 4 since we cannot obtain the exact value of $T_i$ of censored data. As a result, the returned confidence band is guaranteed under uncensored distribution $\mathcal{P}_{X \mid \Delta = 1}$. However, as mentioned before, there might be a distribution shift between censored data and uncensored data, leading to the requirement of weighted conformal inference (Tibshirani & Foygel, 2019).

In weighted conformal inference, one needs to calculate the weight $w$ based on $w(x)$, where

$$
 w(x) = \frac{d\mathcal{P}_X(x)}{d\mathcal{P}_{X \mid \Delta = 1}(x)} = \frac{\mathbb{P}(T = 1)}{\mathbb{P}(T = 1 \mid X = x)}. \quad (5)
$$

Intuitively, $w(x)$ helps transfer the guarantee over $\mathcal{P}_{X \mid \Delta = 1}$ to $\mathcal{P}_X$. In the following of the paper, we use the regularized weight $p_i$ in the algorithm, namely

$$
p_i = \frac{w(X_i)}{\sum_{i \in \mathcal{I}_{ca}} w(X_i) + w(X')}.
$$

where we denote $X_i$ as the samples from the calibration fold and $X'$ as the testing point.

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2The simulation dataset is from Kvamme et al. (2019)
**Algorithm 1 WCCI: Weighted Conformalize Censoring Inference**

**Input:** Level $\alpha$

**Input:** data $\mathcal{Z} = (X_i, Y_i, \Delta_i)_{i \in I}$, testing point $X'$

**Input:** function $\hat{w}(x; D)$ to fit the weight function at $x$ using $D$ as data

1. Randomly split $\mathcal{Z}$ into a training fold $\mathcal{Z}_{tr} \triangleq (X_i, Y_i, \Delta_i)_{i \in I_{tr}}$, and a calibration fold $\mathcal{Z}_{ca} \triangleq (X_i, Y_i, \Delta_i)_{i \in I_{ca}}$
2. Use $\mathcal{Z}_{tr}$ to train $\hat{g}(\cdot)$ to estimate the predictor function
3. For each $i \in I_{ca}$ with $\Delta_i = 1$, compute the non-conformity score $V_i = \log(\sum_{k \in R(T_i) \cap I_{ca}} \exp[\hat{g}(X_k) - \hat{g}(X_i)])$
4. For each $i \in I_{ca}$ with $\Delta_i = 1$, compute the weight $W_i = \hat{w}(X_i; \mathcal{Z}_{tr})$
5. Calculate the normalized weights $\hat{p}_i = \frac{W_i}{\sum_{i \in I_{ca}} W_i + \hat{w}(X_i; \mathcal{Z}_{tr})}$ and $\hat{p}_\infty = \frac{\hat{w}(X'; \mathcal{Z}_{tr})}{\sum_{i \in I_{ca}} W_i + \hat{w}(X'; \mathcal{Z}_{tr})}$
6. Calculate the $(1 - \alpha)$-th quantile $Q_{1-\alpha}$ of the distribution $\sum_{i \in I_{ solv}} \hat{p}_i \delta_{V_i} + \hat{p}_\infty \delta_\infty$
7. Calculate $T^w(X')$ as the smallest value such that its conformity score $V'$ (dependent on $T^w(X')$) is larger than $Q_{1-\alpha}$

**Output:** $\hat{C}^1(X') = [0, T^w(X')]$.

**Exchangeability.** In conformal inference, we assume that the non-conformity score satisfies exchangeability (See Assumption 2). However, as shown in Equation 4, there is a summation term in the non-conformity score, where we need to sum up all the samples at risk at time $T_j$. Unfortunately, it breaks the exchangeability when we use the at-risk samples in the calibration fold. As an alternative, we use the at-risk samples in the training fold. The non-conformity scores in the calibration fold $V_i$, $i \in [n]$ then satisfies exchangeability given the training fold (See Equation 6).

$$(V_1, \ldots, V_n | D_{tr}) \overset{d}{=} (V_{\pi(1)}, \ldots, V_{\pi(n)} | D_{tr}), \quad (6)$$

with arbitrary permutation $\pi$.

**The recreation of confidence band.** Based on the non-conformity score proposed in Equation 4, we can reconstruct the confidence band for the survival time. We remark that we calculate the one-sided band $[0, T^w(X')]$ although the two-sided band directly follows. For a new sample $X'$, we first calculate the $(1 - \alpha)$ quantile of (weighted) distribution of the non-conformity score, denoted as $Q_{1-\alpha}$. We then calculate the smallest $T^w(X')$ that makes its non-conformity score $V' = V'_\delta(X', T)$ larger than $Q_{1-\alpha}$, formally,

$$Q_{1-\alpha} = \text{Quantile} \left(1 - \alpha, \sum_{i \in I_{ca}} p_i V_i \right)$$

$$T^w(X') = \inf \{ T : V'_\delta(X', T) \geq Q_{1-\alpha} \}.$$ 

**Algorithm.** Based on the discussions above, we conclude our algorithm in Algorithm 1. In training process, we use training fold to train the estimated predictor $\hat{g}(X)$ (defined in Equation 2) and calculate the weight function (defined in Equation 5). We then use calibration fold to calculate the non-conformity score. We finally construct confidence band $[0, T^w(X')]$ for a given testing point $X'$.

**Robustness on $\hat{w}$.** The weighted conformal inference has guaranteed coverage under the true weight $w(x)$ as shown in Lemma 1. However, we can only obtain its estimator $\hat{w}(x)$ in practice. In the following Theorem 4.1, we prove how the estimation influences the coverage. Note that as $\lim_{\mathcal{Z}_{tr} \to \infty} |\hat{w}(x) - w(x)| \to 0$, the coverage can be provably larger than $1 - \alpha$.

**Theorem 4.1 (Provable Guarantee)** Let $\hat{w}(x)$ be an estimate of the weight $w(x)$. Assume that $\mathbb{E}[w(X)|\mathcal{Z}_{tr}] = 1$ and $\mathbb{E}[w(X)] = 1$. Denote $C^1_n(x)$ as the output band of Algorithm 1 with $n$ calibration samples, then for a new data $X'$, its corresponding survival time satisfies

$$\lim_{n \to \infty} \mathbb{P} \left( T' \in C^1_n(X') \right) \geq 1 - \alpha - \frac{1}{2} \mathbb{E}[|\hat{w}(X) - w(X)|],$$

where the probability $\mathbb{P}$ on the left hand side is taken over $(X', T') \sim \mathcal{P}_X \times \mathcal{P}_{T|X}$, and all the expectation operators $\mathbb{E}$ are taken over $X \sim \mathcal{P}_{X|\Delta=1}$.

Theorem 4.1 proves the lower bound for WCCI. However, it is insufficient to derive the upper bound under the weighted conformal inference framework. To derive the upper bound, we propose the algorithm T-SCI in the next section.

**5. T-SCI: Improved Estimation**

In the previous section, we propose WCCI, which has lower bound coverage guarantees. However, for better data efficiency, we want not only lower bound but also lower bounds. To reach the goal, we propose a two-stage algorithm T-SCI, which returns nearly perfect coverage.

The intuition is from Lemma 2, stating that the quantile conformal inference (QCI) returns a nearly perfect guarantee. Inspired by Lemma 2, we first use Algorithm 1 to return a temporal confidence band and then apply Quantile Conformal Inference to modify this band. We summarize the whole algorithm in Algorithm 2.

**Remark 1.** To apply T-SCI in practice, we split the dataset into $\mathcal{Z}_{tr}$, $\mathcal{Z}_{ca1}$ and $\mathcal{Z}_{ca2}$. We first apply Algorithm 1 with $\mathcal{Z}_{tr}$ and $\mathcal{Z}_{ca1}$ and return a confidence band. We then do calibration in Algorithm 2 with $\mathcal{Z}_{ca2}$. 
Algorithm 2: T-SCI: Two-Stage Conformal Inference

Input: Level \( \alpha \)
Input: additional data: \( Z_{ca2} = (X_i, Y_i, \Delta_i)_{i \in I_{ca2}} \), testing point \( X' \)
Input: First-stage band \([\hat{q}_{\alpha_{ls}}(X'; Z_{tr}, Z_{ca1}), \hat{q}_{\alpha_{ls}}(X'; Z_{tr}, Z_{ca1})]\) output from Algorithm 1 \(^3\)
Input: function \( \hat{w}(x; D) \) to fit the weight function at \( x \) using \( D \) as data

1. For each \( i \in I_{ca2} \) with \( \Delta_i = 1 \), compute the non-conformity score \( \hat{V}_i = \max\{\hat{q}_{\alpha_{ls}}(X_i; Z_{tr}) - T_i, T_i - \hat{q}_{\alpha_{ls}}(X_i; Z_{tr})\} \)
2. For each \( i \in I_{ca2} \) with \( \Delta_i = 1 \), compute the weight \( W_i = \hat{w}(X_i; Z_{tr}) \)
3. Calculate the normalized weights \( \hat{p}_i = \frac{W_i}{\sum_{i \in I_{ca2}} W_i + \hat{w}(X'; Z_{tr})} \) and \( \hat{p}_\infty = \frac{\widehat{w}(X'; Z_{tr})}{\sum_{i \in I_{ca2}} W_i + \hat{w}(X'; Z_{tr})} \)
4. Calculate \( \eta \) as the \((1 - \alpha)\)-th quantile of the distribution \( \sum_{i \in I_{ca}} \hat{p}_i \delta_{V_i} + \hat{p}_\infty \delta_\infty \)

Output: \( C^2(X') = [\hat{q}_{\alpha_{ls}}(X'; Z_{tr}, Z_{ca1}) - \eta, \hat{q}_{\alpha_{ls}}(X'; Z_{tr}, Z_{ca1}) + \eta] \).

Remark 2. In Algorithm 2, we modify the conformal score to be the absolute form again for clarity, since we have already derived an interval estimator of \( T \) in Algorithm 1.

Note that there are two conformal inference procedures in Algorithm 2. When the context is clear, the weight function \( \hat{w}(x) \) and the non-conformity score \( \hat{V}_i \) refers to those in the second conformal inference. Before stating the theorem, we denote \( H(X) \) to measure how well the quantile estimators \( \hat{q}_{\alpha_{ls}}(X), \hat{q}_{\alpha_{ls}}(X) \) are.

\[
H(X) = \max\{|\hat{q}_{\alpha_{ls}}(X) - q_{\alpha_{ls}}(X)|, |\hat{q}_{\alpha_{ls}}(X) - q_{\alpha_{ls}}(X)|\}
\]

(7)

We next show in Theorem 5.1 that Algorithm 2 returns a guaranteed coverage either the weight or the temporal confidence band is estimated well.

Theorem 5.1 (Lower Bound) Let \( \hat{w}(x) \) be an estimate of the weight \( w(x), \hat{q}_{\alpha_{ls}}(x), \hat{q}_{\alpha_{ls}}(x) \) be the quantile estimator returned by WCCI, and \( H(X) \) be defined as Equation 7. Assume that \( \mathbb{E}[\hat{w}(X)|Z_{tr}] = 1 \) and \( \mathbb{E}[w(X)] = 1 \), where all the expectation operators \( \mathbb{E} \) are taken over \( X \sim \mathcal{P}_{X|\Delta=1} \).

Denote \( \hat{C}^2_n(x) \) as the output band of Algorithm 2 with \( n \) calibration samples, and denote \( X' \) as the testing point.

From the weight perspective, under assumptions (A1):

A1. \( \mathbb{E}_{X|\Delta=1}[\hat{w}(X) - w(X)] \leq M_1 \),

we have:

\[
\lim_{n \to \infty} \mathbb{P}\left(T' \in \hat{C}^2_n(X')\right) \geq 1 - \alpha - \frac{1}{2} M_1.
\]

From the quantile perspective, under assumptions (B1-B3):

B1. \( H(X) \leq M_2 \) a.s. w.r.t. \( X \);

B2. There exists \( \delta > 0 \) such that \( \mathbb{E}[\hat{w}(X)]^{1+\delta} < \infty \);

B3. There exists \( \gamma, b_1, b_2 > 0 \) such that \( \mathbb{P}(T = t|X = x) \in [b_1, b_2] \) uniformly over all \( (x, t) \) with \( t \in [q_{\alpha_{ls}}(x) - 2M_2 - 2\gamma, q_{\alpha_{ls}}(x) + 2M_2 + 2\gamma] \cup [q_{\alpha_{ls}}(x) - 2M_2 - 2\gamma, q_{\alpha_{ls}}(x) + 2M_2 + 2\gamma] \), we have:

\[
\lim_{n \to \infty} \mathbb{P}\left(T' \in \hat{C}^2_n(X')\right) \geq 1 - \alpha - b_2(2M_2 + \gamma) - \frac{16b_2^2}{M_2 + \gamma} \]

Theorem 5.1 demonstrates that when \( M_1 \to 0 \) or \( M_2, \gamma \to 0 \) as \( |Z_{tr}| \to 0 \), the confidence band has guaranteed coverage with lower bound \( 1 - \alpha \). Compared to Theorem 4.1, Theorem 5.1 is doubly robust since the coverage is guaranteed when either (A1) or (B1-B3) holds. We next prove the upper bound in Theorem 5.2.

Theorem 5.2 (Upper Bound) Let \( \hat{w}(x) \) be an estimate of the weight \( w(x), \hat{q}_{\alpha_{ls}}(x), \hat{q}_{\alpha_{ls}}(x) \) be the quantile estimator returned by WCCI, and \( H(X) \) be defined as Equation 7. Assume that \( \mathbb{E}[\hat{w}(X)|Z_{tr}] = 1 \) and \( \mathbb{E}[w(X)] = 1 \), where all the expectation operators \( \mathbb{E} \) are taken over \( X \sim \mathcal{P}_{X|\Delta=1} \).

Let \( F_{V, \delta} \triangleq \sum_{i \in I_{ca}} \hat{p}_i \delta_{V_i} + \hat{p}_\infty \delta_{\infty} \) be CDF, and assume \( V_i \) has no ties. Denote \( \hat{C}^2_n(x) \) as the output band of Algorithm 2 with \( n \) calibration samples, and \( X' \) as the testing point.

Under assumptions (C1-C4):

C1. \( \forall s \subset I_{ca2}, \sum_{i \in s} (\hat{w}(X_i) - \hat{w}(X_i)) \leq M'_1 \);

C2. \( H(X) \leq M'_2 \) a.s. w.r.t. \( X \);

C3. \( F_{V, t + L} - F_{V, t} \geq KL \) for all \( t, L \);

C4. there exists \( b_1, b_2 > 0 \) such that \( \mathbb{P}(T = t|X = x) \in [b_1, b_2] \) uniformly over all \( (x, t) \) with \( t \in [q_{\alpha_{ls}}(x) - r, q_{\alpha_{ls}}(x) + r] \cup [q_{\alpha_{ls}}(x) - r, q_{\alpha_{ls}}(x) + r] \), where \( r = 2M'_2 + 2M'_1/K \) We have

\[
\lim_{n \to \infty} \mathbb{P}\left(T' \in \hat{C}^2_n(X')\right) \leq 1 - \alpha + b_2(2M'_2 + \frac{M'_1}{K}).
\]

Theorem 5.2 demonstrates that when the weight function \( \hat{w}(x) \) and the quantile function \( \hat{q}_{\alpha_{ls}}(x), \hat{q}_{\alpha_{ls}}(x) \) are estimated well (C1-C2), the returned coverage T-SCI has a lower bound guarantee. Combining Theorem 5.1 and Theorem 5.2 leads to a “nearly perfect” guaranteed coverage for T-SCI.

6. Experiments

This section aims at verifying some key arguments: (1) T-SCI returns valid coverage with small length interval; (2) Weight plays an essential role in the algorithm; (3) Censoring is more challenging than uncensoring settings. The results support these arguments both in synthetic data and real-world data, see Table 1.
6.1. Setup

Datasets and Environment. We conduct extensive experiments to test the efficiency of the algorithm. We use one synthetic dataset RRNLNPH (from Kvamme et al. (2019)) and two real-world datasets, METABRIC and SUPPORT (See supplementary materials for more details). For each dataset, we test several baseline algorithms along with our proposed algorithms. In each run, 80% data are randomly sampled as the training data, and the two halves of the rest are randomly split as calibration data and test data. We run the experiments 100 times for each algorithm. Moreover, we collect the results under different $\alpha$.

Algorithms. We choose the linear Cox regression (labeled as Cox Reg.) as a baseline. Besides, we conduct CoxPH (Katzman et al., 2018) and CoxCC (Kvamme et al., 2019) (both belong to Cox-MLP) using $S(t)$ to return confidence band although they do not contain a theoretical guarantee. We also choose a kernel-based non-Cox method, (Chen, 2020), labeled as Kernel. We emphasize that Kernel is a different approach since our method is Cox-based.

We integrate our proposed algorithms WCCI and T-SCI with CoxPH and CoxCC, labeled as CoxPH/CoxCC + WCCI/T-SCI. Besides, to ensure that the weights in WCCI and T-SCI are helpful, we test the unweighted version of WCCI and T-SCI, where we set all weights to 1 in WCCI and T-SCI.

Metrics. In the synthetic dataset, our core metric is empirical coverage (EC), defined as the fraction of testing points whose survival time falls in the predicted confidence band. Besides, we calculate the average interval length of the returned band. Given confidence level $\alpha$, a perfect confidence band is expected to return empirical coverage larger than $1 - \alpha$ with a small interval length. In the real-world dataset, we use surrogate empirical coverage (SEC), the upper bound of EC. We defer its formal definition in the supplementary materials.

6.2. Analysis

We summarize the experimental results on RRNLNPH in Table 1 and defer the results on SUPPORT and METABRIC to the supplementary materials due to space limitations.

Coverage and Interval Length. Figure 4 shows the empirical coverage and the interval length of the confidence band returned by algorithms under different confidence levels. Ideally, the confidence band should have large coverage with a small interval length. Notice that WCCI and T-SCI based algorithms outperform their original versions, showing that the proposed algorithms work well. Furthermore, T-SCI is more conservative than WCCI, where T-SCI has larger coverage and interval length. We further remark that T-SCI always returns guaranteed coverage (larger than $1 - \alpha$) under different confidence levels.
Table 1. Performance of Different Models on RRNLNPH.

| Method          | Total  | Censored | Uncensored | Interval Length |
|-----------------|--------|----------|------------|-----------------|
|                 | Mean   | Std.     | Mean       | Std.             | Mean   | Std.   |
| Cox Reg.        | 0.832  | 0.008    | /          | /               | 22.08  | 0.23   |
| CoxPH (Katzman et al., 2018) | 0.829  | 0.008    | 0.554      | 0.016           | 0.978  | 0.004  | 19.65  | 0.21   |
| CoxCC (Kvamme et al., 2019) | 0.830  | 0.008    | 0.556      | 0.016           | 0.975  | 0.003  | 20.17  | 0.24   |
| CoxPH+WCCI      | 0.912  | 0.03     | 0.854      | 0.047           | 0.949  | 0.028  | 21.59  | 0.90   |
| CoxPH+T-SCI     | 0.974  | 0.009    | 0.947      | 0.018           | 0.994  | 0.005  | 29.85  | 0.68   |
| CoxCC+WCCI      | 0.919  | 0.03     | 0.862      | 0.043           | 0.955  | 0.026  | 21.55  | 1.27   |
| CoxCC+T-SCI     | 0.974  | 0.009    | 0.946      | 0.017           | 0.995  | 0.004  | 29.62  | 0.57   |
| CoxPH+WCCI(unweighted) | 0.907  | 0.020    | 0.830      | 0.049           | 0.949  | 0.006  | 22.06  | 1.27   |
| CoxPH+T-SCI(unweighted) | 0.950  | 0.018    | 0.875      | 0.049           | 0.990  | 0.012  | 27.72  | 3.13   |
| CoxCC+WCCI(unweighted) | 0.941  | 0.029    | 0.815      | 0.029           | 0.948  | 0.009  | 22.57  | 0.70   |
| CoxCC+T-SCI(unweighted) | 0.955  | 0.020    | 0.877      | 0.048           | 0.992  | 0.007  | 28.92  | 1.04   |
| Kernel (Chen, 2020) | 0.951  | 0.024    | 0.858      | 0.093           | 0.993  | 0.014  | 51.63  | 32.92  |

Figure 5. **Weight Rationality.** We compare the weighted version (green) with its corresponding unweighted version (yellow). The weighted versions contain less bias for WCCI (closer to the expected 95%) and less variance for T-SCI (shorter boxes).

The rationality of weight $w(x)$. We show the comparison between weighted and unweighted versions in Figure 5. For WCCI algorithms, the weighted version has coverage closer to $1 - \alpha$. For T-SCI algorithms, the weighted version has lower variance. These results show that weighted versions outperform the unweighted versions, which validates the importance of weight $w(x)$.

The difficulty in censoring. Figure 6 shows the algorithms’ performance on censored and uncensored data, respectively. All the algorithms perform larger coverage and less variance on the uncensored data, meaning that censored data is more challenging to deal with than uncensored data.

Analysis of Table 1. We show RRNLNPH results in Table 1, and results of SUPPORT and METABRIC perform similarly. Firstly, notice that WCCI always does not reach the expected coverage mainly due to the inaccurate estimation on the weight, while T-SCI reaches it due to milder requirements in Theorem 5.1 (double robustness). Secondly, notice that Cox Reg., CoxPH, CoxCC (they all lack theoretical guarantee) all fail to return the proper coverage. Thirdly, unweighted versions all suffer from poor performances on censored data due to the lack of weight, showing that weight is vital in covariate shift. Finally, we emphasize that the Kernel method suffers from large interval length and large variance despite the moderate coverage. As a comparison, WCCI and T-SCI often perform more stably.

7. Conclusion

In this paper, we derive confidence band for Cox-based models. We first introduce WCCI by proposing a new non-conformity score. We then propose T-SCI, a two-stage conformal inference applying WCCI as input. Theoretical analysis shows that T-SCI returns nearly perfect coverage, meaning both lower and upper bound guarantee. We conduct extensive experiments on both synthetic data and real-world data to show the proposed algorithm’s correctness.
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Supplementary Materials

We complement the omitted proofs in Section A. We then provide the additional experimental results in Section B. Furthermore, in Section C, we give supplementary notes for some statements in the main text.

A. Proofs

A.1. Proof of Theorem 4.1

Theorem 4.1 (Provable Guarantee) Let \( \hat{\omega}(x) \) be an estimate of the weight \( \omega(x) \). Assume that \( \mathbb{E}[\hat{\omega}(X)|Z_{tr}] = 1 \) and \( \mathbb{E}[\omega(X)] = 1 \). Denote \( \tilde{C}_n^1(x) \) as the output band of Algorithm 1 with \( n \) calibration samples, then for a new data \( X' \), its corresponding survival time satisfies

\[
\lim_{n \to \infty} \mathbb{P} \left( T' \in \tilde{C}_n^1(X') \right) \geq 1 - \alpha - \frac{1}{2} \mathbb{E}[\hat{\omega}(X) - \omega(X)],
\]

where the probability \( \mathbb{P} \) on the left hand side is taken over \( (X', T') \sim \mathcal{P}_X \times \mathcal{P}_{T|X} \), and all the expectation operators \( \mathbb{E} \) are taken over \( X \sim \mathcal{P}_{X|\Delta=1} \).

Firstly, consider a new sample \( (\hat{X}', \hat{T}') \) generated from \( \hat{P}_X \times \mathcal{P}_{T|X} \), where we assume that

\[
d\tilde{P}_X(x) = \hat{\omega}(x) dP_{X|\Delta=1}(x).
\]

As a comparison, due to the definition of \( \omega(x) \), we have

\[
dP_X(x) = \omega(x) dP_{X|\Delta=1}(x).
\]

We remark that \( \tilde{P}_X(x) \), \( P_X(x) \) are indeed distribution since we assume \( \mathbb{E} \omega(X) = \mathbb{E} \hat{\omega}(X) = 1 \), where the expectation is taken over \( P_{X|\Delta=1} \).

We would first prove that the probability \( \hat{T}' \) falls in the derived confidence interval \( \tilde{C}_n^1(X') \) is larger than \( 1 - \alpha \), where \( \alpha \) is the given significance level. The intuition is that, since the derived \( \tilde{C}_n^1(X') \) is derived based on the estimated weight \( \hat{\omega}(x) \), the sample \( \hat{T}' \) is then guaranteed to fall in the confidence interval with probability at least \( 1 - \alpha \).

We derive that

\[
\mathbb{P} \left( \hat{T}' \in \tilde{C}_n^1(\hat{X}') | Z_{tr} \right) = \mathbb{P} \left( \hat{T}' \leq \tau^u(\hat{X}') \right) = \mathbb{P} \left( V(\hat{X}', \hat{T}') \leq V(\hat{X}', \tau^u(\hat{X}') | Z_{tr}) \right) \geq \mathbb{P} \left( V(\hat{X}', \hat{T}') \leq \text{Quantile}(1 - \alpha; \sum_{i=1}^n \tilde{p}_i \delta_{v_i} + \tilde{p}_\infty \delta_\infty) | Z_{tr} \right),
\]

where the last inequality is due to the fact that \( V(\hat{X}', \tau^u(\hat{X}') \geq \text{Quantile}(1 - \alpha; \sum_{i=1}^n \tilde{p}_i \delta_{v_i} + \tilde{p}_\infty \delta_\infty) \). We also use the non-decreasing property of \( V(X, T) \) on \( T \). Furthermore, by Lemma 3, we can replace the \( \delta_\infty \) in the quantile term by \( \delta_V(\hat{X}', \hat{T}') \), therefore,

\[
\mathbb{P} \left( V(\hat{X}', \hat{T}') \leq \text{Quantile}(1 - \alpha; \sum_{i=1}^n \tilde{p}_i \delta_{v_i} + \tilde{p}_\infty \delta_\infty) | Z_{tr} \right) = \mathbb{P} \left( V(\hat{X}', \hat{T}') \leq \text{Quantile}(1 - \alpha; \sum_{i=1}^n \tilde{p}_i \delta_{v_i} + \tilde{p}_\infty \delta_V(\hat{X}', \hat{T}') | Z_{tr} \right).
\]

Besides, we know from Lemma 4 that

\[
V(\hat{X}', \hat{T}') | Z_{tr}, \mathcal{E}(V) \sim \sum_{i=1}^n \tilde{p}_i \delta_{v_i} + \tilde{p}_\infty \delta_V(\hat{X}', \hat{T}'),
\]
We next introduce Lemma 4 which provides the distribution of the non-conformity score. Therefore, we derive that

\[
\mathbb{P} \left( V \left( \tilde{X}', \tilde{T}' \right) \leq \text{Quantile} \left( 1 - \alpha; \sum_{i=1}^{n} \hat{p}_{i} \delta_{v_{i}} + \hat{p}_{\infty} \delta_{V \left( \tilde{X}', \tilde{T}' \right)} \right) \mid Z_{tr} \right) \\
= \mathbb{E}_{x} \mathbb{P} \left( V \left( \tilde{X}', \tilde{T}' \right) \leq \text{Quantile} \left( 1 - \alpha; \sum_{i=1}^{n} \hat{p}_{i} \delta_{v_{i}} + \hat{p}_{\infty} \delta_{V \left( \tilde{X}', \tilde{T}' \right)} \right) \mid Z_{tr}, \mathcal{E} \left( V \right) \right) \\
\geq 1 - \alpha.
\]

Combining the Equation 8, Equation 9 and Equation 10 leads to

\[
\mathbb{P} \left( \tilde{T}' \in \tilde{C}_{n}^{1} \left( \tilde{X}' \right) \mid Z_{tr} \right) \geq 1 - \alpha.
\]

Furthermore, we need to transform the above results into random sample \( (X', T') \sim dP_{X} \times dP_{T \mid X} \). This directly follows Lemma 5 that

\[
\mathbb{P} \left( T' \in \tilde{C}_{n}^{1} \left( X' \right) \mid Z_{tr} \right) - \mathbb{P} \left( \tilde{T}' \in \tilde{C}_{n}^{1} \left( X' \right) \mid Z_{tr} \right) \leq d_{TV} \left( P_{X} \times P_{T \mid X}, \tilde{P}_{X} \times P_{T \mid X} \right) = d_{TV} \left( P_{X}, \tilde{P}_{X} \right).
\]

We can express the total-variation distance between \( Q_{X} \) and \( \tilde{Q}_{X} \) as

\[
d_{TV} \left( P_{X}, \tilde{P}_{X} \right) = \frac{1}{2} \int \left| \hat{w} \left( X \right) dP_{X \mid \Delta=1} \left( X \right) - w \left( X \right) dP_{X \mid \Delta=1} \left( X \right) \right| = \frac{1}{2} \mathbb{E}_{X \sim P_{X \mid \Delta=1}} \left| \hat{w} \left( X \right) - w \left( X \right) \right|.
\]

Combine the above results and take expectations on the training set, we conclude that

\[
\mathbb{P} \left( T' \in \tilde{C}_{n}^{1} \left( X' \right) \right) = \mathbb{E}_{x} \mathbb{P} \left( T' \in \tilde{C}_{n}^{1} \left( X' \right) \mid Z_{tr} \right) \geq 1 - \alpha - \frac{1}{2} \mathbb{E} \left| \hat{w} \left( X \right) - w \left( X \right) \right|.
\]

where the expectation is taken over the training set space and \( X \sim P_{X \mid \Delta=1} \)

**Technical Lemmas.** In this part, we give some technical lemmas used in the proof. We first introduce Lemma 3 which is commonly used in conformal inference. By Lemma 3, we can use \( \delta_{\infty} \) to replace \( \delta_{V \left( \tilde{X}', \tilde{T}' \right)} \) without changing the probability.

**Lemma 3 (Equation(2) in Lemma 1 from Barber et al. (2019a).)** For random variables \( v_{i} \in \mathbb{R}, i \in \left[ n + 1 \right] \), let \( p_{i} \in \mathbb{R}, i \in \left[ n + 1 \right] \) be the corresponding weights summing to 1. Then for any \( \beta \in \left[ 0, 1 \right] \), we have

\[
V \left( \tilde{X}', \tilde{T}' \right) \leq \text{Quantile} \left( \beta, \sum_{i=1}^{n} p_{i} \delta_{v_{i}} + p_{\infty} \delta_{\infty} \right) \iff V \left( \tilde{X}', \tilde{T}' \right) \leq \text{Quantile} \left( \beta, \sum_{i=1}^{n} p_{i} \delta_{v_{i}} + p_{\infty} \delta_{V \left( \tilde{X}', \tilde{T}' \right)} \right).
\]

We next introduce Lemma 4 which provides the distribution of the non-conformity score.

**Lemma 4 (Equation(A.5) from Lei & Candès (2020).)**

\[
\left( V \left( \tilde{X}', \tilde{T}' \right) \mid \mathcal{E} \left( V \right) = \mathcal{E} \left( V^{*} \right), Z_{tr} \right) \sim \text{Quantile} \left( \sum_{i=1}^{n} \hat{p}_{i} \delta_{v_{i}} + \hat{p}_{\infty} \delta_{V \left( \tilde{X}', \tilde{T}' \right)} \right)
\]

where \( \mathcal{E} \left( V^{*} \right) \) is the unordered set of \( V^{*} = \left( v_{1}^{*}, v_{2}^{*}, \ldots, v_{n}^{*}, V \left( \tilde{X}', \tilde{T}' \right) \right) \).

Thirdly, we introduce Lemma 5 which shows a basic property of the total variance distance.

**Lemma 5 (Equation(10) from Berrett et al. (2020).)** Let \( d_{TV} \left( Q_{1X}, Q_{2X} \right) \) denote the total-variation distance between \( Q_{1X} \) and \( Q_{2X} \), then

\[
d_{TV} \left( Q_{1X} \times P_{T \mid X}, Q_{2X} \times P_{T \mid X} \right) = d_{TV} \left( Q_{1X}, Q_{2X} \right).
\]
A.2. Proof of Theorem 5.1

**Theorem 5.1 (Lower Bound)** Let \( \hat{w}(x) \) be an estimate of the weight \( w(x) \), \( \hat{q}_{\alpha_{h,i}}(x) \), \( q_{\alpha_{h,i}}(x) \) be the quantile estimator returned by WCCI, and \( H(X) \) be defined as Equation 7. Assume that \( \mathbb{E}[\hat{w}(X) | Z_{tr}] = 1 \) and \( \mathbb{E}[w(X)] = 1 \), where all the expectation operators \( \mathbb{E} \) are taken over \( X \sim \mathcal{P}_{X|\Delta=1} \). Denote \( \hat{C}_n^{2}(x) \) as the output band of Algorithm 2 with \( n \) calibration samples, and denote \( X' \) as the testing point.

From the weight perspective, under assumptions (A1):

A1. \( \mathbb{E}X_{|\Delta=1}|\hat{w}(X) - w(X)| \leq M_1 \), we have:

\[
\lim_{n \to \infty} \Pr\left(T' \in \hat{C}_n^{2}(X')\right) \geq 1 - \alpha - \frac{1}{2}M_1.
\]

From the quantile perspective, under assumptions (B1-B3):

B1. \( H(X) \leq M_2 \) a.s. w.r.t. \( X \);

B2. There exists \( \delta > 0 \) such that \( \mathbb{E}\left(\hat{w}(X)\right)^{1+\delta} < \infty \);

B3. There exists \( \gamma, b_1, b_2 > 0 \) such that \( \Pr(T = t | X = x) \in [b_1, b_2] \) uniformly over all \( (x,t) \) with \( t \in [q_{\alpha_{h,i}}(x) - 2M_2 - 2\gamma, q_{\alpha_{h,i}}(x) + 2M_2 + 2\gamma] \cup [q_{\alpha_{h,i}}(x) - 2M_2 - 2\gamma, q_{\alpha_{h,i}}(x) + 2M_2 + 2\gamma] \), we have:

\[
\lim_{n \to \infty} \Pr\left(T' \in \hat{C}_n^{2}(X')\right) \geq 1 - \alpha - b_2(2M_2 + \gamma) - \frac{16M_2}{(M_2 + \gamma)^2b_1}.
\]

The proof under (A1) directly follows the proof of Theorem 4.1. Firstly, for a new testing point \( (X', T') \sim \mathcal{P}_X \times \mathcal{P}_{T|X} \), we have

\[
\Pr\left(T' \in \hat{C}_n^{2}(X') | X'\right)
\]

\[
= \Pr\left(T' \in [q_{\alpha_{h,i}}(X') - \eta, \hat{q}_{\alpha_{h,i}}(X') + \eta] | X'\right)
\]

\[
= \Pr\left(\max\{T' - \hat{q}_{\alpha_{h,i}}(X'), q_{\alpha_{h,i}}(X') - T'\} \leq \eta | X\right)
\]

\[
\geq \Pr\left(\max\{T' - q_{\alpha_{h,i}}(X'), q_{\alpha_{h,i}}(X') - T'\} \leq \eta - H(X') | X'\right)
\]

\[
\geq \Pr\left(\max\{T' - q_{\alpha_{h,i}}(X'), q_{\alpha_{h,i}}(X') - T'\} \leq -\epsilon - H(X') | X'\right) - \Pr(\eta < -\epsilon)
\]

\[
\geq \Pr\left(\max\{T' - q_{\alpha_{h,i}}(X'), q_{\alpha_{h,i}}(X') - T'\} \leq -\epsilon - H(X') \mathbb{I}(H(X') \leq \epsilon) | X'\right) - \Pr(\eta < -\epsilon).
\]

Equation (i) follows from Lemma 6, and Equation (ii) follows from:

\[
\Pr\left(\max\{T' - q_{\alpha_{h,i}}(X'), q_{\alpha_{h,i}}(X') - T'\} \leq -\epsilon - H(X') | X'\right) - \Pr\left(\max\{T' - \hat{q}_{\alpha_{h,i}}(X'), \hat{q}_{\alpha_{h,i}}(X') - T'\} \leq \eta - H(X') | X'\right)
\]

\[
\leq \Pr(\eta - H(X') < \max\{T' - q_{\alpha_{h,i}}(X'), q_{\alpha_{h,i}}(X') - T'\} \leq -\epsilon - H(X') | X'\)
\]

\[
\leq \Pr(\eta - H(X') < -\epsilon - H(X') | X')
\]

\[
= \Pr(\eta < -\epsilon).
\]

Equation (iii) can be derived simply based on the discussion on the value of \( \mathbb{I}(H(X') \leq \epsilon) \).

By Assumption (B3), since \( -\epsilon - H(X') \mathbb{I}(H(X') \leq \epsilon) \leq -2\epsilon \), when \( \epsilon \leq M_2 + \gamma \), we have

\[
\Pr\left(\max\{T' - q_{\alpha_{h,i}}(X'), q_{\alpha_{h,i}}(X') - T'\} \leq -\epsilon - H(X') \mathbb{I}(H(X') \leq \epsilon) | X'\right)
\]

\[
\geq \Pr\left(\max\{T' - q_{\alpha_{h,i}}(X'), q_{\alpha_{h,i}}(X') - T'\} \leq 0 | X'\right) - b_2(\epsilon + H(X') \mathbb{I}(H(X') \leq \epsilon))
\]

\[
\geq \Pr\left(\max\{T' - q_{\alpha_{h,i}}(X'), q_{\alpha_{h,i}}(X') - T'\} \leq 0 | X'\right) - b_2(\epsilon + H(X'))
\]

\[
\geq 1 - \alpha - b_2(\epsilon + H(X')).
\]

Combining Eqn 16 with Eqn 17 and taking expectations over \( X' \), we have:

\[
\Pr\left(T' \in \hat{C}_n^{2}(X')\right)
\]

\[
\geq 1 - \alpha - b_2(\epsilon + \mathbb{E}H(X')) - \Pr(H(X') > \epsilon) - \Pr(\eta < -\epsilon)
\]

\[
\geq 1 - \alpha - b_2(2M_2 + \gamma) - \Pr(\eta < -(M_2 + \gamma)).
\]
The Equation (i) holds by taking $\varepsilon = M_2 + \gamma$. Due to Assumption (B1), we have $\mathbb{E} H (X') \leq M_2$ and $\mathbb{P} (H (X') > \varepsilon) = 0$. Note that $\varepsilon = M_2 + \gamma$ does not break the condition of Equation 17.

We next show that $\lim_{n \to \infty} \mathbb{P} (\eta < -(M_2 + \gamma)) \leq \frac{16 M_2}{(M_2 + \gamma)^2 b_1}$. Firstly, by Lemma 7, we have

$$\lim_{n \to \infty} \mathbb{P} (\eta < -(M_2 + \gamma)) \leq \frac{16 M_2}{(M_2 + \gamma)^2 b_1} \mathbb{E} \omega (X) H (X) = \frac{16 M_2}{(M_2 + \gamma)^2 b_1}.$$

The inequality is due to Assumption (B1) and $\mathbb{E} \omega (X) = 1$.

The proof is done.

**Technical Lemmas.** In this part, we give some technical lemmas used in the proof. The following Lemma 6 shows that the difference between non-conformity score under true quantile $q$ and non-conformity score under estimated quantile $\hat{q}$ is upper bounded by $H (X')$.

**Lemma 6** Under notations in Theorem 5.1, we have $|\max \{T' - \hat{q}_{\alpha h} (X'), \hat{q}_{\alpha l o} (X') - T'\} - \max \{T' - q_{\alpha h} (X'), q_{\alpha l o} (X') - T'\}| \leq H (X')$.

**Proof.** We investigate the results via situations on the operator $\max$.

If $\max \{T' - q_{\alpha h} (X'), \hat{q}_{\alpha l o} (X') - T'\} = T' - q_{\alpha h} (X')$ and $\max \{T' - q_{\alpha h} (X'), q_{\alpha l o} (X') - T'\} = T' - q_{\alpha h} (X')$, the conclusion follows the definition of $H (X')$.

If $\max \{T' - q_{\alpha h} (X'), \hat{q}_{\alpha l o} (X') - T'\} = T' - \hat{q}_{\alpha h} (X')$ and $\max \{T' - q_{\alpha h} (X'), q_{\alpha l o} (X') - T'\} = q_{\alpha l o} (X') - T'$, we have

$$\max \{T' - q_{\alpha h} (X'), \hat{q}_{\alpha l o} (X') - T'\} - \max \{T' - q_{\alpha h} (X'), q_{\alpha l o} (X') - T'\}$$

$$= (T' - \hat{q}_{\alpha h} (X')) - (q_{\alpha l o} (X') - T')$$

$$\leq (T' - \hat{q}_{\alpha h} (X')) - (T' - q_{\alpha h} (X'))$$

$$= q_{\alpha h} (X') - \hat{q}_{\alpha h} (X')$$

$$\leq H (X').$$

Similarly,

$$\max \{T' - q_{\alpha h} (X'), \hat{q}_{\alpha l o} (X') - T'\} - \max \{T' - q_{\alpha h} (X'), q_{\alpha l o} (X') - T'\}$$

$$= (T' - \hat{q}_{\alpha h} (X')) - (q_{\alpha l o} (X') - T')$$

$$\geq (q_{\alpha l o} (X') - T') - (q_{\alpha h} (X') - T')$$

$$= q_{\alpha l o} (X') - q_{\alpha h} (X')$$

$$\geq - H (X').$$

Therefore, we have

$$|\max \{T' - q_{\alpha h} (X'), \hat{q}_{\alpha l o} (X') - T'\} - \max \{T' - q_{\alpha h} (X'), q_{\alpha l o} (X') - T'\}| \leq H (X').$$

The other two situations are derived similarly.

We next introduce Lemma 7 which provides the upper bounds of the term $\lim_{n \to \infty} \mathbb{P} (\eta < -\varepsilon)$.

**Lemma 7** Under the assumptions in Theorem 5.1, the following inequality holds.

$$\lim_{n \to \infty} \mathbb{P} (\eta < -\varepsilon) \leq \frac{16}{\varepsilon^2 b_1} \mathbb{E} \omega (X) H (X) = \frac{16 M_2}{(M_2 + \gamma)^2 b_1}.$$

**Proof.** By combining Equation (A.10), (A.11), (A.12), (A.13) in Lei & Candès (2020), and apply the Assumption (B2) we have

$$\lim_{n \to \infty} \mathbb{P} (\eta < -\varepsilon) \leq \mathbb{P} \left( \sum_{i=1}^{n} \omega (X_i) H (X_i) \geq \frac{\varepsilon^2 b_1 n}{16} \right).$$
And by Markov inequality, we have
\[ P \left( \sum_{i=1}^{n} \tilde{w} (X_i) H (X_i) \geq \epsilon^2 b_1 n \right) \leq \frac{16}{\epsilon^2 b_1} \sum_{i=1}^{n} E[\tilde{w} (X_i) H (X_i)] = \frac{16}{\epsilon^2 b_1} E[\tilde{w} (X) H (X)]. \]

The proof is done.

A.3. Proof of Theorem 5.2

**Theorem 5.1 (Lower Bound)** Let \( \tilde{w}(x) \) be an estimate of the weight \( w(x), q_{\alpha_h}(x), \tilde{q}_{\alpha_h}(x) \) be the quantile estimator returned by WCCI, and \( H(X) \) be defined as Equation 7. Assume that \( E[\tilde{w}(X)|Z_{tr}] = 1 \) and \( E[w(X)] = 1 \), where all the expectation operators \( E \) are taken over \( X \sim P_{X|\Delta=1} \). Denote \( \hat{C}^2_n(x) \) as the output band of Algorithm 2 with \( n \) calibration samples, and denote \( X' \) as the testing point.

From the weight perspective, under assumptions (A1):

**A1.** \( E_{X|\Delta=1}[\tilde{w}(X) - w(X)] \leq M_1 \), we have:

\[ \lim_{n \to \infty} P \left( T' \in \hat{C}^2_n(X') \right) \geq 1 - \alpha - \frac{1}{2} M_1. \]

From the quantile perspective, under assumptions (B1-B3):

**B1.** \( H(X) \leq M_2 \) a.s. w.r.t. \( X \);

**B2.** There exists \( \delta > 0 \) such that \( E[\tilde{w}(X)^{1+\delta}] < \infty \);

**B3.** There exists \( \gamma, b_1, b_2 > 0 \) such that \( P(T = t|X = x) \in [b_1, b_2] \) uniformly over all \((x,t)\) with \( t \in [q_{\alpha_h}(x) - 2M_2 - 2\gamma, q_{\alpha_h}(x) + 2M_2 + 2\gamma] \cup [q_{\alpha_h}(x) - 2M_2 - 2\gamma, q_{\alpha_h}(x) + 2M_2 + 2\gamma] \), we have:

\[ \lim_{n \to \infty} P \left( T' \in \hat{C}^2_n(X') \right) \geq 1 - \alpha - b_2(2M_2 + \gamma) - \frac{16M_2}{(M_2 + \gamma)^2 b_1}. \]

We now show the proof of Theorem 5.2. For a new testing point \((X', T') \sim P_X \times P_{T|X}, \) we have

\[ P \left( T' \in \hat{C}^2_n(X') | X' \right) \]

\[ = P \left( T' \in \tilde{q}_{\alpha_h}(X') - \eta, \tilde{q}_{\alpha_h}(X') + \eta | X' \right) \]

\[ = P \left( \max \{T' - \tilde{q}_{\alpha_h}(X'), \tilde{q}_{\alpha_h}(X') - T' \} \leq \eta | X \right) \]

\[ \leq P \left( \max \{T' - q_{\alpha_h}(X'), q_{\alpha_h}(X') - T' \} \leq \eta + H(X') | X \right) \]

\[ \leq P \left( \max \{T' - q_{\alpha_h}(X'), q_{\alpha_h}(X') - T' \} \leq \eta_{q,w} + \epsilon + H(X') | X \right) + P(\eta - \eta_{q,w} > \epsilon) \]

\[ \leq P \left( \max \{T' - q_{\alpha_h}(X'), q_{\alpha_h}(X') - T' \} \leq \eta_{q,w} + \epsilon + H(X') I(H(X') \leq \epsilon) | X \right) + I(H(X') > \epsilon) + P(\eta - \eta_{q,w} > \epsilon). \]

(19)

where we denote \( \eta_{q,w} = \text{Quantile} \left( 1 - \alpha; \sum_{i=1}^{n} p_i \delta V^*_{i} + p_{\infty} \delta V_{\infty} \right) \), and obviously, \( \eta_{q,w} = 0 \) by the definition of the non-conformity score, where \( V^*_i \) is calculated based on \( q_{\alpha_h}(\cdot) \) and \( q_{\alpha_h}(\cdot) \).

Equation (i) follows from Lemma 6, and Equation (ii) follows from:

\[ P \left( \max \{T' - q_{\alpha_h}(X'), q_{\alpha_h}(X') - T' \} \leq \eta + H(X') | X \right) - P \left( \max \{T' - \tilde{q}_{\alpha_h}(X'), \tilde{q}_{\alpha_h}(X') - T' \} \leq \eta_{q,w} + \epsilon + H(X') | X \right) \]

\[ \leq P(\eta_{q,w} + \epsilon + H(X') < \max \{T' - q_{\alpha_h}(X'), q_{\alpha_h}(X') - T' \} \leq \eta + H(X') | X) \]

\[ \leq P(\eta_{q,w} + \epsilon + H(X') < \eta + H(X') | X') \]

\[ = P(\eta - \eta_{q,w} > \epsilon). \]

Equation (iii) can be derived simply based on the discussion on the value of \( I(H(X') \leq \epsilon) \).
By Assumption (C4), since $\varepsilon + H(X') \mathbb{I}(H(X') \leq \varepsilon) \leq 2\varepsilon$, when $\varepsilon \leq M_2 + \gamma$, we have
\[
\lim_{n \to \infty} P(\max\{T' - q_{a_1}, X'\}, q_{a_2} - T') \leq \eta_{q,w} + \varepsilon + H(X') \mathbb{I}(H(X') \leq \varepsilon) | X') \\
\leq \lim_{n \to \infty} P(\max\{T' - q_{a_1}, X'\}, q_{a_2} - T') \leq \eta_{q,w} X') + b_2 (\varepsilon + H(X') \mathbb{I}(H(X') \leq \varepsilon)) \\
\leq \lim_{n \to \infty} P(\max\{T' - q_{a_1}, X'\}, q_{a_2} - T') \leq 0 X') + b_2 (\varepsilon + H(X')) \\
\leq 1 - \alpha + b_2 (\varepsilon + H(X')).
\] (20)

The last inequality is from Lemma 2. Combining Eqn 19 with Eqn 20 and taking expectations over $X'$, we have:
\[
\lim_{n \to \infty} P(T' \in \hat{C}_n^2(X')) \\
\leq 1 - \alpha + b_2 (\varepsilon + \mathbb{E}H(X')) + P(H(X') > \varepsilon) + \lim_{n \to \infty} P(\eta - \eta_{q,w} > \varepsilon).
\]
By taking $\varepsilon = M_2' + M_1'/K$, and plugging in Assumption (B1), the above equation is equivalent to
\[
\lim_{n \to \infty} P(T' \in \hat{C}_n^2(X')) \leq 1 - \alpha + b_2 (2M_2' + M_1'/K) + \lim_{n \to \infty} P(\eta - \eta_{q,w} > M_2' + M_1'/K).
\] (21)

The left is to show that
\[
\lim_{n \to \infty} P(\eta - \eta_{q,w} > M_2' + M_1'/K) = 0.
\] (22)
First we denote $\eta_q = \text{Quantile}(1 - \alpha; \sum_{i=1}^{n} \hat{p}_i \delta_{V_i} + \hat{p}_\infty \delta_{V_\infty})$ where $\hat{p}_i$ is the estimator of $p_i$. Equation 22 holds by applying Lemma 8 and Lemma 9.

The proof is done.

**Technical Lemmas.** In this part, we give some technical lemmas used in the proof. We first prove the following Lemma 8 which gives an upper bound of $|\eta - \eta_q|$.

**Lemma 8** Under assumptions of Theorem 5.2, $|\eta - \eta_q| \leq M_2'$

**Proof.** Notice that $\eta$ is the quantile of distribution $\sum_{i=1}^{n} \hat{p}_i \delta_{V_i} + \hat{p}_\infty \delta_{V_\infty}$ and $\eta_q$ is the quantile of distribution $\sum_{i=1}^{n} \hat{p}_i \delta_{V_i} + \hat{p}_\infty \delta_{V_\infty}$, where $V_i$ is calculated based on $\hat{q}_{a_1}, \hat{q}_{a_2}$.

When $\eta = \eta_q$, the conclusion directly follows. When $\eta \neq \eta_q$, notice that the two distribution share the same weight $\hat{w}$, there must exist a $V''$ and $V'''$ such that
\[
V''' \leq \eta, V'' \geq \eta_q \\
V''' \geq \eta, V'' \leq \eta_q.
\]
This leads to the following two inequalities by Assumption (C2) and Lemma 7.
\[
\eta - \eta_q \geq V''' - V'' \geq -H(X) \geq -M_2' \\
\eta - \eta_q \leq V''' - V'' \leq H(X) \leq M_2'.
\] (23)
Therefore,
\[
|\eta - \eta_q| \leq M_2'.
\]
The proof is done.

We next prove Lemma 9 which provides an upper bound of $|\eta_q - \eta_{q,w}|$.

**Lemma 9** Under assumptions of Theorem 5.2, $|\eta_q - \eta_{q,w}| \leq M_1'/K$

**Proof.** WLOG, assume $\eta_{q,w} - \eta_q = \Delta > 0$. Denote $F(\cdot) = \sum_{i=1}^{n} p_i \delta_{V_i} + p_\infty \delta_{V_\infty}$ and $G(\cdot) = \sum_{i=1}^{n} \hat{p}_i \delta_{V_i} + \hat{p}_\infty \delta_{V_\infty}$.

By the definition of $\eta_q, \eta_{q,w}$, we have
\[
F(\eta_{q,w}) = G(\eta_q) = 1 - \alpha.
\]
Therefore, on the one hand, by Assumption (C1) and Assumption $E_w (X) = E \hat{w} (X) = 1$

$$
F (\eta_{q, w}) = F (\eta_q) \\
= G (\eta_q) - F (\eta_q) \\
\leq \sup_i G (\eta_q) - F (\eta_q) \\
\leq \sup S \left| \sum_{i \in S} w (X_i) - \hat{w} (x_i) \right| \\
\leq M_1'.
$$

(24)

On the other hand, by Assumption (C3)

$$
F (\eta_{q, w}) - F (\eta_q) \\
= F (\eta_q + \Delta) - F (\eta_q) \\
\geq K \Delta.
$$

(25)

Combining Equation 24 and Equation 25 leads to

$$
\eta_{q, w} - \eta_q \leq M_1' / K.
$$

The conclusion directly follows.

Combining Lemma 8 and Lemma 9 leads to the upper bound of $|\eta - \eta_{q, w}|$.

**B. Supplemental Experiment Results**

All codes are available at [https://github.com/thutzr/Cox](https://github.com/thutzr/Cox).

**B.1. Experiment Process**

**Data Pre-processing.** There are both numerical features and categorical features in our datasets. We normalize numerical features on both training set and test set.

**Process.** In each run, the experiment runs as follows:

- We first randomly split 80% data as the training set while the rest is splitted randomly into calibration set and test set.

- Following (Chen, 2020), we randomly sample 100 data points, which are used to construct prediction intervals, from test set. Denote these points as $X_{\text{centers}}$.

- For each point $x_0 \in X_{\text{centers}}$:
  
  - We sample 100 data points in test set with respect to sampling probability proportional to $K(x, x_0)$, where $K(\cdot)$ is the Gaussian kernel.
  
  - For these 100 test points, we use algorithm 1 and 2 to calculate the predicted survival interval with respect to the given confidence level $\alpha$ and check if the true survival time of each point is included in the predicted interval. The fraction of points that are covered in the calculated confidence interval is the empirical coverage. And the difference of upper confidence band and its lower counterpart is interval length. In our experiments, the upper interval band is likely to be infinity sometimes. We truncate those upper bands to the maximum duration of the according dataset.

We run the above procedure for different confidence level $\alpha$s. Results show that our algorithms are robust and effective for different $\alpha$s. In our experiments, $\alpha$ is chosen to be 0.6, 0.7, 0.8, 0.9, 0.95, respectively.
B.2. Model and Hyperparameters

We use pycox and PyTorch to implement CoxCC, CoxPH and neural network model respectively. Then we combine them together to Cox-MLP models. We implement a neural network model with three hidden layers, where each layer has 32 hidden nodes. Between each two layers, we use ReLU as the activation function. We apply batch normalization and dropout which drop 10% nodes at one epoch. Adam is chosen to be the optimizer. In the training process, we feed 80% data as training data and the rest as validation data. Note that here the total data set (training data + validation data) is the training data mentioned in the main article. Each batch contains 128 data points. We train the network for 512 epochs and the trained model is used as the MLP part in our Cox-MLP model.

B.3. Supplemental Results

The empirical coverage and predicted interval length of different models are listed in Table 2 and Table 3. The results are similar to that of RRNLNPH. It should be noticed that unweighted WCCI has very poor performance on censored data in SUPPORT. Both Kernel and unweighted models variate a lot on length of prediction interval.

Prediction on censored data and uncensored data are compared in Figure 7. Performance on censored data are much better than that of uncensored data. The standard deviation is also larger on uncensored data than censored data. This is consistent with our intuition as we do not have exact information of censored data.

Comparison on weighted and unweighted models are shown in Figure 8. Performance of unweighted models are much
weaker than weighted models. This shows the effectiveness of weighted conformal inference.

We also compare performance on different $\alpha$’s on both SUPPORT and METABRIC. Results similar with RRNLNPH are shown in Figure 9, and 10. The empirical coverage of our algorithms exceed the given confidence level and the standard deviation of prediction is relatively low.
T-SCI: A Two-Stage Conformal Inference Algorithm with Guaranteed Coverage for Cox-MLP

Figure 9. Different Model’s Empirical Coverage of Different $\alpha$(SUPPORT)

Figure 10. Different Model’s Empirical Coverage of Different $\alpha$
C. Supplementary Notes

We make some supplementary notes in this section.

C.1. Stability of Non-conformity Score

We state in Section 4 that the non-conformity score is usually more stable when it is single-peak. A multi-peak situation implies that samples with different covariate may have different coverage, namely,

\[ P(T \in C_n(X)|X = x_1) \neq P(T \in C_n(X)|X = x_2), \]

where \( x_1, x_2 \) belong to different peaks. Therefore, we describe the above formula as “unstable” since it provides distinct coverage for distinct groups, although the overall coverage (for the population) is still \( 1 - \alpha \).

The multi-peak phenomenon comes from the fact that we calculate the \( 1 - \alpha \) quantile of \( V_i \) based on all samples. For example, consider a two-peak distribution where the first group has \( 1 - \alpha \) populations. Then the algorithm returns zero coverage (probability equal to zero) for the second group and returns one coverage (probability equal to one) for the first group, which causes instability.

C.2. Censoring Mechanism

There are several other censoring mechanisms considered in Cox-based models. For example, Type-I censoring where the censoring time is a constant, and Type-II censoring where the experiment is terminated when a fixed fraction of samples have occurred the event. Fortunately, Type-I, Type-II, and random censoring share the same likelihood, although the censoring mechanism differs. Moreover, all of these types of censoring cause covariate shifts. Therefore, our algorithm (WCCI and T-SCI) can directly apply to these different censoring mechanisms.

C.3. Surrogate Empirical Coverage

In the experiment part, we use empirical coverage to evaluate the algorithm on a synthetic dataset, defined as the fraction of testing points whose survival time falls in the predicted confidence band.

In the real-world dataset, we calculate surrogate empirical coverage (SEC) instead of empirical coverage due to the lack of survival time. SEC calculates the number when the censoring time is no larger than the band’s upper bound for censored data. We emphasize that SEC is the upper bound of EC.

For example, denote the returned confidence band as \( \hat{C}(X_i) = [T^l(X_i), T^u(X_i)] \) and denote \( I_{test} \) as the training set index, its empirical coverage is defined as:

\[ EC = \frac{1}{|I_{test}|} \sum_{i \in I_{test}} \mathbb{I}(T_i \in \hat{C}(X_i)) \]

its surrogate empirical coverage is defined as:

\[ SEC = \frac{1}{|I_{test}|} \sum_{i \in I_{test}} \left( \mathbb{I}(Y_i \in \hat{C}(X_i), \Delta_i = 1) + \mathbb{I}(Y_i \leq T^u(X_i), \Delta_i = 0) \right) \]