Model-free Bootstrap and Conformal Prediction in Regression: Conditionality, Conjecture Testing, and Pertinent Prediction Intervals

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Abstract

Predictive inference under a general regression setting is gaining more interest in the big-data era. In terms of going beyond point prediction to develop prediction intervals, two main threads of development are conformal prediction and Model-free prediction. Recently, Chernozhukov et al. [2021] proposed a new conformal prediction approach exploiting the same uniformization procedure as in the Model-free Bootstrap of Politis [2015]. Hence, it is of interest to compare and further investigate the performance of the two methods. In the paper at hand, we contrast the two approaches via theoretical analysis and numerical experiments with a focus on conditional coverage of prediction intervals. We discuss suitable scenarios for applying each algorithm, underscore the importance of conditional vs. unconditional coverage, and show that, under mild conditions, the Model-free bootstrap yields prediction intervals with guaranteed better conditional coverage compared to quantile estimation. We also extend the concept of ‘pertinence’ of prediction intervals in Politis [2015] to the nonparametric regression setting, and give concrete examples where its importance emerges under finite sample scenarios. Finally, we define the new notion of ‘conjecture testing’ that is the analog of hypothesis testing as applied to the prediction problem; we also devise a modified conformal score to allow conformal prediction to handle one-sided ‘conjecture tests’, and compare to the Model-free bootstrap.

Keywords: Asymptotic validity, confidence intervals, significance, nonparametric regression, predictive inference, undercoverage.

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1 Introduction

Regression is a ubiquitous tool in statistical literature and practice. To discuss it, let $X \in \mathbb{R}^d$ denote the random regressor/covariate, and $Y \in \mathbb{R}$ the (univariate) response associated with $X$. A general form of a regression setup is the following: the relationship between the response $Y$ and covariate $X$ is described via their (assumed continuous) joint cumulative distribution function (CDF) $F$, i.e.,

$$(X,Y) \sim F$$

(1.1)

with the observations $\{(X_i,Y_i)\}_{i=1}^n$ arising from (1.1) are assumed independent, identically distributed (i.i.d.). This general regression setup has allowed researchers to study valid statistical procedures for inference and prediction problems.

The focus in this paper is predictive inference, specifically, the aim to generate a valid prediction interval (PI) for the response $Y_f$ associated with a future covariate $x_f$ of interest; the PI should have a predetermined coverage level/size. Formally, we call $C_{1-\alpha}(X_f)$ an ‘oracle’ PI of size $1-\alpha$ at a new covariate $X_f = x_f$, if under (1.1),

$$P(Y_f \in C_{1-\alpha}(X_f)|X_f = x_f) = 1 - \alpha.$$

In practice, the oracle PI is unknown; it has to be estimated through a statistical procedure, i.e., given data $\{(X_i,Y_i)\}_{i=1}^n$ the statistician produces an estimate $\hat{C}_{1-\alpha}(X_f)$ such that $P(Y_f \in \hat{C}_{1-\alpha}(X_f)|X_f = x_f) \approx 1 - \alpha$. This estimated PI is called conditionally valid by some authors, see e.g., Lei and Wasserman [2014]; we will further discuss the issue of conditionality in prediction intervals in Section 4.

Under the general regression setup of (1.1), there are at least three avenues in constructing prediction intervals, namely: naive quantile estimation, conformal prediction, and the Model-free Bootstrap (MFB); they are all discussed in detail in Section 2.2.

To give a short preview: quantile estimation(QE) amounts to estimating the conditional distribution of $Y$ given $X$; the term ‘naive’ is due to the fact that using the quantiles of the estimated conditional distribution of $Y_f$ given $X_f = x_f$ to create a PI for $Y_f$ sweeps under the carpet the variability of estimation which invariably results in undercoverage, i.e., the size of the PI will be less than then nominal $1 - \alpha$ in finite samples.

First proposed in Vovk et al. [2005], conformal prediction (CP, for short) is an ingenious technique for generating prediction intervals for i.i.d. or just exchangeable data $Z_1, \ldots, Z_n$; its basic idea is to
gauge how well a new data point $Z_{n+1}$ “conforms” to the observed sample $\{Z_i\}_{i=1}^n$ via a self-chosen “conformity score”. A tutorial on conformal prediction can be found in Shafer and Vovk [2008].

There has been a recent surge in extending the conformal prediction idea to non-i.i.d. statistical setups. Notably, Lei et al. [2013](see also Lei et al. [2018]) extended this idea to the regression setup (1.1), where the newly proposed conformal prediction algorithm constructs $\hat{C}_{1-\alpha}$ that satisfies the following no-undercoverage guarantee:

$$P(Y_f \in \hat{C}_{1-\alpha}(X_f)) \geq 1 - \alpha.$$  (1.2)

The PI is marginally valid as the probability is evaluated unconditionally, based on the randomness of $\{(X_i,Y_i)\}_{i=1}^n \cup (X_f,Y_f)$; its coverage guarantee relies on the exchangeability of the $n + 1$ data pairs $(X_i,Y_i)$ as implied by (1.1). However, the PI generated by the algorithm does not guarantee conditional validity as shown in Lei and Wasserman [2014] where a new algorithm was proposed to construct a PI with asymptotic ”local validity”. In Romano et al. [2019], the authors proposed a conformalized quantile regression approach which offers further improvement for heteroscedastic data. A recent endeavor to extend regression based conformal prediction to guarantee conditional validity is due to Chernozhukov et al. [2021]; see Section 2.2 for details.

The fact that the bootstrap –by generating a large number of artificial samples– can also capture the variability of estimated quantities inherent in prediction makes it an ideal candidate for predictive inference. Recall that the original bootstrap of Efron [1979] is applicable to i.i.d. data that are then sampled with replacement to produce the bootstrap resample. Politis [2015] proposed the “Model-free prediction principle” which amounts to using an invertible transformation to map a complex, non-i.i.d. dataset, to a dataset consisting of i.i.d. variables. The motivation is that prediction is easier –even trivial– with i.i.d. data; one can carry out the prediction in the i.i.d. domain and then map back via the inverse transformation. Furthermore, the “Model-free bootstrap” amounts to performing the standard bootstrap in the i.i.d. domain and then map back, yielding bootstrap PIs in the complex data domain. In a general regression setting, Politis [2013] suggested the use of the probability integral transform (PIT) –based on locally estimated conditional distributions– in order to transform the response data $Y_1, \ldots, Y_n$ to a sample of $n$ i.i.d. variables.

Our main focus of the paper is to understand the commonalities and differences between quantile estimation, conformal prediction and the Model-free Bootstrap (MFB). In Section 2, we contrast model-free to model-based regression, and discuss several different PI constructions. In Section 3, we carry out a preliminary asymptotic analysis for the coverage probability under the different
methods. Then, in Section 4 we discuss how PI validity could/should be assessed, i.e., conditionally or not, and prove a key lemma that reconciles conditional with unconditional validity in a big data setting. In Section 5, we discuss further differences of the three algorithms in terms of their ranges of applicability, and show theoretically that MFB intervals achieve better coverage compared to QE. The implicit reason is that MFB can produce pertinent PIs, a notion introduced by Politis [2015] in the setting of model-based, nonparametric regression; we extend this notion to model-free regression. Finally, in Section 6 we introduce the new concept of conjecture testing that is the analog of hypothesis testing as applied to the prediction problem; we also devise a modified conformal score to allow conformal prediction to handle one-sided ‘conjecture tests’, and compare to the Model-free bootstrap. Our theoretical findings are backed by simulation studies in Section 7.

2 Model-free vs. model-based regression

2.1 Model-based regression

The study of interval estimation is almost a century old, with its origins dating back to Neyman and Jeffreys [1937]. The extension to prediction intervals (PI) was soon to follow; see Patel [1989] and Geisser [1993] for a historical introduction. The traditional—although now outdated—approach was to construct $C_{1-\alpha}$ based on the normal distribution assumption. To describe it, consider first the rather trivial case where the $Y_i$ do not depend on the $X_i$ at all.

**Case I: I.i.d. responses** Assume for a moment that the responses $Y_1, \ldots, Y_n$ are i.i.d.; to conform with the classical tradition, let us assume that the common distribution is $N(\mu, \sigma^2)$. Then the interval

$$C_{1-\alpha}(x_f) = (\mu + z_{\alpha/2}\sigma, \mu - z_{\alpha/2}\sigma) \quad (2.1)$$

is an oracle PI of size $1 - \alpha$. Here, $z_{\alpha/2}$ is the lower $\alpha/2$ quantile of the standard normal distribution.

Since both parameters of the normal distribution are unknown, (2.1) has to be estimated by replacing $\mu$ and $\sigma$ by their unbiased estimators $\hat{\mu}$ and $\hat{\sigma}$, i.e., sample mean and sample variance of data $\{Y_i\}_{i=1}^n$. However, in order to achieve the exact size $1 - \alpha$, we also need to adjust the quantile to be from a $t_{n-1}$ distribution instead of the normal distribution, forming the estimated PI as

$$\hat{C}_{1-\alpha}(x_f) = \left(\hat{\mu} + t_{n-1,\alpha/2}\hat{\sigma}\sqrt{1 + \frac{1}{n}}, \hat{\mu} - t_{n-1,\alpha/2}\hat{\sigma}\sqrt{1 + \frac{1}{n}}\right) \quad (2.2)$$
where $t_{n-1,\alpha/2}$ is the lower $\alpha/2$ quantile of the $t$ distribution with $n-1$ degrees of freedom. The above is based on the fact that
\[
\frac{Y_f - \hat{\mu}}{\hat{\sigma} \sqrt{1 + \frac{1}{n}}} \sim t_{n-1}
\]
instead of $\mathcal{N}(0,1)$.

If we did not account for the randomness of $\{Y_i\}_{i=1}^n$, that precipitates the randomness of $\hat{\mu}$ and $\hat{\sigma}$, then we would simply use (2.1) plugging in $\hat{\mu}$ and $\hat{\sigma}$ for $\mu$ and $\sigma$ respectively. Since $z_{\alpha/2} > t_{n-1,\alpha/2}$, this would lead to undercoverage, as it does not take into account the variance related to the estimation procedure. The estimation variance is also present in the extra $1/n$ term inside the square root; although $1/n$ vanishes asymptotically, ignoring it in finite samples further induces undercoverage.

The above simple example provides a framework towards understanding the contribution of this paper, i.e., that it is imperative to take into account the variance related to model-fitting and estimation of all features that are to be plugged-in the oracle PI. We can now attempt some further generalizations.

**Case II: Model-based linear regression** Assume the data are generated by the model
\[
Y_i = \beta' X_i + Z_i \quad \text{for} \quad i = 1, \ldots, n
\] (2.3)
where $\beta \in \mathbb{R}^d$ is the (unknown) parameter vector, and the errors $Z_i$ are i.i.d. $\mathcal{N}(0,\sigma^2)$.

**Remark 2.1.** We may now assume that the regressors $X_i$ are fixed, i.e., non-random, or that they are random but independent of the errors; in the latter case, the following discussion will be understood in terms of the conditional probability given $X_i = x_i$ for $i = 1, \ldots, n$.

Letting $\hat{\beta}$ and $\hat{\sigma}^2$ denote the Least Squares (LS) estimator of $\beta$ and $\sigma^2$, the analog of (2.2) is
\[
\hat{C}_{1-a}(x_f) = \left( \frac{\hat{\beta}' x_f + t_{n-d,\alpha/2} \hat{\sigma}}{\sqrt{1 + x_f' (X'X)^{-1} x_f}} \right) \left( \frac{\hat{\beta}' x_f - t_{n-d,\alpha/2} \hat{\sigma}}{\sqrt{1 + x_f' (X'X)^{-1} x_f}} \right)
\] (2.4)
where $X$ is the $n \times d$ matrix having $X_i'$ as its $i$th row.

**Case III: Model-based nonparametric regression** Assume now the data are generated by the model
\[
Y_i = \mu_{X_i} + Z_i \quad \text{for} \quad i = 1, \ldots, n
\] (2.5)
where \( \mu_x \) is an unknown (but assumed smooth) function of \( x \in \mathbb{R}^d \), and the errors \( Z_i \) are i.i.d. \( N(0, \sigma^2) \); the caveat of Remark 2.1 still applies.

The quantity \( \mu_x \) can be estimated by any smoothing method, e.g., kernel smoothing, local polynomials, etc. resulting in the estimator \( m_x \). There is no exact distribution (like the \( t \) distribution) to use here, so we must resort to asymptotic normality of \( m_x \). The analog of (2.4) is the PI

\[
\hat{C}_{1-\alpha}(x_f) = (m_{x_f} - z_{\alpha/2}\hat{\sigma}V_{x_f}, m_{x_f} + z_{\alpha/2}\hat{\sigma}V_{x_f})
\]

that only has approximate/asymptotic coverage \( 1 - \alpha \). Here, \( \hat{\sigma} \) is the natural estimate of \( \sigma \), and \( V_{x_f} \) is a feature of the smoothing method; see eq. (3.17) of Politis [2015] for a concrete example based on kernel smoothing.

Model (2.5) can be extended to allow for heteroscedasticity, i.e., letting

\[
Y_i = \mu_{X_i} + \sigma_{X_i}\epsilon_i \quad \text{for} \quad i = 1, \ldots, n
\]

where \( \mu_x \) and \( \sigma_x \) are unknown (but assumed smooth) functions of \( x \in \mathbb{R}^d \), and the errors \( \epsilon_i \) are i.i.d. \( N(0,1) \). An analogous PI to (2.6) ensues, having first estimated \( \sigma_x \) via nonparametric smoothing. Nevertheless, this PI, as well as the previously mentioned PIs, i.e., (2.2), (2.4) and (2.6), are only valid if/when the regression errors are \( \text{exactly} \) normal, an assumption that is rarely justifiable nowadays.

Furthermore, it is of interest to go beyond the assumption of a regression equation driven by i.i.d. errors since even the most general/flexible such equation, namely (2.7), is unnecessarily restrictive. For example, (2.7) implies that the skewness and kurtosis of the response \( Y_i \) is constant, i.e., does not depend on \( X_i \). In that respect, (2.7) can not be assumed to hold even for \( \text{cps71} \), a dataset available within the \( \text{np} \) package of R that has served as a workhorse for nonparametric regression for decades; see Politis [2013] for details.

Note that in the random regressor case, a model equation such as (2.7), or any one of the more restrictive homogeneous and/or parametric versions such as (2.3) or (2.5), all imply (1.1) —under the caveat of Remark 2.1— but not vice versa. Therefore, assumption (1.1) is less restrictive even than general nonparametric regression as defined by eq. (2.7). Working under assumption (1.1) has been termed \textit{Model-free regression} by Politis [2015] in the sense that it is devoid of a model equation such as (2.3), (2.5) or (2.7); this is the subject of the following subsection.
2.2 Model-free regression

We now revert to the “Model-free” setup of eq. (1.1) which is re-stated for convenience here:

\[(X_i, Y_i) \text{ for } i = 1, \ldots, n \text{ are i.i.d. from } F.\]  

(2.8)

Note that the above implies a random design; it is also possible to conduct Model-free regression with a fixed design as discussed in [Politis 2015] but we limit the present discussion to setup (2.8).

Naive quantile estimation. The quantile estimation (QE) approach is straightforward; an oracle PI would be

\[\left( F^{-1}_{y|x_f}(\alpha/2), F^{-1}_{y|x_f}(1 - \alpha/2) \right). \]  

(2.9)

Since the conditional quantile \( F^{-1}_{y|x_f}(p) = \inf \{ y \in \mathbb{R} : F(y|x) \geq p \} \) is unknown, we may estimate it by the appropriate quantile of the CDF estimator, i.e.,

\[\hat{F}^{-1}_{y|x_f}(p) = \inf \{ y \in \mathbb{R} : \hat{F}(y|x) \geq p \}.\]

There is a wide range of selections when it comes to estimating the conditional CDF estimation, which we will mention in section 2.3. Having settled on an choice of estimator, we could plug it in (2.9) resulting in the PI

\[\left( \hat{F}^{-1}_{y|x_f}(\alpha/2), \hat{F}^{-1}_{y|x_f}(1 - \alpha/2) \right). \]  

(2.10)

The above plug-in approach is termed ‘naive’ because it does not account for the estimation error of the quantiles; hence, the PI (2.10) is typically characterized by undercoverage in finite samples. In the next section, asymptotic analysis shows both the bias and variance of this error will affect coverage performance.

Model-free bootstrap. Consider an arbitrary point predictor \( \hat{Y}_f \) for the response to be observed at future point \( x_f \); mathematically, \( \hat{Y}_f \) is a function of the observed data \( \{(X_i, Y_i)\} \) and \( x_f \), i.e.,

\[\hat{Y}_f = g(\{(X_i, Y_i)\}_{i=1}^n, x_f) ; \]  

\( \hat{Y}_f \) can also be regarded as some functional of the estimated predictive distribution, denoted by \( \mathcal{J}(\hat{F}_{y|x_f}) \). In addition, let \( \mathcal{J}(F_{y|x_f}) \) be the true point predictor that \( \hat{Y}_f \) is estimating. The prediction error \( R_f = Y_f - \hat{Y}_f \) is termed the "predictive root" in bootstrap literature; through resampling \( R_f \), we can approximate the quantiles of the distribution of \( R_f \), which then can be used to calculate the bootstrap PI centered at \( \hat{Y}_f \).

The original bootstrap of [Efron 1979] is applicable to i.i.d. data that are then sampled with replacement to produce the bootstrap resample. [Politis 2015] proposed the “Model-free prediction
principle” which amounts to using an invertible transformation to map a complex, non-i.i.d. dataset, to a dataset consisting of i.i.d. variables. The motivation is that prediction is easier—even trivial— with i.i.d. data; one can carry out the prediction in the i.i.d. domain and then map back via the inverse transformation. Furthermore, the “Model-free bootstrap” (MFB) amounts to performing the standard bootstrap in the i.i.d. domain and then map back, yielding bootstrap PIs in the complex data domain.

In the model-free regression setting, [Politis 2013] suggested the use of the probability integral transform (PIT) –based on locally estimated conditional distributions– in order to transform the response data \(Y_1, \ldots, Y_n\) to a sample of \(n\) i.i.d. variables. To elaborate, define the ranks \(U_i = F(Y_i|X_i)\) that are i.i.d. \(Unif(0,1)\) due to the PIT, assuming \(F_{y|x}\) is continuous in \(y\) for all \(x\); hence, this transformation performs a uniformization of the responses. Meanwhile, we can recover the data \(Y_i\) by the identity \(Y_i = F^{-1}_{Y|X}(U_i)\), i.e., by utilizing the inverse PIT. Asymptotic validity of the MFB for bootstrap confidence –as opposed to prediction– intervals was recently shown in [Wang and Politis 2021].

Remark 2.2. Note that by letting \(U_i = F(Y_i|X_i = x_i)\) where \(x_i\) was the realization of \(X_i\), and finding that the distribution of \(U_i\) conditionally on \(X_i = x_i\) is \(Unif(0,1)\), i.e., not depending on the value of \(x_i\), implies that (a) the unconditional distribution of \(U_i\) is also \(Unif(0,1)\), and (b) that \(U_i\) is independent of \(X_i\). Hence, the collection of conditional CDFs \(\{F_{y|x} : x \in \mathbb{R}^d\}\) connects two equivalent probability spaces: one is the space of \(\{(X_i, Y_i)\}_{i=1}^n\), the other is the space of \(\{(X_i, U_i)\}_{i=1}^n\), where \(X_i\) and \(U_i\) are two mutually independent sequences. In the latter, the regression/prediction problem has been trivialized, bringing it to the i.i.d. setting of Case I of Section 2.1.

Here, we propose the following model-free bootstrap algorithm for predictive inference under the distributional setup in (2.8). The original MFB algorithm of [Politis 2015] treated the design points \(X_i\) as fixed during the resampling; the algorithm below is similar albeit the \(X_i\)’s are also resampled.

Algorithm 2.1. MFB prediction interval at future point \(x_f\)—random regressor case:

1. Use the given data \(\{(X_i, Y_i)\}_{i=1}^n\) to estimate the conditional CDF \(\hat{F}_n(\cdot|X_i)\) and its inverse.

2. Calculate estimated ranks \(\hat{U}_i = \hat{F}_n(Y_i|X_i)\).

3. Choose a type of predictor \(\hat{Y}_f = g((X_i, Y_i)_{i=1}^n, x_f)\), i.e., choose the function \(g\), that will be the center of the prediction interval. The predictive root is defined by \(R_f = Y_f - \hat{Y}_f\).
4. Create $X_1^*, \ldots, X_n^*$ by resampling the regressors $\{X_i\}_{i=1}^n$, i.e., by randomly sampling with replacement from the set $\{X_1, \ldots, X_n\}$.

5. Create $U_1^*, \ldots, U_n^*$ by resampling the $\{\hat{U}_i\}_{i=1}^n$. Let $Y_i^* = \hat{F}^{-1}(U_i^*|X_i^*)$. Let $Y_f^*$ be a sample from distribution $\hat{F}(y|X = x_f)$, and $\hat{Y}_f^* = g((X_i^*, Y_i^*))_{i=1}^n, x_f)$. The bootstrap predictive root is
\[ R_f^* = Y_f^* - \hat{Y}_f^*. \]

6. The above step is repeated $B$ times to create $B$ replicates of $R_f^*$. Denote by $q_{\alpha}^*$ the $\alpha$–quantile of the empirical distribution of the $B$ replicates of $R_f^*$. The bootstrap prediction interval is then defined as
\[ (\hat{Y}_f + q_{\alpha/2}^*, \hat{Y}_f + q_{1-\alpha/2}^*). \quad (2.11) \]

For comparison, we state below the original algorithm model-free bootstrap algorithm, i.e., Algorithm 4.4.1 in [Politis 2015]

Algorithm 2.2. MFB prediction interval at future point $x_f$—fixed regressor case:
The algorithm is identical to Algorithm 2.1 except that we replace Step 4 by:

4’. Let $X_i^* = X_i$.

Remark 2.3. [Politis 2015] also proposed some different variations to the basic Algorithm 2.2. For example, the Limit model-free bootstrap omits step (2) that calculates estimated ranks. Instead, in step 3 the $U_i^*$’s are directly sampled from a $Unif(0, 1)$ distribution, thus reducing computational cost and simplifying the analysis for proofs. For predictive inference, the author also recommends using the predictive model-free approach, which estimates the $t^{th}$ rank $\hat{U}_i^{(-t)} = \hat{F}^{(-t)}(Y_i|X_i)$ where $\hat{F}^{(-t)}$ is estimated through the delete-$t$ dataset $\{(X_i, Y_i)\}_{i=1}^n/(X_t, Y_t)$.

Distributional conformal prediction. As mentioned in the Introduction, a recent endeavor to extend conformal prediction to guarantee conditional validity in regression is distributional conformal prediction (CP). This was proposed by [Chernozhukov et al. 2021] who used the aforementioned uniformization transformation –based on a locally estimated PIT– to calculate the conformity score as follows.
For a candidate $y \in \mathbb{R}$ for which we want to test whether it belongs to the PI, $\hat{F}_{n+1}(-|x)$ is an estimator for the conditional distribution function $F(-|x)$, based on $n+1$ data $\{(X_i, Y_i)\}_{i=1}^n \cup (X_f, y)$. Define the sample conditional ranks $\hat{U}_i(X_f, y) = \hat{F}_{n+1}(Y_i|X_i)$ for $i = 1, \cdots, n$ and $\hat{U}_{n+1}(X_f, y) = \hat{F}_{n+1}(y|X_f)$. The conformity scores are defined as $\hat{V}_i(y) = |\hat{U}_i(X_f, y) - 1/2|$, and the $p$-value for the null hypothesis that $y$ conforms to the data is
\[
\hat{p}(y) = \frac{1}{n+1} \sum_{i=1}^{n+1} 1(\hat{V}_i(y) \geq \hat{V}_{n+1}(y)).
\]
The $1 - \alpha$ prediction interval is defined as the range of $y$ where $\hat{p}(y) > \alpha$, i.e.
\[
\hat{C}_{1-\alpha}(X_f) = \{y : \hat{p}(y) > \alpha\}.
\]
With certain assumptions, Chernozhukov et al. [2021] showed that this procedure will guarantee not only unconditional validity, i.e., a finite-sample guarantee of unconditional coverage not less than $1 - \alpha$, but also asymptotic conditional validity in the following sense:
\[
\mathbb{P}(Y_f \in \hat{C}_{1-\alpha}(X_f)|X_f = x_f) \rightarrow 1 - \alpha
\]
as $n \rightarrow \infty$. Interestingly, this is what bootstrap prediction intervals, such as (2.11), typically satisfy. Hence, it is of interest to further compare the CP intervals with the MFB ones.

### 2.3 On choosing conditional CDF and quantile estimator

The conditional CDF and its quantiles plays an important role in all three above mentioned methods. The two quantities are directly related in that we can construct a valid quantile estimator from a CDF estimator, and vice versa. For example, by inverting the CDF estimator, we get the quantile estimator; to construct the CDF estimator from estimated quantiles, the following relationship is convenient:
\[
F_{y|x}(u) = \int_0^1 1(F_{y|x}^{-1}(\tau) \leq u) d\tau.
\]
As one of the fundamental problem in statistics, there exists a plethora of estimators with guarantees of consistency. Considering the volume of different types of distributions, methods that do not rely on a particular parametric model for the conditional distribution are preferred in practice. We now list two such methods which will be used for our comparisons of the three PI methods.
1. **Nonparametric CDF estimation.** This method constructs the estimator via nonparametric kernel smoothing as follows:

\[
\hat{F}(y|x) = \frac{\frac{1}{n} \sum_{i=1}^{n} W_h(X_i, x) K\left(\frac{Y_i - y}{h_0}\right)}{\bar{W}_h(x)},
\]

with \(W_h(X_i, x) = \frac{1}{n} \prod_{s=1}^{d} w\left(\frac{X_{is} - x_s}{h}\right)\) and \(\bar{W}_h(x) = \frac{1}{n} \sum_{i=1}^{n} W_h(X_i, x)\); \(w(\cdot)\) is a univariate, symmetric density function with bounded support, and \(K\) is a proper CDF; \(h\) and \(h_0\) are bandwidths that converge to 0, whose optimal rates depend on asymptotic analysis. Under finite sample setting, we choose \(h\) and \(h_0\) according to existing empirical rule or through cross validation, see Ch. 6, Li and Racine [2006]. Nonparametric kernel estimation works well when the dimension \(d\) of the covariates is low, e.g., \(d \leq 3\). When dealing with high-dimensional covariates, using the formulation in Equation (2.13) may lead to poor performance as a result of curse of dimensionality. Instead of using a product kernel, Ch.4, Politis [2015] demonstrated a simplifying approach by exploiting the univariate kernel combined with a certain form of distance function \(d_\theta(\cdot, \cdot)\) in \(R^d\), and \(W_h(X_i, x) = \frac{1}{h} w\left(d_\theta(\cdot, \cdot)/h\right)\). This helps when the dimension of \(X_i\) is high, or even with functional-type covariates whose dimension is infinite.

Equation (2.13) is suitable for estimation when \(x\) is not a boundary point in the range of covariates. Near the boundary, local linear –as opposed to local averaging– estimation is preferable; see Das and Politis [2020] for details.

2. **Regression quantiles.** The regression quantile approach can alleviate the curse of dimensionality when estimating conditional quantiles with high-dimensional covariates, and has attracted attention both in statistics and econometrics. It seeks to estimate \(F_{y|x}^{-1}(\tau)\) by searching in the linear span of the covariates \(\{X^\prime \beta, \beta \in R^d\}\) such that the expected quantile loss \(E\rho_\tau(Y - X^\prime \beta)\) is minimized. Here, \(\rho_\tau(r) = r(\tau - 1)(r < 0)\) is the check function. The rationale behind using regression quantiles is that the global minimizer \(q(x)\) to \(E\rho_\tau(Y - q(x))\) is exactly the \(\tau\)–quantile \(F_{y|x}^{-1}(\tau)\), and we restrict our search for \(q(x)\) in the linear span of \(x\). \(\beta\) is estimated by the minimizer of the sample quantile loss:

\[
\hat{\beta} = \arg \min_{\beta} \sum_{i=1}^{n} \rho_\tau(Y_i - X_i^\prime \beta),
\]

which is often calculated via numerical algorithms. The optimization problem in eq. (2.14) can be further adjusted to estimate \(\hat{\beta}\) under high-dimensional sparse scenarios, see Chap.15 of Koenker et al. [2017].
3 Preliminary asymptotic analysis

The methods introduced in Section 2 share some common features. Besides the fact that all of them use the conditional CDF function as an indispensable tool, the distributional conformal prediction and Model-free bootstrap both utilize the PIT to get estimated ranks \( \hat{U}_i \) as a middle step towards further inference. However, there are also important differences that distinguish them apart, and may result in different performance. In this section, we conduct asymptotic analysis for the three methods, with a focus on the coverage probability unconditional on the data \((X_n, Y_n) = \{(X_i, Y_i)\}_{i=1}^n\), and conditioning on the future covariate, i.e.

\[
\mathbb{P}_{x_f}(Y_f \in \hat{C}_{1-\alpha}(X_f)) := \mathbb{P}(Y_f \in \hat{C}_{1-\alpha}(X_f)|X_f = x_f).
\]  

(3.1)

As a first step, we perform analysis for the QE method to examine the factors that can affect coverage. This, along with analysis for the other two methods in the appendix, facilitates a conclusion on the commonalities of factors that contribute to coverage bias, which we later put forth as a claim below.

**Naive quantile estimation.** In the example of QE, the estimated conditional quantile \( \hat{F}^{-1}_{y|x_f}(p) \) is used to construct the prediction interval. Rewriting the conditional coverage probability \( \mathbb{P}_{x_f}(Y_{n+1} \in \hat{C}_{1-\alpha}(X_{n+1})) \) under this setup, we have:

\[
\mathbb{P}_{x_f}(Y_{n+1} \in \left( \hat{F}^{-1}_{y|x_f}(\alpha/2), \hat{F}^{-1}_{y|x_f}(1 - \alpha/2) \right)).
\]  

(3.2)

Denoting the quantile estimation errors \( A_n = \hat{F}^{-1}_{y|x_f}(\alpha/2) - F^{-1}_{y|x_f}(\alpha/2) \) and \( B_n = \hat{F}^{-1}_{y|x_f}(1 - \alpha/2) - F^{-1}_{y|x_f}(1 - \alpha/2) \), the above probability equals to

\[
\mathbb{E}_BnF_{y|x_f}\left(F^{-1}_{y|x_f}(1 - \alpha/2) + B_n\right) - \mathbb{E}_A\mathbb{F}_{y|x_f}\left(F^{-1}_{y|x_f}(\alpha/2) + A_n\right)
\]  

(3.3)

By a second order Taylor expansion, expression (3.3) equals to

\[
(1 - \alpha) + f_{y|x_f}\left(F^{-1}_{y|x_f}(1 - \alpha/2)\right)\mathbb{E}(B_n) - f_{y|x_f}\left(F^{-1}_{y|x_f}(1 - \alpha/2)\right)\mathbb{E}(A_n) + \frac{1}{2}f'_{y|x_f}\left(F^{-1}_{y|x_f}(1 - \alpha/2)\right)\mathbb{E}(B_n^2) - \frac{1}{2}f'_{y|x_f}\left(F^{-1}_{y|x_f}(1 - \alpha/2)\right)\mathbb{E}(A_n^2) + \text{higher-order terms}.
\]  

(3.4)

With the decomposition \( \mathbb{E}(A_n^2) = \text{Var}(A_n) + \mathbb{E}^2(A_n) \), Equation (3.4) can also be written in the form of a bias-variance expansion.

Different choices of CDF estimators affect the rate of convergence for coverage bias. In the case of the nonparametric CDF estimator, we have the rate for for the bias and variance as follows (also see Theorem 6.4, Li and Racine [2006]):
Lemma 3.1. When $\hat{F}_{y|x}$ is the nonparametric kernel estimator, both $A_n$ and $B_n$ converge to 0 in probability at rate of $O_p(h^2 + 1/\sqrt{n}h)$, with $E(A_n) = O(h^2)$ and $\text{Var}(A_n) = O(1/nh)$.

This lemma can be used to indicate the rate of the optimal bandwidth $h$ such that the asymptotic rate of convergence of the nonparametric kernel estimator $\hat{F}_{y|x}$ is optimal; as usual, with nonnegative kernels the optimal rate for $h$ is of order $n^{-1/5}$.

In the case of quantile regression, we can achieve asymptotic efficiency, i.e., a $\sqrt{n}$-convergence rate for the estimated quantiles, provided the implied linear regression model for the quantiles is correct; when the model is false, however, the bias can be non-negligible and further leads to incorrect coverage.

The takeaway of the above calculations is that the first two moments regarding the model estimation error, $A_n$ and $B_n$, contribute the most to the bias in conditional coverage probability. Consequently, we do not have a no-undercoverage guarantee in finite samples for this simple method. As it turns out, asymptotic analysis for the other two methods also agrees with this conclusion, which we state as a claim below.

Claim 3.1. Let $e_{\text{total}}$ be the total estimation error regarding the procedures of QE, CP or MFB. Then the first two factors contributing to the coverage bias are the first and second moments of $e_{\text{total}}$; i.e.,

$$\text{Coverage bias} = O(E_n e_{\text{total}}) + O(\text{Var}_n(e_{\text{total}})).$$

Granted, $e_{\text{total}}$ takes on different forms for the three methods. For example, since QE and CP are essentially based on the estimated quantiles, $e_{\text{total}}$ will be the sum of the quantile estimation errors. However, in MFB the total error also includes the error of predictor estimation, and $e_{\text{total}}$ of MFB has extra terms comparing with to QE/CP. Since all errors must converge to 0 in order for each method to be asymptotically valid, validity for MFB requires more assumptions, as we later show in Theorem 5.2. We argue that extra terms in $e_{\text{total}}$ do not necessarily mean more undercoverage – the sign of coefficients for the extra error terms controls this matter.

The derivation of asymptotic results for CP and MFB are presented in the Appendix section. Note that asymptotic theory will play a less important role in a finite-sample setting, and the performance between them can vary as well. Hence, empirical experiments and simulation are typically conducted to compare predictive performance in finite samples.
4 The conditionality problem

One exciting result about conformal prediction which inspired many recent explorations in this area is the marginal/unconditional validity property as given in eq. (1.2). The basis of (1.2) relies on both \((X_n, Y_n)\) and \((X_f, Y_f)\) being random and exchangeable, or more relevantly, i.i.d. in the model-free regression setup (2.8); in addition, the coverage probability should be unconditional with respect to the data. Discussions about appropriateness of assumptions are mostly focused on the data itself, such as the i.i.d. assumption for the data \((X_n, Y_n)\) which is standard in the regression literature; or equi-distribution assumption for the future pair \((X_f, Y_f)\), which led to recent advances in conformal prediction that proposed solutions when there is a distributional shift for \(X_f\), see e.g., Tibshirani et al. [2019].

What is equally important but less focused on, is the appropriate level of conditionality with which we should evaluate the PI’s coverage probability. More specifically, at which level should we integrate randomness of data into the probability evaluation. This so-called conditionality problem has been a crucial concept in statistical inference going beyond prediction intervals. Ever since the proposal of the conditionality principle of Cox [1958] and its connection to the likelihood principle (see Birnbaum [1962]), statisticians have debated on the correctness of these principles and their implications in statistical inference. For a review, see Robins and Wasserman [2000], which also points out that the issue of conditionality does not involve mathematical rigor; instead, arguments regarding its virtue are purely a statistical concern.

In resonance with conditionality for parameter inference problems, new findings are recently discovered regarding the impact of conditioning for prediction problems under a regression setup; see e.g., Rosset and Tibshirani [2020] and Bates et al. [2021], where new tools are also developed for better predictive inference under conditioning. In this section, we study the evaluation of coverage probabilities under different levels of conditioning, and derive relationships between them. We connect different conditioning setups with real world scenarios, and suggest the appropriate level of conditioning under different circumstances. The conditionality problem also leads to further analysis of the MFB algorithm in Section 5.

As a first step, we introduce three probability measures with different levels of conditioning. For
simplicity, they are denoted as \( P_1, P_2, P_3 \) respectively:
\[
\begin{align*}
P_1(\cdot) &= P_{x_f}(\cdot) = P(\cdot|X_f = x_f), \\
P_2(\cdot) &= P(\cdot|X_f = x_f; X_n), \\
P_3(\cdot) &= P(\cdot|X_f = x_f; (X_n, Y_n)).
\end{align*}
\]

We have the following tower property regarding the hierarchical relationship between \( P_k : k \in \{1, 2, 3\} \).

**Lemma 4.1.** *(Tower property)* Let \( A \in \sigma (X_n, Y_n, X_f, Y_f) \) be an arbitrary measurable event; here \( \sigma (\cdot) \) denotes \( \sigma \)-algebra. Then, we have that \( P_2(A) = E_{Y_n|X_n}P_3(A) \) and \( P_1(A) = E_{X_n,Y_n}P_3(A) \).

**Remark 4.1.** Bootstrap calculations (including the MFB) are typically conducted conditionally on the data. The so-called ‘bootstrap world’ is governed by probability measure \( P_3 \), and bootstrap validity is typically proven in probability (or almost surely) with respect to the ‘real world’ probability \( P \). Note that showing validity (or asymptotic validity) under \( P_3 \) is stronger, implying validity (or asymptotic validity) under \( P_2 \) or \( P_1 \). To see why, assume \( P_3(A) \to 1 - \alpha \) in probability; then the expectation of \( P_3(A) \) will also tend to \( 1 - \alpha \) by the bounded convergence theorem, i.e., \( P_1(A) \to 1 - \alpha \) and \( P_2(A) \to 1 - \alpha \). Hence, working under a \( P_3 \) performance measure which is more stringent may be generally preferable. Remark 4.2 below offers a reconciliation of the different viewpoints in a big data setting.

Consider the following data scenarios.

**A. Scenarios with respect to data.** The data \( \{(X_i, Y_i)\}_{i=1}^n \) belong to one of the following conditions:

1. Both \( X_i \) and \( Y_i \) are random, with i.i.d. \((X_i, Y_i) \sim F\).

2. \((X_1, \cdots, X_n)\) are fixed covariates; \( \{Y_i\}_{i=1}^n \) are considered random with distribution \( Y_i|X_i \sim F_{y|x_i} \).

3. The data \( \{(X_i, Y_i)\}_{i=1}^n = (X_n, Y_n) \) are observations that were drawn from the joint distribution \( F \) but are now treated as fixed.

The above three scenarios are directly coupled with the above probability measures, i.e., scenario (A.i) corresponds to \( P_i \), for any \( i = 1, 2, 3 \).
Remark 4.2. [Big data vs. limited data.] By definition of \( P_3 \) in eq. (4.1), the instance-specific \( P_3 \) is a random probability measure which inherits its randomness from the observations \((X_n, Y_n)\); from lemma [4.1] it follows that \( P_1 \) and \( P_2 \) are expectations of \( P_3 \). By the Strong Law of Large Numbers, \( P_3(A) \) will converge to \( P_1(A) \) for any \( A \in \sigma(X_n, Y_n, X_f, Y_f) \) as the sample size \( n \to \infty \). Therefore, under a **big data** regime, \( P_1 \) and \( P_2 \) are not very different from \( P_3 \), and are equally suitable for coverage evaluation. As setups (A.1) and (A.2) are coupled with \( P_1 \) and \( P_2 \) respectively, we see that treating the data as random has validity under the big data regime. On the other hand, when \( n \) is finite, \( P_3 \) can be very different from the other two probability measures; this phenomenon was recently put forth in Bates et al. [2021]. Contrary to the big data regime, the finite-\( n \) case is a **limited data** regime where the data should be regarded as fixed observations, i.e., setup (A.3); this suggests the use of \( P_3 \) as being more appropriate for coverage evaluation with limited data.

To make more concrete the above big data vs. limited data dichotomy, we provide three leading examples to illustrate scenarios (A.1), (A.2) and (A.3) respectively.

1. **Randomized experiments.** Commonly known as A/B testing, randomized experiments is a prevalent tool for treatment effect estimation. Given a large pool of data \( \{X_i\}_{i=1}^n \), it involves random selection and assignment of candidates into control/treatment groups. Formally put, \( S_1, S_2 \subset \{1, \cdots, n\} \) are disjoint random index sets with \( \max(|S_1|, |S_2|) < n \), and \( \{X_{s_1}\}_{s_1 \in S_1}, \{X_{s_2}\}_{s_2 \in S_2} \) are the covariates of treatment/control groups, with responses \( \{Y_{s_1}\}_{s_1 \in S_1}, \{Y_{s_2}\}_{s_2 \in S_2} \) are collected for these covariates. In this case, the data pair \((X, Y)\) in each group should be regarded as random, and \( P_1 \) should be the correct measure for conditional coverage evaluation.

2. **Regression for categorical data.** Given continuous covariates \( X \) and response \( Y \), binning (categorization) is a common practice that transforms \( X \) into a handful of categories in order to eliminate unnecessary randomness in the covariates and reduce complexity of data. While \( Y \) can still be considered random, binning is a procedure that interpolates between random design and fixed design. It is therefore reasonable to consider \( P_2 \) when the binning procedure produces fixed covariates.

3. **Few-shot learning and modeling of rare events.** The phrase ”few-shot learning” is adapted from the machine learning community which describes scenarios where training data \((X, Y)\) is extremely limited in quantity; this is naturally a limited data scenario. In the case of rare events, \( X \) and \( Y \) are observations that are extreme values compared to the population.
distribution. In this case, the coverage probability conditioning on these observations are clearly distinct from one without conditioning. Therefore, $\mathbb{P}_3$ should be the correct probability measure for coverage.

**Remark 4.3. [Conditionality under prediction.]** The conditionality principle was originally proposed in a parameter estimation context; in one of its many versions it states the following: Let $\theta$ be a parameter of interest, then inference with respect to $\theta$, such as evaluating coverage of a CI, should be conditioned on all ancillary statistics, and also relevant subsets; see [Robins and Wasserman] [2000] for details.

Under a prediction context, the different levels of conditioning also represent whether we think the data is ancillary and/or relevant subsets with respect to PI coverage. In this regard, $\mathbb{P}_2$ and $\mathbb{P}_3$ can be better measures of coverage comparing to $\mathbb{P}_1$ under certain circumstances. In the above examples, example 2 is related to viewing the covariates as ancillary statistics; while example 3 is related to viewing the entire observations as relevant subsets.

Together with scenarios (A.1), (A.2) and (A.3), we also introduce a second set of scenarios about the future covariate $X_f$.

**B. Distribution assumption for the future covariate.**

1. $X_f$ is random with distribution $F_{X_f}$.

2. $X_f$ is a fixed future design point in $\mathbb{R}^d$.

(B.1) assumes that the future covariate is randomly chosen; therefore the marginal coverage $\mathbb{P}(Y_f \in C(X_f))$ is actually a weighted average of conditional coverages: $\mathbb{E} \mathbb{P}_{X_f}(Y_f \in C(X_f))$. Being able to achieve a $1 - \alpha$ marginal coverage does not imply an $1 - \alpha$ conditional coverage. On the other hand, an $1 - \alpha$ conditional coverage will guarantee $1 - \alpha$ marginal coverage. To this aspect, validity under (B.2) is stronger than that under (B.1).

In recent years, CP has gained increasing interest in the machine learning community in that it is able to guarantee no undercoverage for a finite number of data under exchangeability; this is a consequence of (A.1) and (B.1)—see [Lei et al.] [2018]. However, CP does not guarantee conditional validity. The CP variant of [Chernozhukov et al.] [2021] offers improvement to [Lei et al.] [2018] in that it achieves asymptotic conditional validity under (A.1) and (B.2). Yet asymptotically this method is on par with the performance of naive QE when considering conditional coverage, as demonstrated
in section 3 and appendix A.1. Thus, CP may be better suited for big data scenarios, where data and future covariate can be regarded random.

It has been known that there is no algorithm that has finite sample no-undercoverage guarantees for conditional validity; see Lemma 1 of Lei and Wasserman [2014]. Instead, correctness of a prediction algorithm is demonstrated via asymptotic conditional validity. As we will show rigorously in the following section, the MFB approach delivers asymptotic coverage validity under any combination of conditions in scenario A and B. Granted, this alone does not justify using MFB over QE and CP as both of them are also asymptotically conditionally valid. Therefore, besides asymptotic validity, we will introduce two extra properties of MFB prediction intervals, namely pertinence and improved coverage over the other two methods.

5 Further analysis of Model-free bootstrap

Recall the two MFB algorithms from Section 2.2. Algorithm 2.1 is referred to as the random regressor scheme, while Algorithm 2.2 is the fixed regressor scheme—which can also be considered when inference is to be made conditionally on the design covariates $X_n$. Algorithm 2.1 takes advantage of the distributional setup of the covariates, and conforms to the setup where the study of interest is the coverage probability unconditional on the data $X_n, Y_n$. Since both $P_2$ and $P_3$ assume that the design covariates $X_n$ is fixed, Algorithm 2.2 is tailored for scenarios (A.2) and (A.3), while Algorithm 2.1 is more suitable for (A.1). Asymptotically, the two algorithms are equivalent.

5.1 Asymptotic pertinence and better coverage guarantees

In terms of interval prediction algorithms, while asymptotic validity guarantees correctness, it alone does not justify good finite sample coverage performance. Section 3.6 of Politis [2015] made a clear illustration of this point and defined the notion of “pertinence” of prediction intervals. Formally speaking, a “pertinent” prediction interval should be able to capture both the variability of future response $Y_f$ correctly, as well as the variance due to estimation. Although the latter is usually asymptotically negligible, being able to capture it will improve finite sample performance. As far as we know, to capture the variance due to estimation (without resorting to simplifying assumptions such as normality) requires some form of bootstrap.
Politis [2015] formulated the notion of “pertinent” prediction intervals in a model-based regression setting such as (2.7). Here, we extend the definition of asymptotic pertinence to the model-free regression setup of (2.8).

**Definition 5.1. Asymptotic pertinence of a model-free prediction interval.** A prediction interval generated by the bootstrap predictive root $R^*_f$ (as defined in Algorithms 2.1 and 2.2) is asymptotically pertinent if it satisfies all of the following:

1. Both $R_f$ and $R^*_f$ can be decomposed into the following representations:

   \[
   R_f = \epsilon_f + e_f, \\
   R^*_f = \epsilon^*_f + e^*_f
   \]

   Here, $\epsilon_f = Y_f - \mathcal{J}(F_{y|x})$ is the non-degenerate variable concerning the distribution of future response $Y_f$, and $e_f$ is model estimation error which converges to 0 in probability; $\epsilon^*_f$ and $e^*_f$ are their bootstrap analogues.

2. $\sup_x |\mathbb{P}^*(\epsilon^*_f \leq x) - \mathbb{P}(\epsilon_f \leq x)| \xrightarrow{P} 0$ as $n \to \infty$.

3. There is a diverging sequence of positive numbers $a_n$ such that $a_n \epsilon_f$ and $a_n \epsilon^*_f$ converge to nondegenerate distributions, and $\sup_x |\mathbb{P}^*(a_n \epsilon^*_f \leq x) - \mathbb{P}(a_n \epsilon_f \leq x)| \xrightarrow{P} 0$ as $n \to \infty$.

4. $\epsilon_f$ is independent of $e_f$ in the real world, i.e., in unconditional probability $\mathbb{P}_1$; similarly, $\epsilon^*_f$ is independent of $e^*_f$ in the bootstrap world, i.e., in conditional probability $\mathbb{P}_3$.

In section 5.2, we give closed forms for the decompositions of part (1) of Definition 5.1 and show that the MFB algorithm produces asymptotic pertinent prediction intervals, a unique advantage compared to both QE and CP, which do not satisfy the decomposition in Definition 5.1. The effect of pertinence will also be shown in section 7, where we run parallel comparison for experiments with large vs. small sample size $n$, and show that asymptotic validity and pertinence each plays a more important role in the two separate cases.

In addition, we now state a general claim that will be substantiated in what follows.

**Claim 5.1.** Under mild conditions, the MFB has better coverage probability compared with QE regardless of the type of CDF/quantile estimator one chooses, and regardless of which of the three probability measures $\mathbb{P}_k$ one chooses to evaluate coverage.
To elaborate, we will show that there exist an integer \( N \) and \( \alpha_0 \in (0, 1) \), such that for all \( \alpha < \alpha_0 \) and \( n \geq N \), we have

\[
P_k \left( Y_f \in \hat{C}_{1-\alpha}^{MF}(X_f) \right) > P_k \left( Y_f \in \hat{C}_{1-\alpha}^{QE}(X_f) \right) \quad \text{for any} \quad k \in \{1, 2, 3\}.
\] (5.1)

Note that for the case of \( k = 3 \), Equation (5.1) holds in probability.

**Remark 5.1.** In Section 3, we showed that QE and CP have almost identical asymptotic expressions in terms of conditional coverage probability, see Equation (A.2) in Appendix A.1. Thus for large \( n \), we may replace \( P_k \left( Y_f \in \hat{C}_{1-\alpha}^{QE}(X_f) \right) \) with \( P_k \left( Y_f \in \hat{C}_{1-\alpha}^{CP}(X_f) \right) \) in Equation (5.1), showing that MFB will also have better coverage than CP for large enough \( n \).

### 5.2 Required technical assumptions

The idea of proving the property of asymptotic pertinence and also Equation (5.1) goes as follows. We first consider the setup of (A.3), which is both the natural real-world scenario as well as the correct setup in the bootstrap world. We show that under (A.3) the decomposition of Definition 5.1 holds for MFB, in contrast with QE and CP. Next, to prove Equation (5.1), we make mild assumption on the estimator \( \hat{p} \), under which the convolution of \( \hat{p} \) with a (asymptotic negligible) Gaussian kernel will lead to more heavy-tailedness of the distribution. In the last step, lemma 4.1 is invoked to extend our result under (A.3) to (A.1) and (A.2).

**Assumption 1.** We make the following general assumptions:

- (C1). The sequence of conditional CDF estimators \( \hat{F}_{y|x_f} \) (indexed by \( n \)) is consistent to a continuous CDF \( F_{y|x} \) in the sup norm:
  \[
  \sup \limits_{u} |\hat{F}_{y|x}(u) - F_{y|x}(u)| \overset{P}{\to} 0.
  \]

- (C2). The MFB is asymptotically valid for the inference problem with respect to \( \hat{Y}_f \) in the following sense, as \( n \to \infty \):

  1. The predictor \( \hat{Y}_f = g(\{(X_i, Y_i)\}_{i=1}^n, x_f) \) and \( \hat{Y}_f^* = g(\{(X_i^*, Y_i^*)\}_{i=1}^n, x_f) \) in the bootstrap world satisfy a central limit theorem: \( \exists \sigma_{\infty}^2 \in \mathbb{R}_+ \), \( \tau_n \to \infty \) such that

  \[
  \tau_n \left( \hat{Y}_f - \mathbb{E} \hat{Y}_f \right) \overset{D}{\to} \mathcal{N}(0, \sigma_{\infty}^2);
  \]
  \[
  \tau_n \left( \hat{Y}_f^* - \mathbb{E} \hat{Y}_f^* \right) \overset{D}{\to} \mathcal{N}(0, \sigma_{\infty}^2), \quad \text{in probability}.
  \]
Where \( E \hat{Y}_f = \mathcal{J}(F_{y|x_f}) + o_p(1/\tau_n) \) and \( \mathcal{J} \) is a functional that maps the CDF function to \( \mathbb{R} \); similarly, \( E\hat{Y}_f^* = \mathcal{J}(\hat{F}_{y|x_f}) + o_p^*(1/\tau_n) \).

2. \( \mathcal{J}(\hat{F}_{y|x_f}) \overset{P}{\to} \mathcal{J}(F_{y|x_f}) \).

(C3). For large enough \( n \), \( \hat{F}_{y|x_f} \) belongs to the following class of CDFs:

\[
\mathcal{F} = \{ F : \exists \sigma_0, u_0 \in \mathbb{R}_+, \forall \sigma < \sigma_0, u > u_0, \hat{F}(u) < \hat{F} \ast \phi_\sigma(u); \hat{F}(-u) > \hat{F} \ast \phi_\sigma(-u) \}.
\]

Here, \( \hat{F}(u) = 1 - F(u) \) is the tail distribution function and \( \ast \) is the convolution operator; \( \phi_\sigma \) is the density function of the normal distribution \( \mathcal{N}(0, \sigma^2) \).

Remark 5.2. In practice, two types of predictors are typically considered: the mean which minimizes the \( L^2 \) loss between future response \( Y_f \) and the predictor \( \hat{Y}_f \), and the median that minimizes the \( L^1 \) loss. For the median case, under assumption (C1) and Polya’s theorem, item 2 in (C2) is guaranteed and no further assumptions are necessary; while in the case of the mean, on top of (C1), we also need uniform integrability of the sequence \( \hat{F}_{y|x_f} \) to ensure \( \mathcal{J}(\hat{F}_{y|x_f}) \overset{P}{\to} \mathcal{J}(F_{y|x_f}) \).

The above conditions can be easily achieved in general. (C1) and (C2) are classic assumptions regarding validity of statistical procedures. Plus, we make no assumption on the rate of convergence for either the conditional CDF estimator nor the predictor at which we center prediction intervals. (C3) is a less intuitive assumption: it implies that the distribution of \( Y_{x_f} + \sigma Z \) has heavier tails than that of \( Y_{x_f} \) when \( Y_{x_f} \sim \hat{F}_{y|x_f} \) and \( Z \sim \mathcal{N}(0, 1) \) independent of \( Y_{x_f} \). However, we will show there is in fact a large class of distributions that falls into this class. We start with the following lemma:

**Lemma 5.1.** Let \( f(u) \) be a density function defined on \( \mathbb{R} \) where (i) \( \exists u_0 > 0 \) such that \( f(u) \) is third-order differentiable and \( |f^{(3)}(u)| \) is bounded for \( |u| > u_0 \). (ii) \( f(u) \) is convex for \( |u| > u_0 \), i.e. \( f''(u) > 0 \). Then the CDF of \( f \) satisfies (C3).

**Remark 5.3.** (a). Condition (ii) in lemma [5.1] is satisfied by a large class of distributions. Since (C3) is a property of the tail distribution function, it is natural to consider distributions that are in the class of regularly varying functions \( RV(\rho) \) at infinity, where the tail CDF \( \hat{F}(u) \) (as well as \( \hat{F}(-u) \)) satisfies

\[
\frac{\hat{F}(cu)}{\hat{F}(u)} \xrightarrow{u\to\infty} e^{-\rho}, \rho > 0;
\]

so that the tail CDF behaves like a power function \( u^{-\rho} \) at infinity (multiplied by a slowly varying function \( L(u) \)). If \( L, L' \) and \( L'' \) behave “nicely”, such that
1. \( L \) is positive and third-order differentiable near infinity;

2. \( L, L', \text{ and } L'' \) all belong to the following class of functions

\[
\mathcal{H} := \left\{ H : \lim_{|u| \to \infty} \frac{H'(u)}{H(u)/u} = 0 \right\}
\]

then \( \exists C > 0, \ f''(u) \sim Cu^{-(p+3)}L(u) > 0 \). The class \( \mathcal{H} \) is a subset of slowly varying functions, see [Resnick 2007].

(b). Another interpretation related to the convolution problem in (C3) is the following. Given \( \hat{F}_{y|x_f} \) that is consistent to \( F_{y|x_f} \) in the sup norm, then we have that \( \hat{F}_{y|x_f} \ast \phi_\sigma \) is a \( C^\infty \) CDF that approximates \( \hat{F}_{y|x_f} \) in the limit when \( \sigma \to 0 \). In addition, we have the following result:

\[
\sup_x |\hat{F}_{y|x_f} \ast \phi_\sigma(x) - F_{y|x_f} \ast \phi_\sigma(x)| \leq \sup_x |\hat{F}_{y|x_f}(x) - F_{y|x_f}(x)|,
\]

where the equality holds only when \( |\hat{F}_{y|x_f}(x) - F_{y|x_f}(x)| \) equals to the sup norm at every \( x \). Then the implication using the predictive root for bootstrap is two-fold: First of all, the root distribution is more smooth than \( \hat{F}_{y|x_f} \) itself, and this can be beneficial to the bootstrap procedure, see [Silverman and Young 1987]. Secondly, the convoluted CDF has better approximation performance than the plain CDF \( F_{y|x_f} \), this means bootstrapping the predictive root requires less data than only bootstrapping the future response in order to achieve the same performance. This agrees with our numerical findings in Section 7.

5.3 Results for MFB pertinence and Claim 5.1

The main theoretical results for our paper are summarized in the following theorems:

**Theorem 5.2.** (Asymptotic validity) Assume (C1) with \( x = x_f \); then the prediction intervals \( \hat{C}(x_f) \) of QE is asymptotically valid. Further assume (C1) for all \( x \), then CP is also asymptotically valid.

\[
P_k \left( Y_f \in \hat{C}_{1-\alpha}(X_f) \right) \to 1 - \alpha \quad \text{as} \quad n \to \infty \quad \text{for} \quad k \in \{1,2,3\}.
\]

(The convergence is in probability sense for \( k = 2,3 \).) If we also assume \( \hat{Y}_f^{\ast} - \hat{Y}_f \overset{P}{\to} 0 \), then Equation (5.3) holds for the MFB as well.

**Theorem 5.3.** (Asymptotic Pertinence of MFB) Assume (C1) and (C2); then, the predictive root \( R_f \) and \( R_f^{\ast} \) in the Model-free bootstrap is asymptotically pertinent in the sense of Definition 5.1.
Theorem 5.4. (Better performance guarantee) Assume (C1), (C2) and (C3); then the Model-free bootstrap has higher coverage comparing to the quantile estimation method in the sense of Equation (5.1).

The last theorem is in effect verifying our Claim 5.1. Proofs of the three theorems are found in Appendix A.4.

We summarize our findings in Table 1.

|                  | Conformal prediction                                      | Model-free bootstrap                                      |
|------------------|-----------------------------------------------------------|-----------------------------------------------------------|
| Applicable       | Big data                                                  | Big data and limited data                                 |
| scenarios        | Random design                                             | Random/ fixed design                                      |
|                  | Random future covariate                                  | Random/ fixed future covariate                            |
| Validity         | Marginal validity                                        | Asymptotic marginal validity                              |
|                  | Asymptotic conditional validity                           | Asymptotic conditional validity                           |
| Advantage        | Finite-sample marginal coverage guarantee                 | Pertinence of prediction intervals                        |
|                  |                                                           | Guaranteed better coverage than QE.                      |

Table 1: Comparison between conformal prediction and Model-free bootstrap.

6 Conjecture testing

6.1 Prediction vs. estimation

Consider the two general classes of statistical inference: parameter estimation and prediction. While prediction intervals are the analogs of confidence intervals in estimation, there is no clearly defined analog of hypothesis testing as applied to prediction. We aim to fill this gap here by defining the new notion of conjecture testing. Table 2 illustrates these analogies.

Conjecture testing is different from hypothesis testing in the following ways. First of all, conjecture testing attempts to answer a question regarding a future response $Y_f$ which is an unobserved random variable; by contrast, (frequentist) hypothesis testing aims to answer a question regarding an unknown fixed (nonrandom) parameter $\theta$. Secondly, the rejection region of a hypothesis test is derived from the distribution of the target statistic under the null hypothesis; by contrast, the
probability measure by which a conjecture gets tested is one of the three mentioned, i.e., $\mathbb{P}_k$ (for some $k$), which remains unchanged when the null changes. In addition, contrary to hypothesis testing which often relies on central limit theorems to prove consistency of a particular test, validity of conjecture testing is directly associated with validity of prediction intervals, which essentially requires consistent estimation of the predictive distribution $F_{y|x_f}$. In this regard, as sample size grows, the acceptance region of hypothesis testing will shrink towards a single point $\theta$, while the acceptance region of conjecture testing will not degenerate.

### 6.2 Conjecture testing: definition and discussion

Statistical hypothesis testing at a certain significance level $\alpha$ is a fundamental tool in statistical inference. Consider a parameter parameter of interest $\theta$ whose value is estimated by a statistic $\hat{\theta}_n$. After defining the null hypothesis $H_0$ and the alternative $H_1$, a frequentist hypothesis test can be conducted by figuring out the threshold of the test statistic that ensures $P_{H_0}(\text{reject } H_0) \leq \alpha$. Alternatively, the test can be conducted by computing the $p$-value and rejecting $H_0$ only if the $p$-value is less than $\alpha$.

By the duality between hypothesis testing and confidence intervals (CI), we can equivalently construct a $1 - \alpha$ CI for $\theta$ and reject $H_0$ if the CI does not include the $\theta$ value(s) under $H_0$. This duality applies equally to the standard two-sided CIs that correspond to a two-sided null hypothesis, as well as one-sided CIs —where one of the CI bounds are $\pm \infty$— that correspond to a one-sided null hypothesis.

While prediction intervals are the analogs of confidence intervals in estimation, there is no clearly defined analog of hypothesis testing as applied to prediction. We aim to fill this gap here by defining the new notion of conjecture testing. It all starts by formulating two conjectures (i.e., hypotheses) regarding the value of the future response $Y_f$, namely the null conjecture $C_{null}: Y_f \in S_{null}$ vs. the
alternative conjecture $C_{alt} : Y_f \notin S_{null}$ where $S_{null}$ is a set of interest.

By analogy with hypothesis testing, the simplest choices for $S_{null}$ are:

1. $S_{null} = \{y_0\}$
2. $S_{null} = [y_0, \infty)$
3. $S_{null} = (-\infty, y_0]$

where $y_0$ is some given value of interest. Case 1 is a point null (with a two-sided alternative), while Cases 2 and 3 are one-sided tests. The aim is to try to make a decision between the two conjectures $C_{null}$ and $C_{alt}$ while controlling the probability of false rejection of $C_{null}$ to be not more than $\alpha$. The probability of false rejection can be measured with probability $P_k$ for some appropriate $k$.

As in the parameter estimation paradigm, there is also a natural duality between conjecture testing and prediction intervals (PI). For example, in Case 1 of the point null, we could construct a $1 - \alpha$ PI for $Y_f$, and reject $C_{null}$ at level $\alpha$ if $y_0 \notin$ PI. If the PI’s $1 - \alpha$ level is measured with probability $P_k$ (for some $k$), the size of the test will also be according to the same $P_k$.

It is quite common in practice to be interested in the behavior of a future response with respect to the predicted value in a particular direction, i.e., leading to one-sided conjectures and PIs. For example, when excessive risk is associated with response having higher (say) values than the projection; in this case, the practitioner would like to find a region of probable values for $Y_f$ that exclude high-risk extreme values. Applications can be found in many fields, such as climate control, system risk monitoring, Value at Risk (VaR), etc.

The above discussion motivates the one-sided tests of Cases 2 and 3. Focusing on Case 2 —the other case being similar— we may start by constructing a $1 - \alpha$ lower one-sided PI of the type $(-\infty, c_f]$ for $Y_f$, such that $P_k (Y_f \notin (-\infty, c_f]) \approx \alpha$. We can then reject $C_{null} : Y_f \in [y_0, \infty)$ when

$$y_0 \notin (-\infty, c_f].$$

Note that in such a case, $P_k (Y \geq y_0) \leq P_k (Y_f \geq c_f) = \alpha$, i.e., the probability of false rejection of $C_{null}$ will not exceed $\alpha$ as required.

Statistically speaking, under the setup of (2.8) with i.i.d. data and future covariate of interest $x_f$, to construct a one-sided PI we need to find $c \in \mathbb{R}$ such that

$$P_k (Y_f - \hat{Y}_f \leq c) \approx 1 - \alpha$$

(6.2)
for either \( k \in \{1, 2, 3\} \) depending on the appropriate data scenario. The inclusion of \( \hat{Y}_f \) in \( \text{[6.2]} \) rules out using the QE and CP approaches. On the other hand, the Model-free bootstrap works readily since we can estimate \( c \) by the \( 1 - \alpha \) quantile of the bootstrap predictive root \( R_f^* \), i.e., \( \hat{c}^* = \hat{D}_{x_f}^{-1} (1 - \alpha) \). Hence, the threshold \( c_f \) appearing in the rejection region \( \text{[6.1]} \) can be estimated by \( \hat{c}_f = \hat{Y}_f + \hat{c}^* = \hat{Y}_f + \hat{D}_{x_f}^{-1} (1 - \alpha) \).

Constructing a one-sided PI – and inverting it to obtain a one-sided conjecture test – is also possible using QE. To do that, we can simply use the left/right quantiles of the estimated conditional CDF; for example, a \((1 - \alpha)100\%\) one-sided PI based on QE reads: \( [\hat{F}_y(x_f, \alpha), \infty) \) or \( (-\infty, \hat{F}_y^{-1}(1 - \alpha)) \).

**Remark 6.1.** Interestingly, the popular CP methodology is not designed to yield one-sided PIs. One might then think that CP can not handle one-sided conjecture tests. Delving deeper, however, it becomes apparent that this limitation is only due to the two-sided nature of the popular conformity score \( \hat{V}_i(y) = |\hat{U}_i(x_f, y) - 1/2| \). In order to handle one-sided PIs and one-sided conjecture tests via CP we may instead adopt a one-sided conformity measure, such as \( \hat{V}_i(y) = -\hat{U}_i(x_f, y) \) under which the produced PI will have the form \((c, \infty)\). We used this choice in our second simulation in Section \( \text{[7]} \).

In Section \( \text{[7]} \) we give a practical example of applying one-sided conjecture testing to examine accuracy of VaR prediction for high-frequency stock returns data.

## 7 Numerical experiments

### 7.1 Synthetic data

#### 7.1.1 Experiment setup

We consider the following model for simulations. Let \( \{(X_i, Y_i)\}_{i=1}^N \) be i.i.d. samples where

\[
X \sim Unif(0, 1), \\
Y = \sin(\pi X) + \sigma \sqrt{1 + 2X \epsilon}
\]

and \( \epsilon \sim T_5 \). We set the future covariate \( x_f = 0.5 \) to guarantee data balance on the two sides of \( x_f \), such that potential boundary effect will not appear in the simulations. The following procedure is conducted to estimate the conditional coverage probability(CVP) of size \( 1 - \alpha \) prediction intervals averaged on data, i.e., an estimate for \( \mathbb{P}_1(Y_f \in C(x_f)) \): for each \( k \in \{1, \cdots, K\} \), generate \( \{(X_i, Y_i)\}_{i=1}^N \) according to \( \text{[7.1]} \); then apply QE, CP and MFB on the data to form three \( 1 - \alpha \) prediction intervals
\( \hat{C}_{k}^{(QF)}(x_f), \hat{C}_{k}^{(CP)}(x_f) \) and \( \hat{C}_{k}^{(MFB)}(x_f) \). Also, after fixing \( X_f = x_f \), sample from \((\tilde{i}, 1) \) \( M \) times to get \((Y_f)_{i=1}^{M} \), and estimate the \( k \)-th coverage probability by the fraction of \( Y_f \) that are in the prediction interval, that is

\[
\frac{\sum_{i=1}^{M} 1 \left( (Y_f)_i \in \hat{C}_k \right)}{M} \tag{7.2}
\]

The collection of \( \overline{CVP}(\hat{C}_k) \) forms an empirical distribution for the coverage probability under model \((\tilde{i}, 1) \). Then we can estimate \( \mathbb{P}_1(Y_f \in \mathcal{C}(x_f)) \) by the sample average \( \frac{1}{K} \sum_{k=1}^{K} \overline{CVP}(\hat{C}_k) \).

### 7.1.2 Parameter tuning

The aforementioned parameters are set to be the following: \( \sigma = 0.2, \alpha = 0.05, K = 200 \) and \( M = 3000 \). Both the nonparametric and quantile regression based CDF estimators are considered in our simulations. For the nonparametric estimator, the bandwidth parameters \( h \) and \( h_0 \) need to be selected. We apply the following criteria for selection: within a grid of candidate bandwidths, the ones with which the uniformized series \( U_i \) has the largest \( p \)-value in terms of the Kolmogorov-Smirnov test for uniformity are selected. As for the quantile regression based CDF, we apply the Barrodale and Roberts algorithm to estimate \( F^{-1}_{y|x}(\tau) \) for \( \tau \) in the grid \( \{0.01i, 0 \leq i \leq 100\} \) and then calculate \( F_{y|x}(u) \) using a discretized version of \((2.12) \). In the bootstrap algorithm, we set \( B = 1000 \).

### 7.1.3 Asymptotic performance

We plot the estimated coverage probabilities, variances of the estimation \( \text{Var}(\overline{CVP}(\hat{C}_k)) \) (suitably scaled), as well as the average lengths of prediction intervals for different values of \( N \in \{50i, i = 1, \cdots, 8\} \) in Figure[1].
We analyze the results in the following aspects.

1. **Asymptotic validity.** For the nonparametric CDF estimator, QE and MFB exhibit asymptotic validity as the coverage probabilities converge to 95% when $N$ increases; while convergence for CP seems to stabilize around 92%. For the quantile regression based CDF estimator, all three algorithms converge to the nominal level.

2. **Coverage comparison.** The prediction intervals of MFB have higher coverage than QE for both CDF estimators, especially when the sample size $N$ is small. This agrees with our result in Theorem 5.3 and also shows that MFB is able to alleviate undercoverage issue under limited data scenario. The behavior of CP varies based on the choice of CDF estimator: when the nonparametric CDF is used, CP performance is not as good as the other methods; while for the quantile regression CDF, CP in general has good performance except for the case $N = 50$, which we will discuss in further details in the next section.
3. **Quality of estimation.** The quality of prediction intervals is assessed by the variances of coverage probabilities and also the lengths of the prediction intervals. Differences between the algorithms are most observable from the results that use the nonparametric CDF estimator. In terms of the variances, the MFB is consistently lower than QE and CP, while CP has the largest variance among the three methods. This is related to the pertinence property of the MFB that helps tracking the nominal level more consistently than the other methods. As for the lengths of prediction intervals, the MFB has equal length compared with QE while delivering higher coverage. On the contrary, CP has an anomaly at $N = 50$ where the length is significantly larger; as $N$ increases, the lengths drop below those of QE and MFB, as do the coverage probabilities.

7.1.4 **Coverage behaviors under limited data scenario**

The behavior of CP under the limited data scenario ($N = 50$) is abnormal: for both CDF estimators, CP’s lengths of prediction intervals are much higher than competing methods; for the quantile regression based estimator, the coverage is even close to 100%. Hence here, we further investigate the results for $N = 50$. In Figure 2 we plot the histograms of the coverage probabilities. As we see from the graphs, CP will ”overcorrect” the prediction intervals to reach the nominal level 95%. In the case of using the nonparametric CDF estimator, the average coverage of CP is almost identical to that of MFB, but many of the prediction intervals are corrected to reach a 100% coverage, which also cause the interval lengths of CP to be much higher than those of MFB. In the case of using the quantile regression based CDF, this behavior is even more severe, causing the averaged coverage to be almost 100%. Therefore, the reliability of CP to generate conditionally valid prediction intervals is questionable under limited data setting.

7.2 **VaR prediction for intraday stock returns data**

We demonstrate an application of conjecture testing on high-frequency intraday stock returns data. To fix notations, let $S_t$ denote the price process of a stock; $X_t = \log \frac{S_t}{S_{t-1}}$ denotes the log-return log $\frac{S_t}{S_{t-1}}$ at time $t$. The concept of Value-at-Risk (VaR) is a risk measure in the following sense: for a finite time period $m$ and a pre-specified level $\alpha$, the VaR is the threshold $c$ such that the $m$-period return $T_m = \sum_{t=1}^{m} X_t$ is guaranteed to surpass $c$ with probability $1 - \alpha$. In other words, $VaR(\alpha) = F_m^{-1}(\alpha)$, where $F_m$ is the CDF of $T_m$.

This concept can be extended in various ways. First of all, we can extend the statistic of interest
beyond the case of total return $\sum_{k=t+1}^{t+m} X_k$, such as the form $T_m = f(X_1, \cdots, X_m)$ where $f$ is a continuous function. Examples include the worst $m$–period cumulative return, $T_m = \min_{1\leq t \leq m} R_t$, where $R_t = \sum_{k=1}^{t} X_k$, and the worst one-period return $T_m = \min_{k=1}^{m} X_k$. These risk-type statistics will induce different forms of $F_m$. These examples are considered in Bertail et al. [2004].
Another extension is to find appropriate covariate that can have predictive power for future VaR. For this purpose, we introduce additional dependence on the time parameter $t$ for $T_m$: $T_{t+1,m} = f(X_{t+1}, \ldots, X_{t+m})$. Also, let $V_{t,m}$ be the covariate of interest that is $\sigma(X_{t-m+1}, \ldots, X_t)$ measurable. Then given $V_{t,m}$ we want to find the $\alpha$-lower quantile for the conditional random variable $T_{t+1,m} | V_{t,m}$ as our VaR prediction for the future $m$-period returns. This is analogous to the one-sided prediction bounds described in Section 6, and we can use either QE or MFB to estimate the quantile of interest.

In our experiment, we consider 1-minute level return data during trading hours for our simulation. When extracting data, we remove those that are gathered from the first and last 5-minute in each trading day for quality control. We use the past $m$-period realized volatility $V_{t,m} = \sum_{k=t-m+1}^{t} X_k^2$ as the covariate and study its impact on future $T_{t+1,m}$ via VaR. We take $T_{t+1,m}$ to be the worst $m$-period cumulative return for the future data $(X_{t+1}, \ldots, X_{t+m})$, and our experiments show that by choosing appropriate $m$ there exhibits clear heteroscedascity in the paired data $(V_{t,m}, T_{t+1,m})$. Being able to capture the relationship between them will help individual traders to control their risk exposure, especially for day trading practitioners.

We formally setup the experiment as in the following. Let $\{X_n\}_{n=1}^{N}$ be the observed data up to time $N$; our goal is to predict the VaR of $T_{N+1,m}$ conditioning on $V_{N,n}$. The regression model is trained on observed data from the past $\{(V_{i,m}, T_{i+1,m})\}_{i \in I}$ where $I \subset \{m, \ldots, N-m\}$ is some index set. Because both $V_{i,m}$ and $T_{i+1,m}$ are aggregated statistics over $m$ periods, they each tends to have strong serial dependence for adjacent time indices which violates the i.i.d. assumption in our regression setup. To fix this issue, we only consider data from the time grid $I = \{(2k+1)m, k \in \mathbb{N}\}$, such that $(V_{(2k+1)m,m}, T_{(2k+1)m+1,m})$ are based on non-overlapping blocks of data $\{(X_{2mk+1}, \ldots, X_{2m(k+1)}), k \in \mathbb{N}\}$, thereby reducing the sample size by a factor of $2m$.

A new challenge arises from this procedure. On the one hand, as the dynamics of price process is time-varying, to ensure the joint distribution of $(V_{i,m}, T_{i+1,m})$ does not change over time, the past data $\{X_n\}_{n=1}^{N}$ needs to be from a short time frame, e.g., within 2 weeks so that the data size is less than $N_0 = (6.5 \times 60 - 10) \times 10 = 3800$. On the other hand, through our observation, the heteroscedasticity phenomena are most pronounced when $m$ is larger than some threshold $m_0$, e.g. $m_0 = 30$, although the choice of $m_0$ varies for different stocks. By our data trimming procedure above, the sample size of the paired data is at most $|I| = \left\lfloor \frac{N_0}{2m_0} \right\rfloor = 63$. This situation naturally falls into our limited data scenario introduced in Section 4.

We apply QE, MFB as well as CP using the nonparametric CDF estimator to predict the future
VaR on two stocks, AMC and GME listed on NYSE; these two stocks have recently been very popular with day traders, and have exhibited abnormal stock price upsurges despite drops in revenue reported in their financial statements. Coupled with this phenomenon, the volatility and fluctuations in the returns of these two stocks are higher than market average. It is therefore of practical value to devise a more formal testing procedure.

We gathered data from April 10th to July 10th 2021 using the AlphaVantage stock APIs and performed post processing outlined in the above paragraphs to get pairs of \((V, T)\) data. Our VaR predictions are calculated for \(\alpha \in \{0.01, 0.05, 0.1\}\) on \((V_{t,m}, T_{t+1,m})\) with \(m = 45\) for GME and \(m = 30\) for AMC, where the training data used for testing either have \(|Z| = 34\) or \(|Z| = 68\) prior to time \(t\). We perform conjecture testing based on predicted VaRs and future values \(T_{t+1,m}\), with null hypothesis being \(T_{t+1,m} > VaR_{pred}\). This testing procedure is carried out consecutively with respect to \(t\) so that we have a series of accept-reject results. Lastly, we calculate the empirical acceptance rate based on the results and compare it with the nominal level, \(1 - \alpha\). We benchmark the methods by closeness between the empirical acceptance rate and the nominal level.

The results of our experiments are presented in Table 3 and 4. The methods used for comparison are: naïve quantile estimation (QE); Model-free bootstrap with \(L_1\) and \(L_2\) predictors (MFB-\(L_1\) and MFB-\(L_2\) respectively); and (one-sided) distributional conformal prediction (CP).

Based on the empirical results, both QE and MFB still exhibit undercoverage issue, while we find that overall MFB is able to boost the coverage of QE for both \(|Z| = 34\) and \(|Z| = 68\), exemplifying the result of Theorem 5.4 when sample size increases to \(|Z| = 68\), the undercoverage issue is relieved to some level for both methods.

Measured by closeness to the nominal level, for the AMC stock the performance of CP is superior to other participating methods, while for GME the MFB has the edge. Notice that for the GME stock and some datapoints of the AMC stock, there are overcoverage issues for CP, echoing our analysis for the behavior of CP under limited-data scenario in the previous numerical experiment.
Ticker: GME

| Sample size Method | $\alpha = 0.01$ | $\alpha = 0.05$ | $\alpha = 0.1$ |
|--------------------|-----------------|-----------------|----------------|
| $|\mathcal{I}| = 34$ | QE 95.9 94.1 88.2 | MFB-$L^1$ 97.2 94.1 89.1 | MFB-$L^2$ 97.7 94.1 88.6 |
|                   | MFB-$L^1$ 97.2 94.1 89.1 | CP 99.5 97.7 91.4 |
| $|\mathcal{I}| = 68$ | QE 96.7 94.1 89.8 | MFB-$L^1$ 97.3 95.7 89.8 | MFB-$L^2$ 98.6 95.1 89.8 |
|                   | CP 99.4 96.7 92.5 |

Table 3: Empirical acceptance rate results for GME.

Ticker: AMC

| Sample size Method | $\alpha = 0.01$ | $\alpha = 0.05$ | $\alpha = 0.1$ |
|--------------------|-----------------|-----------------|----------------|
| $|\mathcal{I}| = 34$ | QE 95.1 90.8 86.5 | MFB-$L^1$ 95.1 91.6 87.6 | MFB-$L^2$ 95.4 91.4 86.8 |
|                   | CP 98.2 97.1 90.5 |
| $|\mathcal{I}| = 68$ | QE 95.8 91.7 87.9 | MFB-$L^1$ 97.1 92.6 88.2 | MFB-$L^2$ 96.8 92.3 87.9 |
|                   | CP 99.0 95.8 89.8 |

Table 4: Empirical acceptance rate results for AMC.

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A Appendix

A.1 Asymptotic analysis for CP

Denote \( \hat{U}(x, y) = \hat{F}(y|x) \), \( \hat{U}_i = \hat{U}(X_i, Y_i) \), and \( \hat{U}_{(\alpha/2)}, \hat{U}_{(1-\alpha/2)} \) the \( \alpha/2 \) sample quantiles of \( \{\hat{U}_i\} \). Note that in Chernozhukov et al. [2021], the conditional CDF is estimated with both \( \{(X_i, Y_i)_{i=1}^n\} \) and \((X_f, y)\), which results in an augmentation to \( \hat{U}_i \) that is denoted by \( \hat{U}_i'(X_f, y) = \hat{F}_{n+1}(Y_i|X_i) \).

We assert that \( \hat{U}_i \) and \( \hat{U}_i'(X_f, y) \) are asymptotically equivalent. Specifically, let \((X_f, Y_f)\) take on arbitrary values \((x, y)\); then, \(\sup_{i} |\hat{U}_i - \hat{U}_i'(x, y)| = \mathcal{O}_p(1/n)\). As both \( \hat{U}_{(\alpha)} \) and \( \hat{U}_i'(\alpha) \) converge to \( \alpha \) in probability, \( \hat{U}_{(\alpha)} - \hat{U}_i'(\alpha) = \mathcal{O}_p(1) \). Therefore, we can use \( \hat{U}_i \) instead for simplified asymptotic analysis.

Although in Chernozhukov et al. [2021], the estimated ranks \( \hat{U}_i' \) are further transformed to \( \hat{V}_i \) with which the \( p \)-values are calculated, the key to generating prediction interval still relies on the ranks themselves. With this in mind, the conditional coverage probability approximately equals to

\[
P(\hat{U}(X_f, Y_f) \in \left( \hat{U}_{(\alpha/2)}, \hat{U}_{(1-\alpha/2)} \right) | X_f = x_f).
\]

Let \( P_n \) and \( E_n \) denote the probability measure and expectation respectively associated with data \((X_n, Y_n)\). Then, by iterated expectation, (A.1) equals to

\[
E_n \mathbb{E}_{y_f \sim F(\cdot|x_f)} P_{n} \left\{ \hat{U}(x_f, y_f) \in \left( \hat{U}_{(\alpha/2)}, \hat{U}_{(1-\alpha/2)} \right) | X_f = x_f \right\} \\
= E_n \mathbb{E}_{y_f \sim F(\cdot|x_f)} E_{n} \mathbb{1} \left\{ \hat{U}(x_f, y_f) \in \left( \hat{U}_{(\alpha/2)}, \hat{U}_{(1-\alpha/2)} \right) \right\} \\
= E_n \mathbb{E}_{y_f \sim F(\cdot|x_f)} \left\{ y_f \in \left( \hat{F}_{y|x_f}^{-1}(\hat{U}_{(\alpha/2)}), \hat{F}_{y|x_f}^{-1}(\hat{U}_{(1-\alpha/2)}) \right) \right\} \\
\approx E_n F_{y|x_f}(\hat{F}_{y|x_f}^{-1}(\hat{U}_{(1-\alpha/2)}) - F_{y|x_f}(\hat{F}_{y|x_f}^{-1}(\hat{U}_{(\alpha/2)}))
\]

Similarly as before, denote \( A'_n = \hat{F}_{y|x_f}^{-1}(\hat{U}_{(1-\alpha/2)}) - F_{y|x_f}(\hat{U}_{(1-\alpha/2)}) \) and \( B'_n = \hat{F}_{y|x_f}^{-1}(\hat{U}_{(\alpha/2)}) - F_{y|x_f}(\hat{U}_{(1-\alpha/2)}) \) the errors of estimated quantiles; using Taylor expansion we get a similar expansion.
as in Equation (3.4), i.e.,
\[
\mathbb{E}_n F_{y|x_f}(\hat{F}^{-1}(\tilde{U}(1-\alpha/2))) - F_{y|x_f}(\hat{F}^{-1}(\tilde{U}(\alpha/2))) \\
= (1-\alpha) + \mathbb{E}_n(f_{y|x_f}(F_{y|x_f}^{-1}(\tilde{U}(1-\alpha/2))))\mathbb{E}_n(B'_n) - \mathbb{E}_n(f_{y|x_f}(F_{y|x_f}^{-1}(\tilde{U}(\alpha/2))))\mathbb{E}_n(A'_n) \\
+ \frac{1}{2}\mathbb{E}_n(f'_{y|x_f}(F_{y|x_f}^{-1}(\tilde{U}(1-\alpha/2))))Var_n(B'_n) - \frac{1}{2}\mathbb{E}_n(f'_{y|x_f}(F_{y|x_f}^{-1}(\tilde{U}(\alpha/2))))Var_n(A'_n) + \text{higher-order terms.}
\]

(A.2)

Hence, the bias in coverage probability is directly due to the bias and variance of the quantile estimator; in that sense, QE and CP perform very similarly.

The most notable difference between QE and CP is the addition of a new data point \((x_f, y)\) in the original samples \(\{(x_i, y_i)\}_{i=1}^n\) to estimate \(\hat{F}\), which results in the augmentation \(\hat{U}'(x_f, y)\) from \(\hat{U}\). An intuitive interpretation of this is that the new procedure “overfits” on a future observation \((x_f, y)\) and may lead to better coverage with finite sample size. With exchangeability holding, the procedure has guaranteed unconditional validity, while conditional validity holds asymptotically.

### A.2 Asymptotic analysis for MFB

We adopt the usual notation, where \(\mathbb{P}\) denotes the probability measure for the original probability space, and \(\mathbb{P}^*\) the probability measure in the bootstrap world, i.e., conditioning on the data \((X_n, Y_n)\). Given future covariate \(x_f\), let \(D_{x_f}\) denote the distribution of the predictive root \(R_f = Y_f - \hat{Y}_f\) under \(\mathbb{P}\), and let \(\hat{D}_{x_f}^*\) and \(\hat{D}_{x_f}^{*-1}\) denote the distribution and quantile respectively of the bootstrap version \(R_f^*\) under \(\mathbb{P}^*\); also assume that both are continuous functions, i.e., that \(R_f\) is a continuous random variable. The bootstrap prediction interval \(\hat{C}^{MF}(X_f)\) is \((\hat{Y}_f + \hat{D}_{x_f}^{*-1}(\alpha/2), \hat{Y}_f + \hat{D}_{x_f}^{*-1}(1-\alpha/2))\), and is considered a random element under \(\mathbb{P}\). The randomness of \(\hat{C}^{MF}(X_f)\) is due to variability across samples; given the observed sample, \(\hat{C}^{MF}(X_f)\) is a fixed quantity.

For the moment, let us focus our interest on the coverage probability without conditioning on the observed samples; hence the governing law is the original probability measure \(\mathbb{P}\). In addition, we have the following lemma concerning the distribution of bootstrap samples.

**Lemma A.1.** 1. Under \(\mathbb{P}^*\), the distribution of \(X_i^*\) conditioning on \((X_n, Y_n)\) is \(\frac{1}{n} \sum 1\{y \leq X_i\}\); The distribution of \(Y_i^* | X_i^* = X_k\) is \(\hat{F}_{y|x_k}\).
2. Under \(\mathbb{P}\), the distributions of \(X_i^*\) and \(Y_i^*\) are the expectations of their distributions under \(\mathbb{P}^*\). i.e.,
the distribution of \(X_i^*\) is \(F_X\), and \(Y_i^*\) \(X_i^* = x\) follows \(E_n \hat{F}_{y|x}^\prime\).

3. Under \(\mathbb{P}^*\), \(Y_f^*\) is independent of \(\hat{Y}_f^*\), so the distribution of \(R_f^* = Y_f^* - \hat{Y}_f^*\) is the convolution between \(Y_f^* \sim \hat{F}_{y|x_f}\) and the distribution of \(\hat{Y}_f^* = g(\{X_i^*, Y_i^*\}^n_{i=1})\).

4. Under \(\mathbb{P}\), \(Y_f\) is independent of \(\hat{Y}_f\) as well, and the distribution \(D_{x_f}\) is the convolution of \(F_{y|x_f}\) and the distribution of \(\hat{Y}_f\).

Let \(T_z f(x) = f(x + z)\) be the translation operator. For a CDF \(F\), \((T_z F)^{-1}(u) = F^{-1}(u) - z\).

Denote \(\Delta_1^{(u)} = \hat{D}_{x_f}^{(-1)}(u) - \left(T_{\mathcal{J}(\hat{F}_{y|x_f})} \hat{F}_{y|x_f}\right)^{-1}(u); \Delta_2 = \mathcal{J}(\hat{F}_{y|x_f}) - \mathcal{J}(\hat{F}_{y|x_f})\). Also, \(A_n\) and \(B_n\) are the same as in section 3.

Note that \(\hat{Y}_f\) and \(R_f^*\) are dependent on the data as they both depend on the data, so the previous route for coverage calculation can not be directly applied here. To carry out some asymptotic analysis, we make the following extra assumptions: \(\hat{Y}_f\) and \(\hat{Y}_f^*\) converge (respectively) to \(\mathcal{J}(F_{y|x_f})\) and \(\mathcal{J}(\hat{F}_{y|x_f})\), which are estimands of the two, in probability and in \(L^1\). Also assume \(D_{x_f}\) and \(\hat{D}_{x_f}^*\) are uniformly continuous, so that by Taylor expansion (\(\delta\)-method), the distributions \(D_{x_f}(x)\) and \(\hat{D}_{x_f}^*(x)\) converge (respectively) to \(T_{\mathcal{J}(F_{y|x_f})} F_{y|x_f}(x)\) and \(T_{\mathcal{J}(\hat{F}_{y|x_f})} \hat{F}_{y|x_f}(x)\), uniformly in \(x\). As a consequence, \(\forall u \in (0, 1), \hat{D}_{x_f}^{(-1)}(u) \overset{p}{\longrightarrow} \left(\mathcal{J}(F_{y|x_f}) \hat{F}_{y|x_f}\right)^{-1}(u) = \hat{F}_{y|x_f}^{-1}(u) - \mathcal{J}(\hat{F}_{y|x_f})\), and thus \(\Delta^{(u)} \overset{p}{\longrightarrow} 0\).

Consider the following decomposition holds:

\[
\begin{align*}
\hat{Y}_f + \hat{D}_{x_f}^{(-1)}(\alpha/2) &= F_{y|x_f}^{-1}(\alpha/2) + A_n + \Delta_1^{(\alpha/2)} + \Delta_2, \\
\hat{Y}_f + \hat{D}_{x_f}^{(-1)}(1 - \alpha/2) &= F_{y|x_f}^{-1}(1 - \alpha/2) + B_n + \Delta_1^{(1 - \alpha/2)} + \Delta_2
\end{align*}
\]  

Denote the total error in (A.3) \(e_{total} = A_n + B_n + \Delta_1^{(\alpha/2)} + \Delta_1^{(1 - \alpha/2)} + \Delta_2\). Now by iterated expectation and Taylor expansion, the coverage probability for the PI (2.11) is

\[
\begin{align*}
\mathbb{E}_n \left( F_{y|x_f}(\hat{Y}_f + \hat{D}_{x_f}^{(-1)}(1 - \alpha/2)) - F_{y|x_f}(\hat{Y}_f + \hat{D}_{x_f}^{(-1)}(\alpha/2)) \right) \\
= \mathbb{E}_n F_{y|x_f} \left( F_{y|x_f}^{-1}(1 - \alpha/2) + A_n + \Delta_1^{(1 - \alpha/2)} + \Delta_2 \right) - \mathbb{E}_n F_{y|x_f} \left( F_{y|x_f}^{-1}(\alpha/2) + B_n + \Delta_1^{(\alpha/2)} + \Delta_2 \right) \\
= (1 - \alpha) + O(\mathbb{E}_n e_{total} + Var_n(e_{total})) + \text{higher-order terms}.
\end{align*}
\]

Despite different formalization, the above discussion shows the three methods have similar asymptotic behavior for their respective (unconditional) coverage probability, in the sense that the source of coverage bias is from the first two moments of the total estimation error in each method.
A.3 Proof of Lemma 5.1

Proof. First of all, we assume (i) holds for all $u \in \mathbb{R}$. By Taylor’s Theorem,

$$f(u + z) = f(u) + f'(u)z + \frac{f''(u)}{2}z^2 + R(z),$$

where the remainder $R(z)$ has the form

$$R(z) = \frac{f^{(3)}(\xi(z))}{3!}z^3$$

for some $\xi(z) \in (u, u + z)$. Since $|f^{(3)}(\xi(z))|$ is bounded, we have

$$\int_{\mathbb{R}} R(z)\phi_\sigma(z) \, dz = o(\sigma^2),$$

where $\phi_\sigma(z)$ is the density function for the normal distribution $\mathcal{N}(0, \sigma^2)$.

Denote the density of $Y + \sigma Z$, where $Y$ has density $f(u)$ and $\sigma Z \sim \mathcal{N}(0, \sigma^2)$ as $\tilde{f}$. Then by convexity, $\forall |u| > u_0$

$$\tilde{f}(u) = (f * \phi_\sigma)(u) = \int_{\mathbb{R}} f(u + z)\phi_\sigma(z) \, dz$$

$$= \int_{\mathbb{R}} \left( f(u) + f'(u)z + \frac{f''(u)}{2}z^2 + R(z) \right) \phi_\sigma(z) \, dz$$

$$= f(u) + \frac{f''(u)}{2}\sigma^2 + o(\sigma^2)$$

$$> f(u)$$

for small enough $\sigma^2$. As a consequence, $\forall u > u_0$, $\tilde{F} * \phi_\sigma(u) = \int_{-\infty}^{u} \tilde{f}(x) \, dx > \int_{-\infty}^{-u_0} f(x) \, dx = \tilde{F}(u)$. Analogously, $F * \phi_\sigma(u) > F(u)$ for $u < -u_0$.

In the more general case where (i) is satisfied on the restricted domain $|u| > u_0$, $\forall \epsilon > 0$, we can choose $\sigma$ small enough where $\mathbb{P}(|\sigma Z| > u_0) < \epsilon$, so that $\forall |u| > 2u_0$, $|u + \sigma Z|$ is concentrated within $(u_0, \infty)$ with probability greater than $1 - \epsilon$; therefore $f(u + \sigma Z)$ satisfies (i) and (ii) for $|u| > 2u_0$ with probability $1 - \epsilon$. By the same procedure of Equation (A.5), this gives

$$\tilde{f}(u) > f(u)(1 - \epsilon) + \frac{f''(u)}{2} \left( \sigma^2 - \int_{z > c_{\sigma, \epsilon}/2} z^2 \phi_\sigma(z) \, dz \right) + o(\sigma^2)$$

for small enough $\sigma^2$. As a consequence, $\forall u > u_0$, $\tilde{F} * \phi_\sigma(u) = \int_{-\infty}^{u} \tilde{f}(x) \, dx > \int_{-\infty}^{-u_0} f(x) \, dx = \tilde{F}(u)$. Analogously, $F * \phi_\sigma(u) > F(u)$ for $u < -u_0$.
where \( c_{\sigma^2/2} \) is the upper \( \epsilon/2 \) quantile for the \( N(0, \sigma^2) \) distribution. Since \( \epsilon \) is arbitrarily small and \( f \) is convex for \( |u| > 2u_0 \), we conclude that \( \hat{f}(u) > f(u) \) for \( |u| > 2u_0 \). The remainder of the proof is the same as above. \( \square \)

Note that we may relax condition (i) in lemma 5.1 where \( f'' \) exists and is absolutely continuous on \( u > |u_0| \). Then \( f^{(3)} \) exists and the remainder \( R(z) \) has an integral form \( R(z) = \int_{(u, u+z)} \frac{f^{(3)}(t)}{2} (u + z - t)^2 \, dt \), and with bounded \( f^{(3)} \), \( \int_{R} R(z) \phi_{\sigma}(z) \, dz \) is also \( o(\sigma^2) \).

A.4 Proofs of Theorems 5.2, 5.3 and 5.4

Proof of Theorem 5.2. By Lemma 1.2.1 of Politis et al. [1999], under (C1) with \( x = x_f \), \( \hat{F}_{y|x_f}^{-1}(\alpha) \overset{P}{\rightarrow} F_{y|x_f}^{-1}(\alpha), \forall \alpha \in (0, 1) \). As a consequence, the boundary points of \( \hat{C}_{1-\alpha}^{(QF)}(x_f) \) converges to those of \( C_{1-\alpha}(x_f) = \left( F_{y|x_f}^{-1}(\alpha/2), F_{y|x_f}^{-1}(1 - \alpha/2) \right) \), then we have that \( \mathbb{P}( Y_f \in \hat{C}_{1-\alpha}^{(QF)}(X_f) ) \overset{P}{\rightarrow} 1 - \alpha \).

With further assumption that (C1) holds for all \( x \), then \( \hat{U}(Y_i|X_i) \) (and \( \hat{U}'(Y_i|X_i) \)) has asymptotic uniform distribution in \([0, 1]\). To see this, note that for \( X_i = x \) fixed, \( \hat{U}(Y_i|X_i = x) - U(Y_i|X_i = x) \overset{P}{\rightarrow} 0 \), then \( \mathbb{P}( \hat{U}(Y_i|X_i = x) \leq u ) \rightarrow u, \forall u \in [0, 1] \). Now

\[
\mathbb{P}( \hat{U}(Y_i|X_i) \leq u ) = E_{X_i} E_{Y_i|X_i=x} E_{\alpha-1} I(\hat{U}(Y_i|X_i) = x) \leq u ) = E_{X_i} \mathbb{P}( \hat{U}(Y_i|X_i) = x ) \leq u ) ,
\]

then by dominated convergence theorem, \( \mathbb{P}( \hat{U}(Y_i|X_i) \leq u ) \rightarrow u \). Then for CP, the analysis in section 3 shows that \( \hat{C}_{1-\alpha}^{(CP)}(x_f) \) is asymptotically equivalent to \( \hat{C}_{1-\alpha}^{(QF)}(x_f) \).

With the additional assumption \( \hat{Y}_f - \hat{Y}_f \overset{P}{\rightarrow} 0 \), \( \hat{C}_{1-\alpha}^{(MF)}(x_f) \) is asymptotically equivalent to \( \hat{C}_{1-\alpha}^{(QF)}(x_f) \), thus MFB is asymptotically valid.

Proof of Theorem 5.3. We decompose \( R_f \) and \( R_f^* \) as follows.

\[
R_f = Y_f - \hat{Y}_f = (Y_f - \mathcal{J}(F_{y|x_f})) - (\hat{Y}_f - \mathcal{J}(F_{y|x_f})) := \epsilon_f + \epsilon_f^*; \tag{A.6}
\]

\[
R_f^* = Y_f^* - \hat{Y}_f^* = (Y_f^* - \mathcal{J}(\hat{F}_{y|x_f})) - (\hat{Y}_f^* - \mathcal{J}(\hat{F}_{y|x_f})) := \epsilon_f^* + \epsilon_f^*; \tag{A.7}
\]

with \( \epsilon_f = Y_f - \mathcal{J}(F_{y|x_f}) \), \( \epsilon_f^* = Y_f^* - \mathcal{J}(\hat{F}_{y|x_f}) \); and \( \epsilon_f = \mathcal{J}(F_{y|x_f}) - \hat{Y}_f \), \( \epsilon_f^* = \mathcal{J}(\hat{F}_{y|x_f}) - \hat{Y}_f^* \).

Under assumption (C1), (2) in definition 5.1 is satisfied. Under assumption (C2), both \( \tau_n \epsilon_f \) and \( \tau_n \epsilon_f^* \) converge in distribution to normal distributions with equal variances, which shows (3) in definition 5.1.
Observe that $\epsilon_f$ only depends on $Y_f$, and the randomness of $e_f$ depends on the data $(X_n, Y_n) \perp Y_f$, therefore $\epsilon_f \perp e_f$. Similarly, conditioning on the data, $\epsilon_f^* \perp e_f^*$ in the bootstrap world. This shows (4).

**Proof of Theorem 5.4.** Under scenario (A3), assumption (C2) and previous result, the distribution of the bootstrap root $(R_f^*)$ is asymptotically equivalent to the convolution between $\hat{F}_{y|x_f}$ and a Gaussian distribution $\mathcal{N}(0, \tau_n^2)$. Then assumption (C3) guarantees that $\exists \alpha_0 \in (0, 1), n_0 \in \mathbb{N}$ such that $\forall \alpha < \alpha_0$ and $n > n_0$, $\tilde{C}_{1-\alpha}^{(QE)}(x_f) \subseteq \tilde{C}_{1-\alpha}^{(MF)}(x_f)$. This shows Equation (5.1) for $k = 3$. By Lemma 4.1, we can show (5.1) for the other two scenarios.