Inference for Interpretable Machine Learning: Fast, Model-Agnostic Confidence Intervals for Feature Importance

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Abstract

In order to trust machine learning for high-stakes problems, we need models to be both reliable and interpretable. Recently, there has been a growing body of work on interpretable machine learning which generates human understandable insights into data, models, or predictions. At the same time, there has been increased interest in quantifying the reliability and uncertainty of machine learning predictions, often in the form of confidence intervals for predictions using conformal inference. Yet, there has been relatively little attention given to the reliability and uncertainty of machine learning interpretations, which is the focus of this paper. Our goal is to develop confidence intervals for a widely-used form of machine learning interpretation: feature importance. We specifically seek to develop universal model-agnostic and assumption-light confidence intervals for feature importance that will be valid for any machine learning model and for any regression or classification task. We do so by leveraging a form of random observation and feature subsampling called minipatch ensembles and show that our approach provides assumption-light asymptotic coverage for the feature importance score of any model. Further, our approach is fast as computations needed for inference come nearly for free as part of the ensemble learning process. Finally, we also show that our same procedure can be leveraged to provide valid confidence intervals for predictions, hence providing fast, simultaneous quantification of the uncertainty of both model predictions and interpretations. We validate our intervals on a series of synthetic and real data examples, showing that our approach detects the correct important features and exhibits many computational and statistical advantages over existing methods.

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1 Introduction

Reliability and interpretability are crucial ingredients to building trustworthy artificial intelligence and machine learning systems for deployment in high-stakes applications like autonomous vehicles, facial recognition, healthcare, and national security [58, 23, 31, 1]. Recognizing the importance of this area, there is a large and growing literature on interpretable and explainable machine learning [48, 82, 40, 43]. At the same time, there is a surge of interest in being able to quantify levels of reliability of machine learning models, often in the form of measuring model uncertainty [24, 33, 79]. Many have proposed to develop confidence intervals or confidence sets for predictions, typically leveraging approaches from conformal inference [63, 32, 7, 35, 36, 53, 18, 50]. Despite the importance of both reliability and interpretability in machine learning systems, there is relatively little work on quantifying the reliability or uncertainty in machine learning interpretations. This paper focuses on one of the most popular forms of machine learning interpretation: feature importance, defined as the level of influence of a feature on the model predictions. Our specific goal is to develop a novel procedure with accompanying theory to conduct valid statistical inference for feature importance that is computationally fast and model-agnostic so that it can determine statistically significant features for any supervised machine learning model and regression or classification task.

The intersection of machine learning interpretability and reliability / uncertainty quantification is critically important and under-studied, with limited methods available for conducting model-agnostic inference on feature importance. To motivate the significance of our problem, let's consider an example from healthcare. Suppose the task is to predict adverse outcomes for ICU patients based on numerous features recorded in electronic health records. While a predictive model with high accuracy is important, interpreting the model and understanding which clinical features are predictive of adverse outcomes is arguably more crucial, as discovering these key features could prompt changes in clinical care and treatments. But what if the interpretations of feature importance provided by this healthcare model are unreliable, exhibiting a high degree of uncertainty? Preventing clinical care decisions from being made based on potentially unreliable interpretations of features in this healthcare model motivates the need for valid statistical inference of feature importance scores.

1.1 Related Work

Feature importance quantifies the effect of the input features on the predictions, therefore providing insights to scientific discovery and/or model validation, improving the interpretability of machine learning models. Most existing methods use model specific approaches, embedding feature importance measure within the prediction methods, including coefficients in generalized linear model [49], information gained from feature subsampling in tree-based methods [14, 17],

and gradient-based importance in deep learning [59, 62, 87, 42]. On the other hand, many have advocated for model agnostic approaches, including those based on feature permutations [21, 60, 38, 2], Shapley values [44, 45, 61], or feature occlusion [51, 21, 39, 83, 88]. Advantages of model-agnostic approaches include its flexibility in the choice of the predictive model and its unified interpretation across different models. In this paper, we focus on the feature occlusion measure of feature importance due to its applicability to any machine learning algorithms that output predictions.

Our work also builds on the growing literature on uncertainty quantification and inference for machine learning predictions, especially conformal inference approaches [25, 70, 5, 36, 56, 68, 71, 15, 55] which provide distribution-free predictive intervals or sets and enjoy valid finite-sample coverage. We are specifically motivated and inspired by the J+aB approach proposed in [32] that uses observation subsampling or bootstrapping to get fast leave-one-out predictions. Additionally, our work is also related to a recent line of papers on predictive inference for cross validation [10, 9, 46], which will prove useful for our theoretical guarantees.

Despite the significance of this area, there is relatively little work on inferential approaches for feature importance. Most of prior work on feature importance inference are only applicable for specific models, including the post-selection inference [13, 34, 64, 11] and the de-biased Lasso [85, 67, 30] for high-dimensional linear and generalized linear models, and more recently in random forests [47, 72, 73], etc. More general inference methods based on knock-off [16, 6, 8] seek to select features with FDR control, but do not provide intervals for feature importance. Some propose model class reliance (MCR) [21, 60] that investigate the feature importance across a set of well-performed models on the same data set, instead of one particular model in use. More related approaches that construct confidence intervals for feature importance include CPI [75], GCM [57], Floodgate [86], and VIME [78, 77]. Many are only applicable for regression tasks and not classification, others make specific distributional assumptions that might not hold for general ML problems. The approach most closely related to ours is the LOCO-Split inference method of [35, 52]. This method leverages conformal inference via data-splitting to conduct inference on feature occlusion scores. Out of the techniques we have thus far discussed for feature importance inference, LOCO-Split is by far the most general, being both model-agnostic and assumption-light. Despite these advantages, LOCO-Split has several major caveats that prevent its widespread adoption: (i) it is computationally expensive as separate models need to be fit to exclude each feature; (ii) data-splitting doesn't utilize full training data, and many in conformal inference literature have noted the poor performance and high variance of data splitting for inference [7, 69, 84]; and (iii) there is limited theory to support the use of LOCO-Split: its theoretical properties are only studied in the context of regression. In this paper, we address each of these shortcomings of LOCO-Split by developing a new inferential procedure.

Inspired by the subsampling approach of J+aB, our inferential approach is rooted in an

ensemble built by taking tiny random subsamples of both observations and features in tabular data. This idea of double subsampling appears first in the context of random forests [41, 27], linear regression [37], and more recently has been termed "minipatch ensembles" by [65, 80]. We adopt this idea of minipatch ensembles and we are the first to develop inferential approaches using this approach.

1.2 Our Contributions

1. We leverage ideas from minipatch ensembles [80, 26, 81] which subsample both observations and features to develop *a novel procedure to construct model-agnostic confidence intervals for feature importance*. We utilize the leave-one-covariate-out approach [35] while *avoiding data-splitting* and utilizing the full training data. Further, we *avoid model refitting* leading to a fast procedure as computations required for inference are nearly free as part of the ensemble learning process.

2. We provide theoretical guarantees showing that our confidence intervals enjoy *asymptotically correct coverage*, under minimal assumptions for any machine learning model and regression or classification task. Our proof tackles the dependencies of our leave-one-out estimates created by avoiding data splitting, by leveraging recent results [10] on the asymptotics of cross-validation.

3. We further show that our same procedure can provide *valid distribution-free predictive intervals* by extending the recent work of [32]. These predictive intervals are computationally free, with no further computations required.

4. Finally, we validate the coverage of our feature importance intervals in synthetic data; through synthetic and real data experiments, we also show that our approach compares favorably to existing methods in terms of Type I error / coverage, power, width, and computation.

2 Model-agnostic Inference for Feature Importance

In this section, we propose a fast algorithm for constructing confidence intervals for the importance of any target feature, in terms of its predictive power for a new sample. In particular, we leverage the idea of leave-one-covariate-out (LOCO) method [36], which focuses on the following quantity:

$$\Delta_{\text{LOCO},j}^*(\boldsymbol{X}, \boldsymbol{Y}) = \mathbb{E}\left[\text{Error}\left(Y, \mu(X; \boldsymbol{X}, \boldsymbol{Y})\right) - \text{Error}\left(Y, \mu(X_{\setminus j}; \boldsymbol{X}, \boldsymbol{Y})\right) | \boldsymbol{X}, \boldsymbol{Y}\right], \qquad (1)$$

where $\mu(\cdot; \boldsymbol{X}, \boldsymbol{Y})$ is the full predictive model fit on the training data set $(\boldsymbol{X}, \boldsymbol{Y})$, using all features; $\mu(\cdot; \boldsymbol{X}_{:,\setminus j}, \boldsymbol{Y})$ is the predictive model trained on the same data set but without feature j. Error()

is some nonconformity function appropriate for the supervised learning task, and the expectation is taken over a new test data point (X, Y).

Prior method: LOCO-Split To perform statistical inference for (1), [36] propose to construct confidence interval for feature j in regression problems via data splitting (LOCO-Split). Specifically, the N training samples are split into two sets: D_1, D_2. The full model $\mu(\cdot; \boldsymbol{X}_{D_1,:}, \boldsymbol{Y}_{D_1})$ and leave-j-covariate-out model $\mu(\cdot; \boldsymbol{X}_{D_1,:}, \boldsymbol{Y}_{D_1})$ are fit separately on the first part D_1 of the training data. Then they calculate the change of nonconformity on D_2 after removing feature j:

$$\Delta_j(X_i, Y_i) = \text{Error}(Y_i, \hat{\mu}^{-j}(X_i)) - \text{Error}(Y_i - \hat{\mu}(X_i)), \quad i \in D_2, \tag{2}$$

and construct confidence intervals using D_2 via an asymptotic Z-test or non-parametric sign test. However, LOCO-Split can suffer from (i) a *significant loss of information* from data splitting, and (ii) *intensive computation* since it requires re-fitting separate models to exclude each feature.

Leveraging an ensemble learning framework: minipatch learning To make the most use of our training data while also reducing the computational cost incurred in many refitting steps, we leverage the idea of a new ensemble method proposed recently in [65, 81], which is referred to as "minipatch learning". Here, small subsets of both observations and features are randomly selected and used for model training. The full predictor is the ensemble (average) of all the models trained on these random subsets, which are called "minipatches". As an ensemble method, minipatch learning is flexible and can be applied with any machine learning algorithm being the base learner on minipatches; it is also computationally efficient since model fitting on each tiny minipatch can be extremely fast. However, the key property of minipatch learning that we leverage is the fact that both observations and features are randomly selected during the model training, which can make leave-one-covariate-out computation much simpler and faster. For any target feature j, one can easily perform feature occlusion by only averaging over minipatches without feature j, hence *no additional fitting* is required regardless the number of features. Furthermore, leaving one observation out is as simple as leaving one feature out, making it extremely fast to compute the change of non-conformity score in a leave-one-out fashion instead of splitting the training data.

2.1 Target of Inference: Feature Importance Score

Before jumping into our algorithm for constructing confidence intervals, we first formally define our inference target, which is a slight modification of (1) and aligns well with the minipatch learning framework discussed earlier. We focus on the predictors that are ensembled from base learners trained by small minipatches of the training data, and we would like to provide statistical inference for the predictive power with or without the target feature. Specifically, consider a base

learning algorithm $H \colon \mathcal{X} \times \mathcal{Y} \to \mathcal{F}$ that maps the sample space $\mathcal{X} \times \mathcal{Y}$ to a class of predictors $\mathcal{F}$. Examples of this base learner H can be ridge regression, random forest, deep neural networks, etc. Then given a training data set $(\boldsymbol{X}, \boldsymbol{Y})$ independently sampled from some probability distribution $\mathcal{P}$, where $\boldsymbol{X} \in \mathbb{R}^{N \times M}$ includes N observations of M features, and $\boldsymbol{Y} \in \mathbb{R}^{N}$ includes N continuous responses or categorical labels, we consider the predictor $\mu(\cdot; \boldsymbol{X}, \boldsymbol{Y}) \colon \mathbb{R}^{M} \to \mathbb{R}^{d}$ that satisfies the following:

$$\mu(X; \boldsymbol{X}, \boldsymbol{Y}) = \frac{1}{\binom{N}{n}\binom{M}{m}} \sum_{\substack{I \subset [N], |I| = n, \\ F \subset [M], |F| = m}} H(\boldsymbol{X}_{I,F}, \boldsymbol{Y}_{I})(X_{F}), \tag{3}$$

where n and m are the number of observations and features within a minipatch, specified by practitioners. We assume the prediction is of some constant dimension d. Allowing $d \geq 1$ is to accommodate for the classification problems when the output prediction is a probability vector. This is the predictor that a random minipatch learning algorithm would converge to when the number of minipatches tends to ∞. Given a loss function or non-conformity function, $\mathrm{Error}(\cdot, \cdot)$, we can then evaluate the predictive performance of this predictor by $\mathbb{E}_{(X,Y) \sim \mathcal{P}} \mathrm{Error}(Y, \mu(X; \boldsymbol{X}, \boldsymbol{Y}) | \boldsymbol{X}, \boldsymbol{Y})$, where $\mathcal{P}$ is the distribution of test data. For any feature j of interest, we then consider the following feature importance score:

$$\Delta_{j}^{*}(\boldsymbol{X}, \boldsymbol{Y}) = \mathbb{E}_{(X,Y) \sim \mathcal{P}} \left[\mathrm{Error}(Y, \mu(X_{\backslash j}; \boldsymbol{X}_{:,\backslash j}, \boldsymbol{Y})) - \mathrm{Error}(Y, \mu(X; \boldsymbol{X}, \boldsymbol{Y})) | \boldsymbol{X}, \boldsymbol{Y} \right]. \tag{4}$$

We may also use the notation Δ_{j}^{*} to denote $\Delta_{j}^{*}(\boldsymbol{X}, \boldsymbol{Y})$ when the training data $(\boldsymbol{X}, \boldsymbol{Y})$ is clear from the context. Note that our feature importance score shares a very similar form with the inference target $\Delta_{\mathrm{LOCO},j}^{*}(\boldsymbol{X}_{D_{1},:}, \boldsymbol{Y}_{D_{1}})$ of LOCO-Split, with only two differences: (i) $\Delta_{j}^{*}(\boldsymbol{X}, \boldsymbol{Y})$ reflects the additional predictive power of feature j given the full training data set $(\boldsymbol{X}, \boldsymbol{Y})$, while $\Delta_{\mathrm{LOCO},j}^{*}(\boldsymbol{X}_{D_{1},:}, \boldsymbol{Y}_{D_{1}})$ is conditioned on one split D_{1} of the training data; (ii) the prediction algorithms (3) we consider take the average of fitted models trained using small minipatches. Although the form of the feature importance score (4) seems a little strange as it is conditioned on the training data and the predictive model, this is also the case for many other feature importance inference methods [75, 57, 86]. Furthermore, prior works [75, 57] have shown that it is impossible to develop a feature importance test that is valid under any model and also has nontrivial power without conditioning on the predictive model.

2.2 Fast Feature Importance Inference

Inspired by the LOCO-Split [36] and the Jackknife+-after-bootstrap algorithm [32], we propose the LOCO-MP algorithm (Algorithm 1) for constructing $1 - \alpha$ confidence intervals for $\Delta_{j}^{*}(\boldsymbol{X}, \boldsymbol{Y})$ defined in (4). For any base learner H, we first train prediction models for a large number of random minipatches; then we compute the leave-one-out and leave-one-covariate-out predictions for each observation $i = 1, \ldots, N$ and feature of interest j. The prediction error change due to

feature occlusion can then be computed for each sample in the training data set ($\{\Delta_j(X_i, Y_i)\}_{i=1}^N$). Since the conditional expectation of $\Delta_j(X_i, Y_i)$ given $\boldsymbol{X}_{\setminus i,:}, \boldsymbol{Y}_{\setminus i}$ is very close to $\Delta_j^*(\boldsymbol{X}, \boldsymbol{Y})$, we construct our confidence interval centered around their mean $\bar{\Delta}_j$. Although there exists weak dependency between different $\Delta_j(X_i, Y_i)$, we will still show that central limit theorem holds in the following section and the confidence interval $\hat{C}_j$ based on normal approximation has asymptotically correct coverage.

Algorithm 1: Minipatch LOCO Inference

Input: Training pairs $(\boldsymbol{X}, \boldsymbol{Y})$, feature of interest j, minipatch sizes n, m; number of minipatches K; base learner H; confidence level $1 - \alpha$;

1. Perform Minipatch Learning: For $k = 1, ..., K$

   (a) Randomly subsample n observations, $I_k \subset [N]$, and m features, $F_k \subset [M]$.

   (b) Train prediction model $\hat{\mu}_k$ on $(\boldsymbol{X}_{I_k, F_k}, \boldsymbol{Y}_{I_k})$: for any $X \in \mathbb{R}^M$,
   $\hat{\mu}_k(X) = H(\boldsymbol{X}_{I_k, F_k}, \boldsymbol{Y}_{I_k})(X_{F_k})$.

2. Obtain LOO and LOO + LOCO predictions:

   (a) Obtain the ensembled LOO prediction:
   $\hat{\mu}_{-i}(X_i) = \frac{1}{\sum_{k=1}^K \mathbb{I}(i \notin I_k)} \sum_{k=1}^K \mathbb{I}(i \notin I_k)\hat{\mu}_k(X_i)$;

   (b) Obtain the ensembled LOO + LOCO prediction:
   $\hat{\mu}_{-i}^{-j}(X_i) = \frac{1}{\sum_{k=1}^K \mathbb{I}(i \notin I_k)\mathbb{I}(j \notin F_k)} \sum_{k=1}^K \mathbb{I}(i \notin I_k)\mathbb{I}(j \notin F_k)\hat{\mu}_k(X_i)$;

3. Calculate LOO Feature Occlusion:
   $\Delta_j(X_i, Y_i) = \text{Error}(Y_i, \hat{\mu}_{-i}^{-j}(X_i)) - \text{Error}(Y_i, \hat{\mu}_{-i}(X_i))$;

4. Obtain a $1 - \alpha$ interval for Δ_j: $\hat{\mathbb{C}}_j = [\bar{\Delta}_j - \frac{z_{\alpha/2}\hat{\sigma}_j}{\sqrt{N}}, \bar{\Delta}_j + \frac{z_{\alpha/2}\hat{\sigma}_j}{\sqrt{N}}]$, with
   $\bar{\Delta}_j = \frac{1}{N}\sum_{i=1}^n \Delta_j(X_i, Y_i)$ being the sample mean and $\hat{\sigma}_j = \sqrt{\frac{\sum_{i=1}^n (\Delta_j(X_i, Y_i) - \bar{\Delta}_j)^2}{N-1}}$ being the sample standard deviation.

Output: $\hat{\mathbb{C}}_j$

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3 Coverage Guarantees for Feature Importance Confidence Intervals

In this section, we show the asymptotic normality of $\bar{\Delta}_j - \Delta_j^*$ and the consistency of the sample variance $\hat{\sigma}_j^2$ for the population variance, which together imply the asymptotic $1 - \alpha$ coverage of the confidence interval we constructed in Algorithm 1. For theoretical convenience, we first define some notations and auxiliary functions.

3.1 Notations and Definitions of Auxiliary Functions

Let
$$h_j(X, Y; \boldsymbol{X}, \boldsymbol{Y}) = \text{Error}(Y, \mu(X_{\setminus j}; \boldsymbol{X}_{:,\setminus j}, \boldsymbol{Y})) - \text{Error}(Y, \mu(X; \boldsymbol{X}, \boldsymbol{Y})) \tag{5}$$

be the feature importance of feature j evaluated at training data set $(\boldsymbol{X}, \boldsymbol{Y})$ and test data point (X, Y). Recall our definition of the inference target Δ_j^* in the main paper, one can see that

$$\Delta_j^* = \mathbb{E}_{X,Y}(h_j(X, Y; \boldsymbol{X}, \boldsymbol{Y})|\boldsymbol{X}, \boldsymbol{Y})$$

is the expectation of $h_j(X, Y; \boldsymbol{X}, \boldsymbol{Y})$ taken over the test data point.

In addition, we define
$$h_j(X, Y) = \mathbb{E}_{\boldsymbol{X}, \boldsymbol{Y}}[h_j(X, Y; \boldsymbol{X}, \boldsymbol{Y})] \tag{6}$$

as the expectation of $h_j(X, Y; \boldsymbol{X}, \boldsymbol{Y})$ over the training data set; $\hat{h}_j(X_i, Y_i; \boldsymbol{X}_{\setminus i,:}, \boldsymbol{Y}_{\setminus i}) = \Delta_j(X_i, Y_i)$, the LOO feature occlusion score calculated in Algorithm 1; $\tilde{h}_j(X_i, Y_i; \boldsymbol{X}_{\setminus i,:}, \boldsymbol{Y}_{\setminus i}) = h_j(X_i, Y_i; \boldsymbol{X}_{\setminus i,:}, \boldsymbol{Y}_{\setminus i}) - h_j(X_i, Y_i)$. For convenience, in the following proofs, we denote $\mu(X_{\setminus j}; \boldsymbol{X}_{\setminus i,\setminus j}, \boldsymbol{Y}_{\setminus i})$, $\mu(X; \boldsymbol{X}_{\setminus i,:}, \boldsymbol{Y}_{\setminus i})$, $\mu(X_{\setminus j}; \boldsymbol{X}_{:,\setminus j}, \boldsymbol{Y})$, and $\mu(X; \boldsymbol{X}, \boldsymbol{Y})$ by $\mu_{-i}^{*-j}(X)$, $\mu_{-i}^*(X)$, $\mu^{*-j}(X)$, and $\mu^*(X)$, respectively. Also, we define $\hat{\mu}_{I,F}(X) = (H(\boldsymbol{X}_{I,F}, \boldsymbol{Y}_{I_k}))(X_F) \in \mathbb{R}^d$ as the prediction of the base learner trained on $(\boldsymbol{X}_{I,F}, \boldsymbol{Y}_I)$.

Since our theory and proof involves many asymptotic statements, here we formally define different convergence modes we will use. For any random variables X and Y where X implicitly depends on the sample size N, we write $X \xrightarrow{p} Y$ if for any $\epsilon > 0$, $\lim_{N \to \infty} \mathcal{P}(|X(N) - Y| > \epsilon) = 0$; $X \xrightarrow{L_1} Y$ if $\lim_{N \to \infty} \mathbb{E}|X(N) - Y| = 0$; $X \xrightarrow{d} Y$ if for any $t \in \mathbb{R}$, $\lim_{N \to \infty} \mathcal{P}(X(N) \leq t) = \mathcal{P}(Y \leq t)$. For any two scalars $a, b \in \mathbb{R}$ that may implicitly depend on sample size N, we write $a = o(b)$, or $b \gg a$, if $\lim_{N \to \infty} \frac{a}{b} = 0$.

For any interval $[a, b] \subset \mathbb{R}$ with $a \leq b$ we use $|[a, b]| = b - a$ to denote its length. For two random variables X, Y, we write $X \stackrel{\text{d.}}{=} Y$ if the distribution of X is the same as the distribution of Y. We use $[N]$ to represent the set $\{1, \ldots, N\}$. For any n, i, we denote the ith canonical vector in $\mathbb{R}^n$ by e_i^n, and we will omit the superscript when the dimension is clear from the context.

3.2 Guarantees for Feature Importance Inference

Assumption 1 (Lipschitz condition for Error function)**.** *The error function satisfies the Lipschitz condition with parameter L:* $|\text{Error}(Y, \hat{Y}_1) - \text{Error}(Y, \hat{Y}_2)| \leq L\|\hat{Y}_1 - \hat{Y}_2\|_2$ *for any* $Y \in \mathbb{R}$ *and predictors* $\hat{Y}_1, \hat{Y}_2 \in \mathbb{R}^d$.

The Lipschitz condition is mild and can be satisfied by many different loss functions and non-conformity scores typically used in regression and classification tasks.

Assumption 2 (Minipatch stability). *For any two minipatches (I, F) and (I', F'), where $I, I' \subset [N]$, $F, F' \subset [M]$, $\|\hat{\mu}_{I,F}(X) - \hat{\mu}_{I',F'}(X)\|_2 \leq B$ for any input X.*

Assumption 2 requires the predictions given by models trained from different minipatches to have bounded difference, so that the algorithm enjoys some stability w.r.t. random sampling of minipatches. Similar assumptions are also seen in the literature on ensemble methods [19].

Assumption 3 (Minipatch size). *The minipatch sizes (m, n) satisfie $\frac{n}{N}, \frac{m}{M} \leq \beta$ for some constant $0 < \beta < 1$, and $n = o(\frac{\sigma_j}{LB}\sqrt{N})$.*

As the total sample size increases, the number of observations in each minipatch can also increase, but should be at a smaller rate than $\sqrt{N}$ so that the algorithm is stable enough for the central limit theorem to hold.

Theorem 1 (Asymptotic distribution of $\bar{\Delta}_j$). *Suppose that all training data $(X_i, Y_i) \overset{i.i.d}{\sim} \mathcal{P}$ and Assumptions 1-3 hold. If the number of random minipatches $K \gg (\frac{L^2 B^2 N}{\sigma_j^2} + \frac{LB\sqrt{N}}{\sigma_j} + 1) \log N$, and the sequence of random variables $\{[h_j(X_i, Y_i) - \mathbb{E}(h_j(X_i, Y_i))]^2 / \sigma_j^2\}_{i=1}^N$ is uniformly integrable, then we have*

$$\sqrt{N}\sigma_j^{-1}(\bar{\Delta}_j - \Delta_j^*) \overset{d}{\to} \mathcal{N}(0, 1),$$

where $\sigma_j^2 = \text{Var}_{(X,Y) \sim \mathcal{P}}(h_j(X, Y))$ with $h_j(\cdot, \cdot)$ being defined in (6).

Remark 1. *Theorem 1 and its proof is closely related to and inspired by a recent work on central limit theorem for cross validation errors [10]. The uniform integrability is a mild assumption also made in [10]. The major difference between our result and [10] is that we consider a random algorithm which leads to extra error terms that we deal with by using the stability of the minipatch algorithm. More specifically, we show that $\frac{1}{\sigma_j\sqrt{N}}\sum_{i=1}^N(\Delta_j(X_i, Y_i) - \Delta_j^*) = \frac{1}{\sigma_j\sqrt{N}}\sum_{i=1}^N[h_j(X_i, Y_i) - \mathbb{E}(h_j(X_i, Y_i)) + \varepsilon_i]$, where $\frac{1}{\sigma_j\sqrt{N}}\sum_{i=1}^N \varepsilon_i$ is a higher order error term that converges to zero in probability, thanks to the stability of the minipatch algorithm. Furthermore, due to the independence of $\{h_j(X_i, Y_i)\}_{i=1}^N$, we can apply the central limit theorem to show asymptotic normality of $\frac{1}{\sigma_j\sqrt{N}}\sum_{i=1}^N[h_j(X_i, Y_i) - \mathbb{E}(h_j(X_i, Y_i))]$.*

Theorem 2 (Consistency of variance estimate). *Consider the sample variance $\hat{\sigma}_j^2$ defined in Algorithm 1. Under the same assumptions as in Theorem 1, we have $\frac{\hat{\sigma}_j^2}{\sigma_j^2} \overset{p}{\to} 1$.*

By combining Theorems 1 and 2, we immediately have the asymptotic correct coverage of our confidence interval $\hat{C}_j$, whose width scales as $1/\sqrt{N}$:

Corollary 1 (Coverage and width of $\hat{\mathbb{C}}_j$). *Under the same assumptions as in Theorem 1, we have*

$$\lim_{N \to \infty} \mathcal{P}(\Delta_j^* \in \hat{\mathbb{C}}_j) = 1 - \alpha, \quad \sqrt{N}\sigma_j^{-1}|\hat{\mathbb{C}}_j| \overset{p}{\to} 2z_{\alpha/2}.$$

The proofs of all our theoretical results are included in Appendix A.

4 Distribution-free Predictive Inference

As can be seen from Algorithm 1, the minipatch learning framework makes the computation of leave-one-out and leave-one-covariate-out predictions nearly free given the fitted models from small minipatches. Inspired by [32] which provides fast and distribution-free predictive inference using Jackknife+ [7] with bootstrap, we propose a novel Jackknife+ Minipatch conformal inference procedure (J+MP) that can additionally take advantage of our fitted leave-one-out (LOO) predictors to construct predictive confidence intervals.

Specifically, given the LOO predictions computed in step 2 of Algorithm 1, we can further compute the non-conformity score for each data point i: $R_i^{(\mathrm{LOO})} = \mathrm{Error}(Y_i, \hat{\mu}_{-i}(X_i))$; Then for any new data point with feature X_{N+1}, we obtain its ensembled LOO prediction: $\hat{\mu}_{-i}(X_{N+1}) = \frac{1}{\sum_{k=1}^{K} \mathbb{I}(i \notin I_k)} \sum_{k=1}^{K} \mathbb{I}(i \notin I_k)\hat{\mu}_k(X_{N+1}), \quad i = 1, \ldots, N$. For a given confidence level $1 - \alpha$, following the construction in [7, 32], our Jackknife+ MP confidence set / interval for Y_{N+1} is defined as follows:

1. In the regression setting, we focus on the absolute error loss, i.e., $\mathrm{Error}(Y, \hat{Y}) = |Y - \hat{Y}|$, and our confidence interval is

$$\hat{C}_\alpha^{\mathrm{J+MP}}(X_{N+1}) = [\hat{q}_{N,\alpha}^{-}\{\hat{\mu}_{-i}(X_{N+1}) - R_i^{(LOO)}\}, \hat{q}_{N,\alpha}^{+}\{\hat{\mu}_{-i}(X_{N+1}) + R_i^{(LOO)}\}], \quad (7)$$

   where we followed the notation in [7]: for any values $\{v_i\}_{i=1}^{N}$, $\hat{q}_{N,\alpha}^{+}\{v_i\}$ is the $\lceil(1-\alpha)(N+1)\rceil$th smallest value in $\{v_i\}_{i=1}^{N}$, and $\hat{q}_{N,\alpha}^{-}\{v_i\}$ is the $\lfloor\alpha(N+1)\rfloor$th smallest value in $\{v_i\}_{i=1}^{N}$.

2. In the classification setting,

$$\hat{C}_\alpha^{\mathrm{J+MP}}(X_{N+1}) = \{Y : \sum_{i=1}^{N} \mathbb{I}(\mathrm{Error}(Y, \hat{\mu}_{-i}(X_{N+1}) \geq R_i^{(LOO)}) \leq (1 - \alpha)(N + 1)\}. \quad (8)$$

The full procedure for constructing predictive interval is summarized in Algorithm 2.

Algorithm 2: J+MP Minipatch Predictive Interval

Input: Training pairs $(\boldsymbol{X}, \boldsymbol{Y})$, test point X_{N+1}, minipatch sizes n, m; number of minipatches K, base learner H, target confidence level $1 - \alpha$;

1. Perform Minipatch Learning: For $k = 1, ..., K$:

    (a) Randomly subsample n observations, $I_k \subset [N]$, and m features, $F_k \subset [M]$.

    (b) Train prediction model $\hat{\mu}_k$ on $(\boldsymbol{X}_{I_k, F_k}, \boldsymbol{Y}_{I_k})$: for any $X \in \mathbb{R}^M$, $\hat{\mu}_k(X) = H(\boldsymbol{X}_{I_k, F_k}, \boldsymbol{Y}_{I_k})(X_{F_k})$.

2. Obtain LOO predictions :

    (a) Obtain the ensembled LOO prediction for $i = 1, ...N$:
    $\hat{\mu}_{-i}(X_i) = \frac{1}{\sum_{k=1}^K \mathbb{I}(i \notin I_k)} \sum_{k=1}^K \mathbb{I}(i \notin I_k) \hat{\mu}_k(X_i)$;
    and ensembled LOO nonconformity scores:
    $R_i^{(LOO)} = \text{Error}(Y_i, \hat{\mu}_{-i}(X_i))$;

    (b) Obtain the ensembled LOO prediction for new observation $N + 1$:
    $\hat{\mu}_{-i}(X_{N+1}) = \frac{1}{\sum_{k=1}^K \mathbb{I}(i \notin I_k)} \sum_{k=1}^K \mathbb{I}(i \notin I_k) \hat{\mu}_k(X_{N+1})$;

3. Calculate Minipatch conformal interval $\hat{C}^{\text{J+MP}}$ as in (7) for regression or (8) for classification.

Output: $\hat{C}_\alpha^{\text{J+MP}}(X_{N+1})$

Similar to [32], we guarantee the coverage of $\hat{C}^{\text{J+MP}}$ with no distributional assumptions.

Assumption 4. $(X_1, Y_1), ..., (X_{N+1}, Y_{N+1})$ *are exchangeable. Formally, for any permutation* σ *on* $\{1, \ldots, N+1\}$, $(X_1, Y_1, \ldots, X_{N+1}, Y_{N+1}) \overset{\text{d.}}{=} (X_{\sigma(1)}, Y_{\sigma(1)}, \ldots, X_{\sigma(N+1)}, Y_{\sigma(N+1)})$

Assumption 5. *The base prediction algorithm H is invariant to the order of input. For $N > 1$, and fixed N-tuple $((X_1, Y_1), ..., (X_N, Y_N))$, and any permutation σ on $\{1, ..., N\}$:*

$$H((X_1, y_1), ..., (x_N, y_N)) = H((X_{\sigma(1)}, Y_{\sigma(1)}), ..., (X_{\sigma(N)}, Y_{\sigma(N)}))$$

Assumption 6. *There exists $\tilde{K} > 0$, such that the number of minipatches in Algorithm 1 is generated from a Binomial distribution $K \sim (\tilde{K}, 1 - \frac{n}{N+1})$.*

These assumptions are standard in the literature of conformal inference [7, 32]. In particular, Assumption 6 follows the Binomial assumption from Theorem 1 in [32]: by generating the number of minipatches at random, it allows symmetrical treatment of samples in our proof.

Theorem 3 (Distribution-free Predictive Inference Guarantee)**.** *Under Assumptions 4-6, the Jackknife+ MP prediction interval satisfies*

$$\mathbb{P}\{Y_{N+1} \in \hat{C}_\alpha^{\text{J+MP}}(X_{N+1})\} \geq 1 - 2\alpha.$$

Our proof, included in Appendix A.3, closely follows the proofs in [7] and [32], while the main difference lies that we also show that features subsampling does not affect the exchangeability among samples.

5 Empirical Studies on Feature Importance Interval

We validate our proposed LOCO-MP empirically with synthetic data sets and real benchmark data sets, showing that it has both computational and statistical advantages over existing methods. In this section, we include (1) a synthetic data study to validate theoretical coverage for inference target; (2) two synthetic data study with different sample sizes and dimensionality for comparisons with competing methods; (3) a real benchmark data study for comparisons with competing methods; (4) a study on the impact of minipatch sizes.

Synthetic Data We set up a linear and a particularly challenging non-linear data generating framework for in both regression and classification scenarios to test our approach. We use a signal-to-noise ratio (SNR) to control the signal level, where features with higher SNR are more informative thus easier to identify. In all simulations, the features $\boldsymbol{X}$ of each data set are created from $N(0, I_M)$. The linear generating framework constructs the regression response by setting $\boldsymbol{Y} = \boldsymbol{X}_S^\top \boldsymbol{\beta} + \epsilon$, where S is the set of important features, $\boldsymbol{\beta} = SNR * 1_S$, and $\epsilon \sim N(0, 1)$; for binary classification response, we use the logistic link function $\mathcal{P}(Y = 1) = \frac{\exp(\boldsymbol{X}_S^\top \boldsymbol{\beta})}{1 + \exp(\boldsymbol{X}_S^\top \boldsymbol{\beta})}$. The non-linear framework uses $\boldsymbol{X}_S$ to construct a multi-layer perceptron with two hidden layers with pre-defined layer weights. We use internal ReLU (tangent) activations and identity (sigmoid) activation in the final layer to generate regression(classification) data. The weights of the first layer are set to be SNR, and the rest weights are randomly generated from $N(0, 1)$ (Uniform$[0, 1]$) in regression (classification). We set bias as one in the first layer and zero for the rest in classification, and all zero in regression.

Validating Theoretical Coverage for Inference Target We first construct an empirical study to demonstrate that the feature importance confidence intervals generated by LOCO-MP can provide valid coverage for the inference target. Since the exact value of the inference target Δ_j^* in (4) involves expectation and hence is unknown, we use Monte Carlo approximation with $10,000$ test data points from the same distribution as the training data and use the sample average on the test data set as a surrogate of the expectation in (4). In particular, this surrogate inference target for feature j is calculated as the mean difference between the prediction error of test data with feature j and without feature j. In addition, instead of using the deterministic minipatch predictor (3) for calculating the target, we approximate it by the random minipatch predictor where each minipatch are chosen uniformly at random with number of minipatches $K = 10,000$ for $N <= 40,000$ and $K = 50,000$ for larger sample sizes.

Here we focus on the linear classification and linear regression scenario, setting the number of features to be 50 and the number of important features to be 5. The sample size of training data N ranges from 100 to $5,000$, and we set minipatch size $m = 0.05M, n = 0.5\sqrt{N}$. Using ridge regression (for regression data) and logistic ridge regression (for classification data) as

the base estimator and error rate $\alpha = 0.1$, we evaluate the coverage and width of LOCO-MP confidence intervals constructed from 200 replicates. As shown in Figure 1, LOCO-MP exhibits valid coverage rate and generates efficient intervals with width decreasing as N increases.
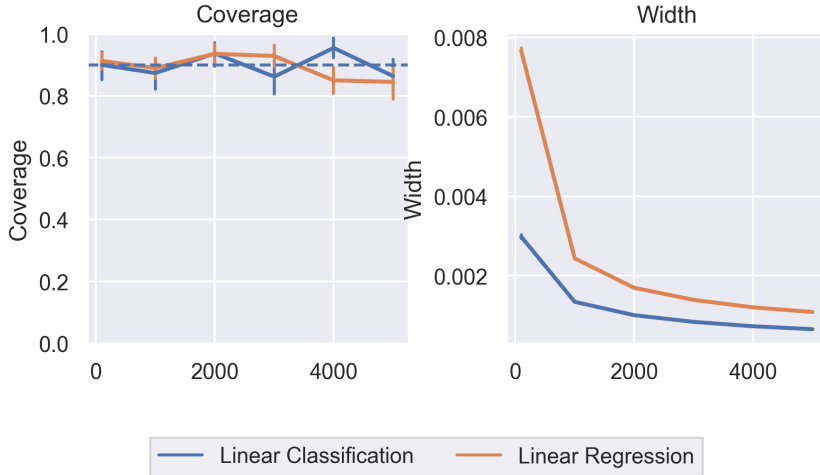

Figure 1: *Coverage for the inference target* (4) *and width of 90% confidence intervals in synthetic linear regression and classification data, using (logistic) ridge as the base estimator. LOCO-MP has valid coverage near 0.9, with small interval width that decreases as the sample size N increases.*

Comparison to Competing Methods: Type I Error, Power, and Computational Time
Now we compare LOCO-MP with some competing methods including the LOCO-Split [35] which is most closely related to our approach, and other model-agnostic feature importance inference methods: CPI [75], GCM, GCM with bootstrap (GCM_boot) [57] and floodgate [86]. For a more complete comparison, we also build a LOCO-SplitMP method, which is LOCO-Split with the minipatch ensemble methods being the prediction algorithm. Although the theoretical inference targets of these methods differ from each other, they share the same goal of identifying the true features as significant under various model settings and supervised learning tasks.

To evaluate the performance of these methods under different scenarios, we generate 500 repeats of synthetic data from linear and non-linear, regression and classification settings explained at the beginning of section 5 with SNR ranging from 0 to 15. We set $N = 200$ observations, $M = 50$ features, and the error rate $\alpha = 0.1$. For the prediction algorithms, We consider ridge (logistic) regression, random forest, and a multilayer perceptron (MLP) with two hidden layers. Since random forest is a tree ensemble method, we compare LOCO-MP using decision tree to other non-ensemble methods using random forest with 200 trees. The MLP prediction algorithms use ReLU activation in the hidden layers and identity activation in the final layer for regression prediction; and tangent activation in the hidden layers and sigmoid activation in the final layer for classification prediction. In terms of hyper-parameter selection, the ridge penalty parameter λ

	Linear regression data				Linear classification data			
	Ridge		Random Forest		Logistic Ridge		Random forest	
	LOCO-MP	LOCO-Split	LOCO-MP	LOCO-Split	LOCO-MP	LOCO-Split	LOCO-MP	LOCO-Split
N=200, M = 50	3.20	**1.77**	**3.22**	20.52	**5.04**	5.73	**4.80**	7.52
N = 500, M = 200	**29.14**	38.02	**30.60**	698.54	**34.11**	194.93	**32.37**	80.57
N = 1000, M = 400	**115.60**	218.29	**120.29**	6574.44	**123.88**	1397.53	**127.09**	470.59
N = 2000, M = 800	**451.38**	1562.62	**478.96**	*gt* 5hr	**513.89**	11259.15	**489.96**	8408.11

Table 1: *Computation time in seconds on linear synthetic data sets with various sample sizes and dimensionality. LOCO-MP shows major computational advantages over LOCO-Split in large data sets by avoiding re-fitting.*

is tuned via bootstrap validations for all inference methods except LOCO-MP, in which λ is a small fixed value (0.0001). We set $K = 1000$, minipatch sizes $n = 0.1N$, $m = 0.1M$ ($m = 0.5M$ for non-linear classification with MLP due to its complicated structure).

We construct confidence intervals of the first signal feature over 500 replicates and measure the power of inference by the proportions of confidence intervals with lower bounds greater than zero. As illustrated in Figure 2, LOCO-MP consistently offers higher power than competing methods. Besides, to show that LOCO-MP at the same time offers dramatically computational savings, we compare the running time of LOCO-MP and LOCO-Split in various settings of sample size in Table 1. In addition, we show the time comparison of the synthetic study, measuring feature importance intervals of all features in Table 2. All of the computation time is recorded on a server with a 32-Core Processor and 252GB of RAM.
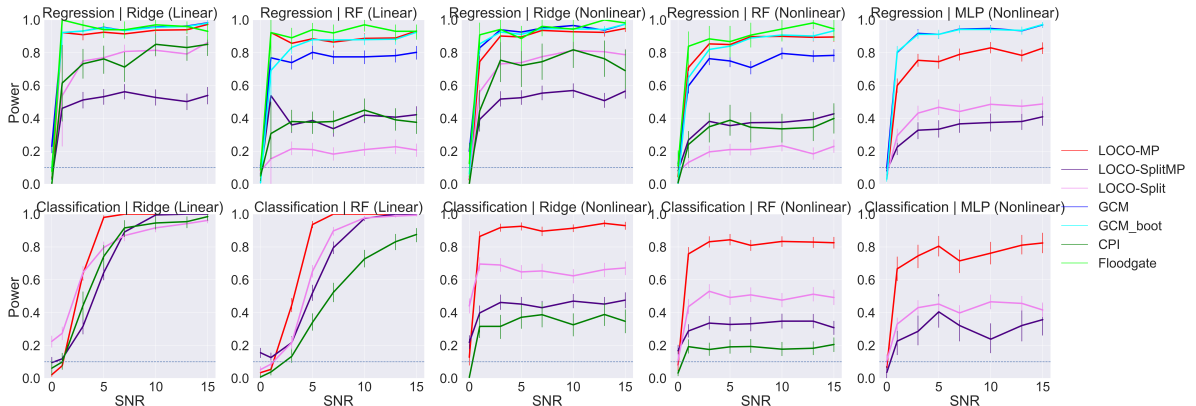

Figure 2: *Inference power on synthetic regression and classification data. LOCO-MP successfully controls type I error in all scenarios (with power < 0.1 when SNR = 0), and is either the best or among the top performers in terms of statistical power across all scenarios.*

Comparison to Competing Methods with larger synthetic data sets   To evaluate the performance of LOCO-MP in data sets with larger sample size and dimensionality, we construct

Regression					
	Ridge (Linear)	RF (Linear)	Ridge (Nonlinear)	RF (Nonlinear)	MLP (Nonlinear)
LOCO-MP	3.20	3.22	3.33	3.38	272.36
LOCO-Split	1.77	20.52	1.67	20.06	26.86
LOCO-SplitMP	21.49	18.20	21.39	18.35	12689.53
GCM	3.60	41.78	3.24	41.16	52.97
GCM_boot	17.95	208.64	16.24	204.14	264.06
CPI	3.09	2.65	3.66	3.02	
Floodgate	9.81	14.53	11.33	15.17	
Classification					
LOCO-MP	5.04	4.80	4.60	4.45	281.8
LOCO-Split	5.73	7.52	5.75	19.75	16.9
LOCO-SplitMP	105.40	87.80	76.90	61.05	13690.6
CPI	3.53	3.20	3.85	3.52	

Table 2: *Computation time in seconds on linear and nonlinear, classification and regression synthetic data sets with $N = 200$, $M = 50$.*

200 replicates of synthetic data with $N = 1000$, $M = 200$ from linear and non-linear, regression and classification settings, with all other settings being the same as before. As shown in Figure 3, LOCO-MP is still among the best methods with the highest power in all scenarios. Besides, we perform computational time comparisons for LOCO methods in these larger data sets. Table 3 demonstrates that LOCO-MP can dramatically improve computational efficiency in large data sets, and is faster than LOCO-Split in most of the cases.
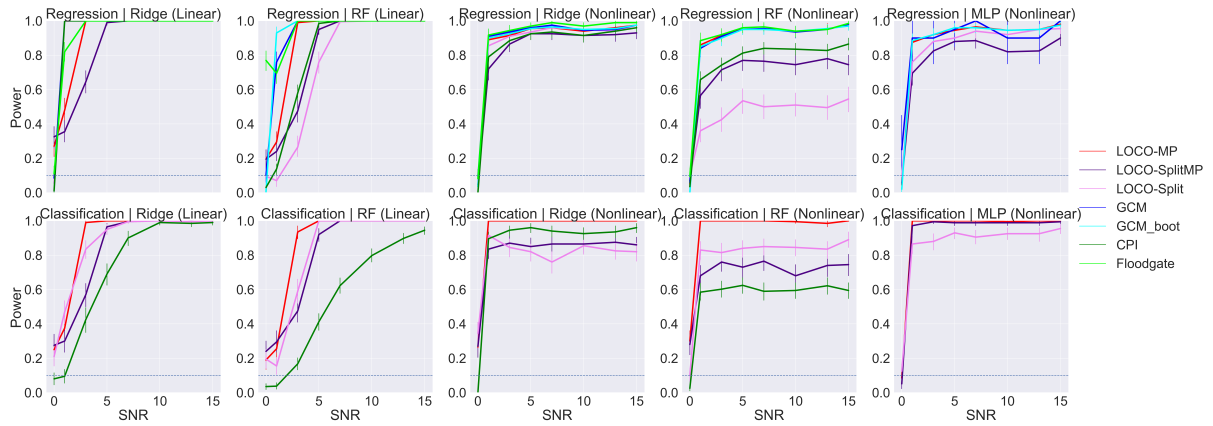

Figure 3: *Inference power on synthetic regression and classification data with larger sample size and dimensionality. LOCO-MP still is either the best or among the top performers in terms of statistical power across all scenarios.*

Regression					
	Ridge (Linear)	RF (Linear)	Ridge (Nonlinear)	RF (Nonlinear)	MLP (Nonlinear)
LOCO-MP	**56.01**	**57.27**	59.04	**58.39**	**487.54**
LOCO-Split	63.45	1657.62	**39.38**	3322.83	521.81
LOCO-SplitMP	152.32	130.16	147.93	132.38	> 10 hr
Classification					
LOCO-MP	**63.29**	**61.65**	**64.10**	**63.96**	**381.18**
LOCO-Split	365.09	467.19	438.61	320.04	6298.95
LOCO-SplitMP	885.80	384.56	719.18	274.16	>10 hr

Table 3: *Computation time in seconds on linear and nonlinear, classification and regression synthetic data sets with $N = 1000$, $M = 200$. LOCO-MP offers dramatic computational time savings over competing methods, including LOCO-Split.*

Case Study on Real Benchmark Data We apply our method to obtain feature importance intervals in benchmark datasets including the Boston house price [28] regression data set of 506 samples and 13 features, and the Africa heart disease data [29, 54] classification data set of 462 samples and 9 features. Note that LOCO-MP is extremely flexible to any data size. We select these benchmark data sets because they are well studied in previous works and contain a small number of features that enables visualization of confidence intervals. We compare the feature importance interval for all features, using decision tree with 1000 minipatches in LOCO-MP and random forest with 200 trees in competing methods. The error rate is set to be $\alpha = 0.1$ with Bonferroni correction for multiplicity.

Figure 4 provides a visualization of the confidence intervals of each feature in the Africa heart disease data and the Boston house price data, where a confidence interval with a lower bound greater than zero suggests a significant feature. Table 4 illustrates the multiplicity adjusted p-values of each feature, averaged over 20 runs of each method. **Reliable and accurate feature inference**: (i) In the Boston house price data set, LOCO-MP discovers the average number of rooms per dwelling (RM) and the % lower status of the population (LSTAT) are classified as important features, which is consistent with previous studies on this data set [22, 20, 75]. LOCO-SplitMP agrees with the findings of LOCO-MP, while all other methods either do not identify both important features or have lots of false positives. (ii) In the Africa heart disease classification data set, LOCO-MP and LOCO-SplitMP identify two significant features: tobacco consumption and age, also matching the feature importance conclusions in the literature [77, 4]. CPI and LOCO-Split failed to identify any significant features. In addition, LOCO-MP has consistently higher interval efficiency with the smallest interval widths in both of the data sets. Besides, another major advantage of LOCO-MP is able to simultaneously construct valid distribution-free predictive intervals, with no extra computational cost.
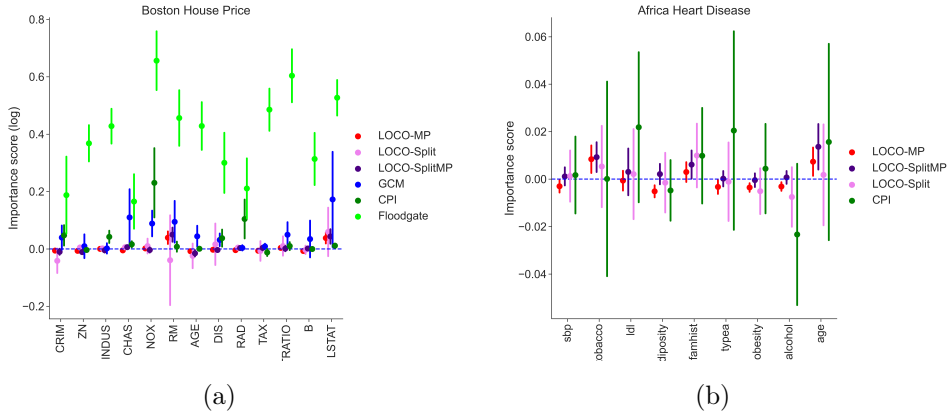
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Figure 4: *Feature inference (multiplicity adjusted) on the Boston House Price regression data and Africa Heart Disease classification data. Features whose lower bounds of confidence interval greater than zero are statistically significant. The confidence intervals with an upper bound smaller than zero indicate that such a feature would hamper prediction. LOCO-MP identifies important features that are consistent with previous studies on each data set, and is among the best in terms of interval efficiency with the smallest widths.*

Boston House Price												
Feature	AGE	B	CHAS	CRIM	DIS	INDUS	**LSTAT**	NOX	PTRATIO	RAD	**RM**	TAX	ZN
LOCO-MP	1.000	1.000	1.000	1.000	1.000	0.982	**0.000**	0.960	0.868	1.000	**0.000**	1.000	1.000
LOCO-Split	0.939	0.976	0.939	0.964	0.794	0.990	0.764	0.881	0.893	0.947	0.378	0.872	0.924
LOCO-SplitMP	0.984	1.000	0.902	0.995	0.958	0.961	**0.001**	0.950	0.852	0.977	**0.010**	0.960	1.000
CPI	0.380	0.410	**0.070**	**0.071**	**0.070**	**0.013**	**0.092**	**0.024**	**0.054**	**0.005**	0.157	0.363	0.369
Floodgate	**0.004**	**0.095**	0.147	**0.015**	**0.000**	**0.000**	**0.000**	**0.000**	**0.000**	**0.097**	**0.000**	**0.000**	**0.001**
GCM	0.165	0.365	0.532	0.280	0.332	0.462	0.161	0.329	0.391	0.441	**0.083**	0.234	0.393
Africa Heart Disease												
Feature	adiposity	age	alcohol	famhist	ldl	obesity	sbp	tobacco	typea			
LOCO-MP	1.000	**0.002**	1.000	0.506	1.000	1.000	1.000	**0.082**	1.000			
LOCO-Split	0.948	0.855	1.000	0.544	0.952	0.979	0.980	0.906	0.929			
LOCO-SplitMP	0.451	**0.015**	0.789	0.192	0.438	0.886	0.776	**0.045**	0.669			
CPI	0.492	0.425	0.693	0.300	0.388	0.462	0.479	0.375	0.314			

Table 4: *Multiplicity adjusted p-values for feature inference in the Boston house price data and Africa heart disease data, averaged over 20 runs (data splits). p-values below $\alpha = 0.1$ are statistically significant and in bold.*

Minipacth Size We aim to evaluate the impact of minipatch sizes on the performance of LOCO-MP in terms of inference power and interval width, as well as the performance of predictive interval J+MP in terms of predictive coverage and interval width. Here we construct 100 replicates synthetic linear regression data with $SNR = 10$, $N = 200$, and $M = 50$. We also generate 100 test data points under the same distribution of the training data to evaluate the performance of J+MP. With $\alpha = 0.1$ and $K = 1000$, we use ridge regression with small penalty (0.0001) and decision tree as base estimator. As shown in Figure 5, LOCO-MP obtains power equaling to 1 in all minipatch sizes combinations, and it provides smaller interval width with smaller minipatch

sizes. In addition, the J+MP predictive interval also offers valid coverage with all minipatch size combinations. However, the predictive interval width would decrease with a larger minipatch. We also recommend a data-driven tuning method for minipatch size selection, which chooses a minipatch size (m, n) that leads to the lowest mean squared error in regression or highest accuracy in classification via bootstrap validation.
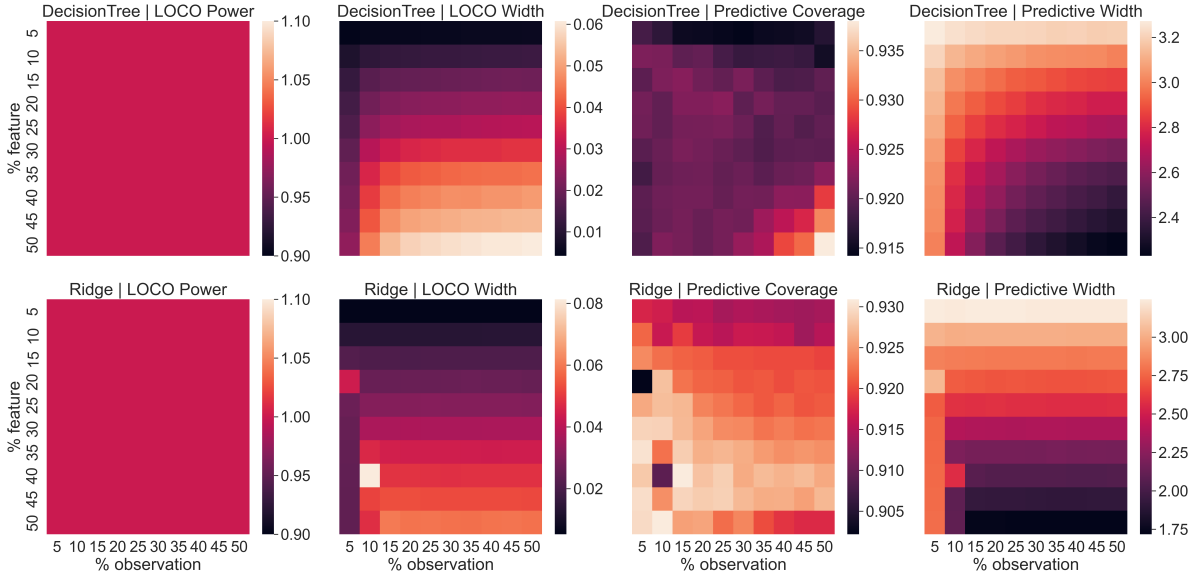

Figure 5: *Inference power and feature importance interval width of LOCO-MP and predictive coverage and predictive interval width of J+MP in synthetic linear regression data, using various combinations of minipacth sizes.*

6 Empirical Studies on Predictive Interval

We evaluate the performance of J+MP predictive inference approach on some larger regression and classification data sets, shown in Table 6. We include two regression tasks: a high dimensional RNA-seq data set from the Religious Orders Study and Memory and Aging Project (ROSMAP) Study [12], and the communities and crime data set [3], as well as one high dimensional classification PANCAN cancer RNA-seq data set [76]. We transform every feature to have mean 0 and variance 1, and the response of the regression problems is also standardized. The results of J+MP predictive intervals are compared to existing conformal inference methods, including split conformal [35], cross conformal [69], Jackknife+ [7] and J+aB [32]. For the base prediction algorithms, we select a linear model (logistic regression for classification) with ridge penalty and a non-linear decision tree as base prediction models. In terms of parameter tuning, J+MP sets the penalty hyperparameter of (logistic) ridge model as 0.0001 and selects the minipatch sizes (m, n) which leads to the lowest mean squared error in regression or highest accuracy in classification via bootstrap validation.

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For other conformal methods, the penalty hyperparameter is selected via bootstrap validation. The number of folds in cross conformal is set to be 5. In addition, we evaluate the J+aB and J+MP methods using a random K drew from $K \sim Binomial(\tilde{K}, 1 - \frac{n}{N+1})$, where $\tilde{K} = 100$. And in J+aB, we apply sampling without replacement in the bootstrap step, and the optimal sampling size is selected via bootstrap validation.

Data	# observations	# features	# classes	Type	Citation
PANCAN	761	13,244	5	Classification	[76]
Communities and Crime	1993	99		Regression	[3]
RNA-seq	507	900		Regression	[12]

Table 5: *Data Sets Used in Empirical Study*

Table 6 validates the performance of conformal intervals in terms of coverage (our target is $1 - \alpha$), interval width (smaller is better), and computational time, under 100 train/test splits on each benchmark data sets with the error rate $\alpha = 0.1$. Empirically, the various forms of J+MP and J+aB do not differ much from each other, respectively. Moreover, the results show that our J+MP and J+aB achieve valid and the most consistent coverage, and the other methods fail to provide 0.9 coverage for the high-dimensional PANCAN classification data set with decision tree model. Secondly, comparing to methods with valid coverage, J+MP and J+aB have similar performance and always outperform with the smallest interval widths. However, there is a trade-off between interval efficiency and computational efficiency. It makes sense that the Jackknife+-based methods are slower than split conformal and cross conformal, but both J+MP and J+aB are significantly faster than Jackknife+. In addition, J+MP further outruns J+aB with dramatically great computational savings, when dealing with large high dimensional data set or with the implementation of nonlinear prediction methods. For example, in the case of PANCAN classification data set, J+MP even outperforms the Conformal Split method with three times less computational costs, and is dramatically faster than Jackknife+, depending on the size of data sets and the based prediction model.

7   Discussion

Impact   This is the first paper to provide a fast, widely applicable, and theoretically valid approach for conducting inference to find statistically significant features in any supervised machine learning model. Due to the wide application of various machine learning methods in every aspect of human society, some being high-stake applications like healthcare, policy making, and scientific discoveries, there have been serious and increasing concerns regarding the reliability and interpretability of these machine learning algorithms. Our proposed method can help to

Base model	Conformal	Coverage			Width			Time (s)		
		RNA-seq	Communities	PANCAN	RNA-seq	Communities	PANCAN	RNA-seq	Communities	PANCAN
(Logistic) Ridge	J+MP	0.925	0.860	0.899	**2.390**	2.189	**0.900**	0.315	0.1097	1159.858
	J+aB	0.935	0.870	0.906	2.447	2.017	0.906	0.269	0.07	30647.633
	J+	0.907	0.890	0.906	2.527	**1.908**	0.906	3.818	0.349	30647.633
	Split	0.916	0.890	0.809	2.779	2.069	0.809	0.00861	0.00531	52.25
	Cross	0.916	0.890	0.900	2.598	1.919	**0.900**	0.0872	0.0115	401.13
Random Forest	J+MP	0.925	0.910	0.891	**2.262**	**1.976**	**0.891**	2.659	0.118	590.289
	J+aB	0.934	0.900	0.906	2.326	2.167	0.906	4.844	0.564	30647.633
	J+	0.972	0.890	0.483	3.267	2.792	0.484	90.517	3.748	28302.148
	Split	0.925	0.930	0.793	3.351	3.774	0.835	0.144	0.0118	37.318
	Cross	0.981	0.910	0.801	3.103	2.785	0.804	1.460	0.096	322.227

Table 6: *Comparative results for predictive intervals constructed via our Minipatch Jacknife+ (J+MP) method in terms of coverage, interval width, and computational time on two regression (RNA-seq, Communities) and one classification (PANCAN) data sets.*

address this problem and make better use of machine learning in a safer and more understandable manner.

Limitations & Future Work 1) Our theoretical results guarantee asymptotic coverage, while it could be of interest in future work to relax the large N assumptions. 2) The inference target of our confidence interval is conditioning on the training set and the specific machine learning algorithm. It is of future interest to investigate the effect of model mis-specification and different training sets theoretically. Our simulation studies suggest, however, that our approach still retains proper coverage / Type I error for possibly mis-speified models and has good power with sufficiently large SNRs. 3) Our empirical studies only focused on tabular data since the minipatch subsampling strategy is not directly applicable to sequential data, image data or other structured data. Extending our approach and theory for these types of data could be of future interest. 4) In this paper, we performed all timing comparisons using sequential computing, but our approach is primed for further computational improvement by using distributed systems for efficient memory and parallel computing. 5) Our method is not applicable to high-dimensional settings where $M > N$, since the additional predictive power of any feature can be vanishing and feature occlusion is fundamentally ill-posed. There does not seem to be a direct extension of our specific approach to the high-dimensional setting, but some other approaches that leverage minipatch subsampling may be worth investigating in future work.

Acknowledgments

Shell Graduate Fellowship.

A   Proofs

In this section, we present the proofs of all our theoretical statements on the valid coverage of our feature importance confidence intervals and distribution-free predictive intervals.

A.1   Proof of Theorem 1

Our proof utilizes some key results in [10], while due to the randomness of our minipatch algorithm, we devote our main analysis to the concentration of the random algorithm on its population version (Proof of Lemma 4). First note that for any $1 \le i \le N$, we have the following decomposition:

$$
\begin{aligned}
&\Delta_j(X_i, Y_i) - \Delta_j^* \\
=&h_j(X_i, Y_i) - \mathbb{E}(h_j(X_i, Y_i)) + \hat{h}_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}) - h_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}) \\
&+ \mathbb{E}[h_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}) | \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}] - \Delta_j^* \\
&+ \tilde{h}_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}) - \mathbb{E}[\tilde{h}_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}) | \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}] \\
=:&h_j(X_i, Y_i) - \mathbb{E}(h_j(X_i, Y_i)) + \varepsilon_{i,j}^{(1)} + \varepsilon_{i,j}^{(2)} + \varepsilon_{i,j}^{(3)},
\end{aligned}
$$

where we have let

$$
\begin{aligned}
\varepsilon_{i,j}^{(1)} =&\hat{h}_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}) - h_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}), \\
\varepsilon_{i,j}^{(2)} =&\mathbb{E}[h_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}) | \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}] - \Delta_j^*, \\
\varepsilon_{i,j}^{(3)} =&\tilde{h}_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}) - \mathbb{E}[\tilde{h}_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}) | \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}].
\end{aligned}
$$

Further define $\varepsilon_j^{(k)} = \frac{1}{\sigma_j \sqrt{N}} \sum_{i=1}^N \varepsilon_{i,j}^{(k)}$. Our goal is to show that

$$
\frac{1}{\sigma_j \sqrt{N}} \sum_{i=1}^N (\Delta_j(X_i, Y_i) - \Delta_j^*) = \frac{1}{\sigma_j \sqrt{N}} \sum_{i=1}^N [h_j(X_i, Y_i) - \mathbb{E}(h_j(X_i, Y_i))] + \sum_{k=1}^3 \varepsilon_j^{(k)}
$$

converges to standard Gaussian distribution. For the error terms $\varepsilon_j^{(k)}$, $k = 1, 2, 3$, the following lemma suggests that they all converge to zero in probability.

Lemma 4. *Under the same conditions as in Theorem 1, $\varepsilon_j^{(k)} \xrightarrow{p} 0$, $k = 1, 2, 3$.*

While for $\frac{1}{\sigma_j \sqrt{N}} \sum_{i=1}^N [h_j(X_i, Y_i) - \mathbb{E}(h_j(X_i, Y_i))]$, applying Lindeberg's central limit theorem and following the same argument as in the proof of Theorem 1 in [10], we have $\frac{1}{\sigma_j \sqrt{N}} \sum_{i=1}^N [h_j(X_i, Y_i) - \mathbb{E}(h_j(X_i, Y_i))] \xrightarrow{d} \mathcal{N}(0, 1)$. Finally, applying Slutsky's theorem finishes the proof of Theorem 1.

A.2 Proof of Theorem 2 and Corollary 1

Proof of Theorem 2. We would like to apply the variance consistency result (Theorem 5 in [10]) in our setting, with the $h_n(Z_i, Z_{B_j})$ under their notation being substituted by $h_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i})$, which is denoted by $\tilde{\Delta}_j(X_i, Y_i)$ in this proof. Let $\bar{\tilde{\Delta}}_j = \frac{1}{N}\sum_{i=1}^{N} \tilde{\Delta}_j(X_i, Y_i)$, and

$$\tilde{\sigma}_j^2 = \text{Var}_{X,Y}(\bar{h}_j(X,Y)),$$

$$\hat{\tilde{\sigma}}_j^2 = \frac{1}{N}\sum_{i=1}^{N}\left(\tilde{\Delta}_j(X_i, Y_i) - \bar{\tilde{\Delta}}_j(X_i, Y_i)\right)^2,$$

where $\mathbb{E}[h_j(X, Y; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i})|X, Y]$ is defined in (10). Then Theorem 5 in [10] suggests that, if $\gamma_{loss}(h_j) = o(\tilde{\sigma}_j^2/N)$ and $\gamma_{ms}(h_j) = o(\tilde{\sigma}_j^2)$ hold, we have $\frac{\hat{\tilde{\sigma}}_j^2}{\tilde{\sigma}_j^2} \xrightarrow{p} 1$. In the following, we will show (i) $\frac{\sigma_j^2}{\tilde{\sigma}_j^2} \xrightarrow{p} 1$; (ii) the stability quantities associated with h_j satisfy $\gamma_{loss}(h_j) = o(\sigma_j^2/N)$, $\gamma_{ms}(h_j) = o(\sigma_j^2)$; (iii) $\frac{\hat{\sigma}_j^2}{\hat{\tilde{\sigma}}_j^2} \xrightarrow{p} 1$. Combining these three results and $\frac{\hat{\tilde{\sigma}}_j^2}{\tilde{\sigma}_j^2} \xrightarrow{p} 1$, we will then have $\frac{\hat{\sigma}_j^2}{\sigma_j^2} \xrightarrow{p} 1$, and our proof will be complete.

(i) To show the closeness between the variances of $\bar{h}_j(X,Y)$ and $h_j(X,Y)$, first we can write out

$$\left|\frac{\tilde{\sigma}_j^2}{\sigma_j^2} - 1\right| = \sigma_j^{-2}\mathbb{E}([\bar{h}_j(X,Y) - \mathbb{E}(\bar{h}_j(X,Y))]^2 - [h_j(X,Y) - \mathbb{E}(h_j(X,Y))]^2).$$

Since for any random variables ξ_1, ξ_2, $|\mathbb{E}(\xi_1^2 - \xi_2^2)| = |\mathbb{E}(\xi_1 - \xi_2)^2 + 2\xi_2(\xi_1 - \xi_2)| \leq \mathbb{E}(\xi_1 - \xi_2)^2 + 2\sqrt{\mathbb{E}(\xi_2^2)}\sqrt{\mathbb{E}(\xi_1 - \xi_2)^2}$, we can further bound $\left|\frac{\tilde{\sigma}_j^2}{\sigma_j^2} - 1\right|$ by

$$\left|\frac{\tilde{\sigma}_j^2}{\sigma_j^2} - 1\right| \leq \sigma_j^{-2}\mathbb{E}[\bar{h}_j(X,Y) - h_j(X,Y) - \mathbb{E}(\bar{h}_j(X,Y) - h_j(X,Y))]^2$$

$$+ 2\sigma_j^{-1}\left(\mathbb{E}[\bar{h}_j(X,Y) - h_j(X,Y) - \mathbb{E}(\bar{h}_j(X,Y) - h_j(X,Y))]^2\right)^{1/2}$$

$$\leq \sigma_j^{-2}\mathbb{E}[\bar{h}_j(X,Y) - h_j(X,Y)]^2 + 2\sigma_j^{-1}\left(\mathbb{E}[\bar{h}_j(X,Y) - h_j(X,Y)]^2\right)^{1/2},$$

where we have applied the fact that for any random variable ξ, $\text{Var}(\xi) \leq \mathbb{E}(\xi^2)$. As has been shown in the last part of the proof of Lemma 4, for any (X, Y), $|\bar{h}_j(X,Y) - h_j(X,Y)| \leq \frac{2LBn}{N}$. Hence $\left|\frac{\tilde{\sigma}_j^2}{\sigma_j^2} - 1\right| \leq \frac{4L^2B^2n^2}{\sigma_j^2 N^2} + \frac{4LBn}{\sigma_j N} = o(1)$ by Assumption 3. Therefore, $\frac{\tilde{\sigma}_j^2}{\sigma_j^2} \xrightarrow{a.s.} 1$, implying $\frac{\sigma_j^2}{\tilde{\sigma}_j^2} \xrightarrow{p} 1$.

(ii) As shown when bounding $\varepsilon_j^{(3)}$ in the proof of Lemma 4, $\gamma_{loss}(h_j) \leq \frac{16L^2B^2n^2}{(N-1)^2} = o(\frac{\sigma_j^2}{N})$. Similar to that proof, here we let (X_{N+1}, Y_{N+1}) be a sample from $\mathcal{P}$ which is independent

from $(\boldsymbol{X}, \boldsymbol{Y})$, and denote by $(\boldsymbol{X}_{\backslash i,:}^{\backslash l}, \boldsymbol{Y}_{\backslash i}^{\backslash l})$ the $N-1$ training set with sample i excluded, and sample l replaced by (X_{N+1}, Y_{N+1}). By the definition of the mean-squared stability in [10],

$$\gamma_{ms}(h_j) = \frac{1}{N-1} \sum_{l \neq i} \mathbb{E}[(h_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,}, \boldsymbol{Y}_{\backslash i}) - h_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,}^{\backslash l}, \boldsymbol{Y}_{\backslash i}^{\backslash l})^2].$$

Then following similar arguments as in the proof of Lemma 4, we have $\gamma_{ms}(h_j) \leq \frac{4L^2 B^2 n^2}{(N-1)^2} = o(\frac{\sigma_j^2}{N})$. Thus Applying Theorem 5 in [10] leads to $\frac{\hat{\tilde{\sigma}}_j^2}{\tilde{\sigma}_j^2} \xrightarrow{p} 1$.

(iii) Now we show the closeness between our own variance estimate $\hat{\sigma}_j^2 = \frac{1}{N}\sum_{i=1}^{N}(\Delta_j(X_i, Y_i) - \bar{\Delta}_j)^2$ and $\hat{\tilde{\sigma}}_j^2 = \frac{1}{N}\sum_{i=1}^{N}(\tilde{\Delta}_j(X_i, Y_i) - \bar{\tilde{\Delta}}_j)^2$. Similar to the proof in (i), we can first write

$$|\hat{\sigma}_j^2 - \hat{\tilde{\sigma}}_j^2|$$
$$\leq \frac{1}{N}\sum_{i=1}^{N}(\Delta_j(X_i, Y_i) - \tilde{\Delta}_j(X_i, Y_i))^2 + 2\hat{\tilde{\sigma}}_j\sqrt{\frac{1}{N}\sum_{i=1}^{N}(\Delta_j(X_i, Y_i) - \tilde{\Delta}_j(X_i, Y_i))^2}.$$

Recall that we have already shown the closeness between $\Delta_j(X_i, Y_i) = \hat{h}_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i})$ and $\tilde{\Delta}_j(X_i, Y_i) = h_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i})$ when bounding $\varepsilon_j^{(1)}$ in the proof of Lemma 4, we would like to reuse some of the notations and intermediate results in that proof. Let $\alpha_i^{(1)} = \|\hat{\mu}_{-i}^{-j}(X_i) - \tilde{\mu}_{-i}^{-j}(X_i)\|_2$, $\alpha_i^{(2)} = \|\hat{\mu}_{-i}(X_i) - \tilde{\mu}_{-i}(X_i)\|_2$, $\alpha_i^{(3)} = \|\tilde{\mu}_{-i}^{-j}(X_i) - \mu_{-i}^{*-j}(X_i)\|_2$, and $\alpha_i^{(4)} = \|\tilde{\mu}_{-i}(X_i) - \mu_{-i}^{*}(X_i)\|_2$, where $\tilde{\mu}_{-i}^{-j}(X_i)$ and $\tilde{\mu}_{-i}(X_i)$ are defined in (9). Then by Assumption 1, we have $|\Delta_j(X_i, Y_i) - \tilde{\Delta}_j(X_i, Y_i)| \leq L\sum_{l=1}^{4}\alpha_i^{(l)}$, and hence

$$|\hat{\sigma}_j^2 - \hat{\tilde{\sigma}}_j^2|$$
$$\leq \frac{L^2}{N}\sum_{i=1}^{N}\left(\sum_{l=1}^{4}\alpha_i^{(l)}\right)^2 + \frac{2L\hat{\tilde{\sigma}}_j}{\sqrt{N}}\sqrt{\sum_{i=1}^{N}\left(\sum_{l=1}^{4}\alpha_i^{(l)}\right)^2}$$
$$\leq \frac{L^2}{N}\left(\sum_{l=1}^{4}\sum_{i=1}^{N}\alpha_i^{(l)}\right)^2 + \frac{2L\hat{\tilde{\sigma}}_j}{\sqrt{N}}\sum_{i=1}^{N}\sum_{l=1}^{4}\alpha_i^{(l)}$$
$$\leq \sigma_j^2\left(\sum_{l=1}^{4}\frac{L}{\sigma_j\sqrt{N}}\sum_{i=1}^{N}\alpha_i^{(l)}\right)^2 + 2\hat{\tilde{\sigma}}_j\sigma_j\left(\sum_{l=1}^{4}\frac{L}{\sigma_j\sqrt{N}}\sum_{i=1}^{N}\alpha_i^{(l)}\right).$$

Recall that we have shown in the proof of Lemma 4 that $|\varepsilon_j^{(1)}| \leq \sum_{l=1}^{4}\frac{L}{\sigma_j\sqrt{N}}\sum_{i=1}^{N}\alpha_i^{(l)} \xrightarrow{p} 0$, and we have just shown in (ii) that $\frac{\hat{\tilde{\sigma}}_j^2}{\sigma_j^2} \xrightarrow{p} 0$. Hence, $\frac{|\hat{\sigma}_j^2 - \hat{\tilde{\sigma}}_j^2|}{\hat{\tilde{\sigma}}_j^2} \xrightarrow{p} 0$, or equivalently, $\frac{\hat{\sigma}_j^2}{\hat{\tilde{\sigma}}_j^2} \xrightarrow{p} 1$, which completes our proof.

$\square$

Proof of Corollary 1. We combine Theorem 1 and Theorem 2, and apply Slutsky's theorem to obtain

$$\sqrt{N}\hat{\sigma}_j^{-1}(\bar{\Delta}_j - \Delta_j^{*}) \xrightarrow{d} \mathcal{N}(0, 1).$$

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Then the coverage probability satisfies

$$\lim_{N \to \infty} \mathcal{P}(\Delta_j^* \in \hat{\mathbb{C}}_j) = \lim_{N \to \infty} \mathcal{P}(\sqrt{N}\hat{\sigma}_j^{-1}|\bar{\Delta}_j - \Delta_j^*| \leq z_{\alpha/2}) = 1 - \alpha.$$

In addition, since $\sqrt{N}\sigma_j^{-1}|\hat{\mathbb{C}}_j| = 2z_{\alpha/2}\frac{\hat{\sigma}_j}{\sigma_j}$ and Theorem 2 suggests that $\frac{\hat{\sigma}_j^2}{\sigma_j^2} \xrightarrow{p} 1$, we have $\sqrt{N}\sigma_j^{-1}|\hat{\mathbb{C}}_j| \xrightarrow{p} 2z_{\alpha/2}$. $\qquad\square$

A.3 Proof of Theorem 3

Our proof closely follows the proofs in [7] and [32], while the main difference lies that our algorithm also subsample features randomly. For completeness, we will write out the full proof, including the steps that are very similar to [7] and [32].

First we suppose that we have access to a new data point (X_{N+1}, Y_{N+1}), and we consider the following "lifted" algorithm that is similar to the one defined in [32] and is symmetric w.r.t. all $N + 1$ data points $(X_1, Y_1), \ldots, (X_{N+1}, Y_{N+1})$. The extended training data is denoted by $(\boldsymbol{X}^*, \boldsymbol{Y}^*)$ with $\boldsymbol{X}^* \in \mathbb{R}^{(N+1) \times M}$ and $\boldsymbol{Y}^* \in \mathbb{R}^{N+1}$.

Algorithm 3: Lifted J+MP Minipatch Predictive Interval

Input: Training data $\{(X_i, Y_i)\}_{i=1}^{N+1}$, minipatch sizes n, m; number of minipatches $\tilde{K}$, base learner H;

1. Perform Minipatch Learning: For $k = 1, ..., \tilde{K}$:

    (a) Randomly subsample n observations, $I_k \subset [N + 1]$, and m features, $F_k \subset [M]$.

    (b) Train prediction model $\hat{\mu}_k$ on $(\boldsymbol{X}_{I_k, F_k}^*, \boldsymbol{Y}_{I_k}^*)$: $\hat{\mu}_k = H(\boldsymbol{X}_{I_k, F_k}^*, \boldsymbol{Y}_{I_k}^*)$.

2. Obtain leave-two-out predictions : For $i_1 \neq i_2 \in [N + 1]$:

    (a) Obtain the ensembled leave-two-out prediction for i_1, i_2:
    $\hat{\mu}_{-i_1,-i_2}(X_{i_1}) = \frac{1}{\sum_{k=1}^K \mathbb{I}(i_1 \notin I_k)\mathbb{I}(i_2 \notin I_k)} \sum_{k=1}^K \mathbb{I}(i_1 \notin I_k)\mathbb{I}(i_2 \notin I_k)\hat{\mu}_k(X_{i_1})$;
    $\hat{\mu}_{-i_1,-i_2}(X_{i_2}) = \frac{1}{\sum_{k=1}^K \mathbb{I}(i_1 \notin I_k)\mathbb{I}(i_2 \notin I_k)} \sum_{k=1}^K \mathbb{I}(i_1 \notin I_k)\mathbb{I}(i_2 \notin I_k)\hat{\mu}_k(X_{i_2})$;

    (b) Obtain the non-conformity score/residual for i_1, i_2:
    $R_{i_1, i_2} = \text{Error}(Y_{i_1}, \hat{\mu}_{-i_1,-i_2}(X_{i_1}))$;
    $R_{i_2, i_1} = \text{Error}(Y_{i_2}, \hat{\mu}_{-i_1,-i_2}(X_{i_2}))$;

Output: Residuals $(R_{i_1, i_2} : i_1 \neq i_2 \in [N + 1])$.

Define matrix $R \in \mathbb{R}^{(N+1) \times (N+1)}$ as the leave-two-out non-conformity score matrix, where R_{i_1, i_2} is the output of Algorithm 3 if $i_1 \neq i_2$, and diagonal entries $R_{i,i} = 0$ for all i. Also define comparison matrix $A \in \mathbb{R}^{(N+1) \times (N+1)}$ by letting $A_{i_1, i_2} = \mathbb{I}(R_{i_1, i_2} > R_{i_2, i_1})$. Let $S(A) = \{i : \sum_{i'=1}^{N+1} A_{i,i'} \geq (1 - \alpha)(N + 1)\}$ denote the indices of samples which have higher non-conformity scores than $(1 - \alpha)(N + 1)$ samples. In the following, we will first show the size of $S(A)$ is small and $\mathcal{P}(N + 1 \in S(A)) \leq 2\alpha$, and then we will build a connection between $N + 1 \in S(A)$ and $Y_{N+1} \notin \hat{C}_\alpha^{\text{J+MP}}$.

By using exactly the same arguments as in the proof of Theorem 1 in [7], we have $|S(A)| <$

$2\alpha(N+1)$. Now we prove that the distribution of $S(A)$ would not change when $\{(X_i, Y_i)\}_{i=1}^{N+1}$ are arbitrarily exchanged. We first note that the residual matrix R is a function of the extended training data $(\boldsymbol{X}^*, \boldsymbol{Y}^*)$ and subsampled minipatches $(I_1, F_1), \ldots, (I_{\tilde{K}}, F_{\tilde{K}})$, and we denote this function by $\mathcal{A}$:

$$R = \mathcal{A}(\boldsymbol{X}^*, \boldsymbol{Y}^*; (I_1, F_1), \ldots, (I_{\tilde{K}}, F_{\tilde{K}})),$$

where each entry of R satisfies

$$R_{i_1, i_2} = \text{Error}(Y_{i_1}, \frac{1}{\sum_{k=1}^{K} \mathbb{I}(i_1 \notin I_k) \mathbb{I}(i_2 \notin I_k)} \sum_{k=1}^{K} \mathbb{I}(i_1 \notin I_k) \mathbb{I}(i_2 \notin I_k) H(\boldsymbol{X}^*_{I_k, F_k}, \boldsymbol{Y}^*_{I_k})(X_{i_1}).$$

Consider an arbitrary permutation σ on $[N+1]$, and let $\Pi_\sigma \in \{0, 1\}^{(N+1) \times (N+1)}$ be its matrix representation, with $(\Pi_\sigma)_{\sigma(i),:} = e_i^\top$ for $i = 1, \ldots, N+1$. Also let $\sigma(I_k) = \{\sigma(i) : i \in I_k\}$. Then we can also write $Y_{i_1} = (\Pi_\sigma \boldsymbol{Y}^*)_{\sigma(i_1)}$, and $H(\boldsymbol{X}^*_{I_k, F_k}, \boldsymbol{Y}^*_{I_k})(X_{i_1}) = H((\Pi_\sigma \boldsymbol{X}^*)_{\sigma(I_k), F_k}, (\Pi_\sigma \boldsymbol{Y}^*)_{\sigma(I_k)})((\Pi_\sigma \boldsymbol{X}^*)_{\sigma(i_1)})$. Thus

$$(\Pi_\sigma R \Pi_\sigma^\top)_{\sigma(i_1), \sigma(i_2)}$$

$$= R_{i_1, i_2}$$

$$= \text{Error}((\Pi_\sigma \boldsymbol{Y}^*)_{\sigma(i_1)}, \frac{\sum_{k=1}^{K} \mathbb{I}(\sigma(i_1) \notin \sigma(I_k)) \mathbb{I}(\sigma(i_2) \notin \sigma(I_k)) H((\Pi_\sigma \boldsymbol{X}^*)_{\sigma(I_k), F_k}, (\Pi_\sigma \boldsymbol{Y}^*)_{\sigma(I_k)})((\Pi_\sigma \boldsymbol{X}^*)_{\sigma(i_1)})}{\sum_{k=1}^{K} \mathbb{I}(\sigma(i_1) \notin \sigma(I_k)) \mathbb{I}(\sigma(i_2) \notin \sigma(I_k))}.$$

Therefore,

$$\Pi_\sigma R \Pi_\sigma^\top = \mathcal{A}(\Pi_\sigma \boldsymbol{X}^*, \Pi_\sigma \boldsymbol{Y}^*; (\sigma(I_1), \sigma(F_1)), \ldots, (\sigma(I_{\tilde{K}}), \sigma(F_{\tilde{K}}))).$$

Since $\{(I_k, F_k)\}_{k=1}^{\tilde{K}}$ are independent random sets with uniform distribution over $[N+1] \times [M]$, $\{(I_k, F_k)\}_{k=1}^{\tilde{K}} \overset{\text{d.}}{=} \{(\sigma(I_k), \sigma(F_k))\}_{k=1}^{\tilde{K}}$. Meanwhile, by Assumption 4 and Assumption 5, $\Pi_\sigma \boldsymbol{X}^* \overset{\text{d.}}{=} \boldsymbol{X}^*$, $\Pi_\sigma \boldsymbol{Y}^* \overset{\text{d.}}{=} \boldsymbol{Y}^*$, and $H(\cdot)$ is invariant to the order of the input. Hence $\Pi_\sigma R \Pi_\sigma^\top \overset{\text{d.}}{=} R$. Since A and $S(A)$ are functions of R, we also have $S(A) \overset{\text{d.}}{=} S(\Pi_\sigma A \Pi_\sigma^\top)$. For any $1 \leq i \leq N$, there exists a permutation $\sigma(i) = N+1$, and thus $\mathcal{P}(N+1 \in S(A)) = \mathcal{P}(N+1 \in S(\Pi_\sigma A \Pi_\sigma^\top)) = \mathcal{P}(i \in S(A))$. Since this holds for all $1 \leq i \leq N$, $\mathcal{P}(N+1 \in S(A)) = \frac{\mathbb{E}(\sum_{i=1}^{N+1} \mathbb{I}(i \in S(A))}{N+1} = \frac{\mathbb{E}(|S(A)|)}{N+1} \leq 2\alpha$.

Now we show a connection between the events $N+1 \in S(A)$ and $Y_{N+1} \notin \hat{C}_\alpha^{\text{J+MP}}$. Let $K = \sum_{k=1}^{\tilde{K}} \mathbb{I}(N+1 \notin I_k)$, then K follows a binomial distribution with parameters $(\tilde{K}, 1 - \frac{n}{N+1})$ since I_k is randomly sampled from $[N+1]$ without replacement. Collect the minipatches $\{(I_k, F_k) : N+1 \notin I_k\}$ and notice that $\{(I_k, F_k) : N+1 \notin I_k\}$ are independent random subsets that are uniformly sampled from $[N] \times [M]$. For each $1 \leq i \leq N$, we ensemble the minipatch predictions from $\{(I_k, F_k) : i, N+1 \notin I_k\}$ for X_i and X_{N+1}, and compute their corresponding non-conformity score, then (i) they are exactly $R_{i,N+1}$ and $R_{N+1,i}$ returned from Algorithm 3; (ii) they also share the same joint distribution as $\{(R_i^{LOO}, \text{Error}(Y_{N+1}, \hat{\mu}_{-i}(X_{N+1}))\}_{i=1}^{N}$ where R_i^{LOO} and $\hat{\mu}_{-i}(X_{N+1}))$ are returned from Algorithm 2. Therefore,

$$\mathcal{P}(\sum_{i=1}^{N} \mathbb{I}(\text{Error}(Y_{N+1}, \hat{\mu}_{-i}(X_{N+1})) \geq R_i^{(LOO)}) \geq (1 - \alpha)(N+1)) = \mathcal{P}(N+1 \in S(A)) \leq 2\alpha,$$

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verifying that for the classification setting, $\mathcal{P}(Y_{N+1} \in \hat{C}_\alpha^{\text{J+MP}}(X_{N+1})) \geq 1-2\alpha$ with $\hat{C}_\alpha^{\text{J+MP}}(X_{N+1})$ being defined in (8). While for the regression setting, note that if $Y_{N+1} \notin \hat{C}_\alpha^{\text{J+MP}}(X_{N+1})$ for $\hat{C}_\alpha^{\text{J+MP}}(X_{N+1})$ defined in (7), we have $\sum_{i=1}^N \mathbb{I}(Y_{N+1} \geq \hat{\mu}_{-i}(X_{N+1}) + R_i^{LOO}) \geq (1-\alpha)(N+1)$ or $\sum_{i=1}^N \mathbb{I}(Y_{N+1} \leq \hat{\mu}_{-i}(X_{N+1}) - R_i^{LOO}) \geq (1-\alpha)(N+1)$ hold, which implies

$$\sum_{i=1}^N |\mathbb{I}(Y_{N+1} - \hat{\mu}_{-i}(X_{N+1})| \geq R_i^{LOO}) \geq (1-\alpha)(N+1).$$

If choosing error function to be the absolute error, we have

$$\mathcal{P}(Y_{N+1} \notin \hat{C}_\alpha^{\text{J+MP}}(X_{N+1}))$$

$$\leq \mathcal{P}(\sum_{i=1}^N |\mathbb{I}(Y_{N+1} - \hat{\mu}_{-i}(X_{N+1})| \geq R_i^{LOO}) \geq (1-\alpha)(N+1))$$

$$\leq \mathcal{P}(\sum_{i=1}^N \mathbb{I}(\text{Error}(Y_{N+1}, \hat{\mu}_{-i}(X_{N+1}) \geq R_i^{(LOO)})) \geq (1-\alpha)(N+1))$$

$$\leq 2\alpha,$$

which finishes our proof.

A.4 Proof of Lemma 4

We prove the convergence in probability results for the three error terms in Lemma 4 separately.

A.4.1 Bounding $\varepsilon_j^{(1)}$

Here we prove the convergence in probability result for $\varepsilon_j^{(1)}$ by concentrating the random minipatch algorithm around its population version. First note that by the Lipschitz condition (Assumption 1), one can show that

$$|\varepsilon_j^{(1)}| \leq \frac{L}{\sigma_j \sqrt{N}} \sum_{i=1}^N \left(\|\mu_{-i}^{*-j}(X_i) - \hat{\mu}_{-i}^{-j}(X_i)\|_2 + \|\mu_{-i}^*(X_i) - \hat{\mu}_{-i}(X_i)\|_2 \right).$$

Recall that we have defined $\hat{\mu}_{I,F}(X_i) = (H(\boldsymbol{X}_{I,F}, \boldsymbol{Y}_{I_k}))(X_{i,F})$ as the prediction of the base learner trained on $(\boldsymbol{X}_{I,F}, \boldsymbol{Y}_I)$. Thus $\hat{\mu}_{-i}(X_i)$, $\hat{\mu}_{-i}^{-j}(X_i)$, $\mu_{-i}^*(X_i)$, and $\mu_{-i}^{*-j}(X_i)$ can be written out as follows:

$$\hat{\mu}_{-i}(X_i) = \frac{1}{\sum_{k=1}^K \mathbb{I}(i \notin I_k)} \sum_{k=1}^K \mathbb{I}(i \notin I_k)\hat{\mu}_{I_k,F_k}(X_i),$$

$$\hat{\mu}_{-i}^{-j}(X_i) = \frac{1}{\sum_{k=1}^K \mathbb{I}(i \notin I_k)\mathbb{I}(j \notin F_k)} \sum_{k=1}^K \mathbb{I}(i \notin I_k)\mathbb{I}(j \notin F_k)\hat{\mu}_{I_k,F_k}(X_i),$$

$$\mu_{-i}^*(X_i) = \frac{1}{\binom{N-1}{n}\binom{M}{m}} \sum_{\substack{I\subset[N],|I|=n,\\F\subset[M],|F|=m}} \mathbb{I}(i\notin I)\hat{\mu}_{I,F}(X_i)$$

$$= \frac{\binom{N}{n}}{\binom{N-1}{n}}\frac{1}{K}\sum_{k=1}^{K}\mathbb{E}[\mathbb{I}(i\notin I_k)\hat{\mu}_{I_k,F_k}(X_i)|\boldsymbol{X},\boldsymbol{Y}],$$

$$\mu_{-i}^{*-j}(X_i) = \frac{1}{\binom{N-1}{n}\binom{M-1}{m}} \sum_{\substack{I\subset[N],|I|=n,\\F\subset[M],|F|=m}} \mathbb{I}(i\notin I)\mathbb{I}(j\notin F)\hat{\mu}_{I,F}(X_i)$$

$$= \frac{\binom{N}{n}\binom{M}{m}}{\binom{N-1}{n}\binom{M-1}{m}}\frac{1}{K}\sum_{k=1}^{K}\mathbb{E}[\mathbb{I}(i\notin I_k)\mathbb{I}(j\notin F_k)\hat{\mu}_{I_k,F_k}(X_i)|\boldsymbol{X},\boldsymbol{Y}].$$

By Assumption 2, $\|\hat{\mu}_{I,F}(X_i) - \hat{\mu}_{I',F'}(X_i)\|_2 \le B$ for any two minipatches (I,F) and (I',F'). Without loss of generality, we will assume that $\|\hat{\mu}_{I,F}(X_i)\|_2 \le B$ for all $i = 1,\ldots,N$, $I\subset[N]$ of size n and $F\subset[M]$ of size m, since both $\|\hat{\mu}_{-i}^{-j}(X_i) - \mu_{-i}^{*-j}(X_i)\|_2$ and $\|\hat{\mu}_{-i}(X_i) - \mu_{-i}^*(X_i)\|_2$ would not change if we subtract each $\hat{\mu}_{I,F}(X_i)$ by its average over all $I\subset[N]$, $F\subset[M]$.

In addition, we define the following quantities that would be helpful in the proofs:

$$\tilde{\mu}_{-i}^{-j}(X_i) = \frac{\binom{N}{n}\binom{M}{m}}{\binom{N-1}{n}\binom{M-1}{m}}\frac{1}{K}\sum_{k=1}^{K}\mathbb{I}(i\notin I_k)\mathbb{I}(j\notin F_k)\hat{\mu}_{I_k,F_k}(X_i),$$

$$\tilde{\mu}_{-i}(X_i) = \frac{\binom{N}{n}}{\binom{N-1}{n}}\frac{1}{K}\sum_{k=1}^{K}\mathbb{I}(i\notin I_k)\hat{\mu}_{I_k,F_k}(X_i). \tag{9}$$

Then $\epsilon_j^{(1)}$ can be further bounded as follows:

$$|\varepsilon_j^{(1)}| \le \frac{L}{\sigma_j\sqrt{N}}\sum_{i=1}^{N}\left[\|\hat{\mu}_{-i}^{-j}(X_i) - \mu_{-i}^{*-j}(X_i)\|_2 + \|\hat{\mu}_{-i}(X_i) - \mu_{-i}^*(X_i)\|_2\right]$$

$$\le \frac{L}{\sigma_j\sqrt{N}}\sum_{i=1}^{N}\left[\|\hat{\mu}_{-i}^{-j}(X_i) - \tilde{\mu}_{-i}^{-j}(X_i)\|_2 + \|\hat{\mu}_{-i}(X_i) - \tilde{\mu}_{-i}(X_i)\|_2 + \right.$$

$$\left.\|\tilde{\mu}_{-i}^{-j}(X_i) - \mu_{-i}^{*-j}(X_i)\|_2 + \|\tilde{\mu}_{-i}(X_i) - \mu_{-i}^*(X_i)\|_2\right].$$

Let

$$\text{I} = \frac{L}{\sigma_j\sqrt{N}}\sum_{i=1}^{N}\|\hat{\mu}_{-i}^{-j}(X_i) - \tilde{\mu}_{-i}^{-j}(X_i)\|_2, \quad \text{II} = \frac{L}{\sigma_j\sqrt{N}}\sum_{i=1}^{N}\|\hat{\mu}_{-i}(X_i) - \tilde{\mu}_{-i}(X_i)\|_2,$$

$$\text{III} = \frac{L}{\sigma_j\sqrt{N}}\sum_{i=1}^{N}\|\tilde{\mu}_{-i}^{-j}(X_i) - \mu_{-i}^{*-j}(X_i)\|_2, \quad \text{IV} = \frac{L}{\sigma_j\sqrt{N}}\sum_{i=1}^{N}\|\tilde{\mu}_{-i}(X_i) - \mu_{-i}^*(X_i)\|_2,$$

and we will upper bound these four terms separately.

1. For term I, since we have assumed $\|\hat{\mu}_{I,F}(X_i)\|_2 \le B$, one can show that

$$|\text{I}| \le \frac{BL\sqrt{N}}{\sigma_j}\max_{1\le i\le N}\left|\frac{K}{\sum_{k=1}^{K}\mathbb{I}(i\notin I_k)\mathbb{I}(j\notin F_k)} - \frac{NM}{(N-n)(M-m)}\right|.$$

Let $\hat{p}_{i,j} = \frac{\sum_{k=1}^{K} \mathbb{I}(i \notin I_k)\mathbb{I}(j \notin F_k)}{K}$ and $p_{i,j} = \frac{(N-n)(M-m)}{NM}$. Then for any $\epsilon > 0$,

$$\mathcal{P}(|\mathrm{I}| > \epsilon) \leq \mathcal{P}\left(\max_{1 \leq i \leq N} |\hat{p}_{i,j}^{-1} - p_{i,j}^{-1}| > \frac{\epsilon \sigma_j}{BL\sqrt{N}}\right)$$

$$\leq \sum_{i=1}^{N} \mathcal{P}\left(|\hat{p}_{i,j}^{-1} - p_{i,j}^{-1}| > \frac{\epsilon \sigma_j}{BL\sqrt{N}}\right).$$

Note that if $|\hat{p}_{i,j} - p_{i,j}| \leq \frac{p_{i,j}}{2}$, $|\hat{p}_{i,j}^{-1} - p_{i,j}^{-1}| = \frac{|\hat{p}_{i,j} - p_{i,j}|}{\hat{p}_{i,j}p_{i,j}} \leq \frac{2|\hat{p}_{i,j} - p_{i,j}|}{p_{i,j}^2}$. Thus $|\hat{p}_{i,j}^{-1} - p_{i,j}^{-1}| > \frac{\epsilon \sigma_j}{BL\sqrt{N}}$ implies

$$|\hat{p}_{i,j} - p_{i,j}| > \min\left\{\frac{p_{i,j}}{2}, \frac{\epsilon \sigma_j p_{i,j}^2}{2BL\sqrt{N}}\right\}.$$

Since $\hat{p}_{i,j} - p_{i,j} = \sum_{k=1}^{K} \frac{1}{K}\left[\mathbb{I}(i \notin I_k)\mathbb{I}(j \notin F_k) - p_{i,j}\right]$ is a sum of independent bounded random variables with mean zero, we can apply the Hoeffding's inequality [see e.g., Proposition 2.5 in 74, and examples therein] to obtain that

$$\mathcal{P}\left(|\hat{p}_{i,j} - p_{i,j}| > \min\left\{\frac{p_{i,j}}{2}, \frac{\epsilon \sigma_j p_{i,j}^2}{2BL\sqrt{N}}\right\}\right) \leq \exp\left\{-K\min\left\{\frac{p_{i,j}^2}{2}, \frac{\epsilon^2 \sigma_j^2 p_{i,j}^4}{2B^2 L^2 N}\right\}\right\},$$

which further implies that

$$\mathcal{P}(|\mathrm{I}| > \epsilon) \leq \sum_{i=1}^{N} \exp\left\{-K\min\left\{\frac{p_{i,j}^2}{2}, \frac{\epsilon^2 \sigma_j^2 p_{i,j}^4}{2B^2 L^2 N}\right\}\right\}$$

$$\leq \exp\left\{\log N - K\min\left\{\frac{\min_i p_{i,j}^2}{2}, \frac{\epsilon^2 \sigma_j^2 \min_i p_{i,j}^4}{2B^2 L^2 N}\right\}\right\}.$$

By Assumption 3, $p_{i,j} = (1 - \frac{n}{N})(1 - \frac{m}{M}) \geq (1 - \beta)^2$. Since $K \gg (\frac{B^2 L^2 N}{\sigma_j^2} + 1)\log N$, there exists $N_0 > 0$ such that when $N \geq N_0$, the number of minipatches $K(N) \geq [\frac{3}{(1-\beta)^8 \epsilon^2} + \frac{3}{(1-\beta)^4}](\frac{B^2 L^2 N}{\sigma_j^2} + 1)\log N$, which implies that

$$\exp\left\{\log N - K\min\left\{\frac{(1-\beta)^4}{2}, \frac{\epsilon^2 \sigma_j^2 (1-\beta)^8}{2B^2 L^2 N}\right\}\right\}$$

$$\leq \exp\left\{\log N - \left(\frac{3}{(1-\beta)^8 \epsilon^2} + \frac{3}{(1-\beta)^4}\right)\left(\frac{B^2 L^2 N}{\sigma_j^2} + 1\right)\min\left\{\frac{3}{2}, \frac{3\sigma_j^2}{2B^2 L^2 N}\right\}\log N\right\}$$

$$\leq \exp\left\{-\frac{1}{2}\log N\right\},$$

when $N \geq N_0$. Therefore, for any $\epsilon > 0$, $\lim_{N \to \infty} \mathcal{P}(|\mathrm{I}| > \epsilon) = 0$, or equivalently, $\mathrm{I} \xrightarrow{p} 0$.

2. For term II, following similar arguments to bounding term I, we have that for any $\epsilon > 0$,

$$\mathcal{P}(|\mathrm{II}| > \epsilon) \leq \sum_{i=1}^{N} \mathcal{P}\left(|\hat{p}_i - p_i| > \min\left\{\frac{p_i}{2}, \frac{\epsilon \sigma_j p_i^2}{2BL\sqrt{N}}\right\}\right)$$

$$\leq \exp\left\{\log N - K \min\left\{\frac{\min_i p_i^2}{2}, \frac{\epsilon^2 \sigma_j^2 \min_i p_i^4}{2B^2 L^2 N}\right\}\right\},$$

where $\hat{p}_i = \frac{\sum_{k=1}^K \mathbb{I}(i \notin I_k)}{K}$ and $p_i = \frac{N-n}{N}$. Since $p_i \geq p_{i,j}$, using the same argument for showing the consistency of I, we have $\lim_{N \to \infty} \mathcal{P}(|\text{II}| > \epsilon) = 0$.

3. While for term III, we first define $Z_k \in \mathbb{R}^{Nd}$ as follows:

$$(Z_k)_{((i-1)d+1):id}$$
$$= \frac{1}{K}\mathbb{I}(i \notin I_k)\mathbb{I}(j \notin F_k)\hat{\mu}_{I_k,F_k}(X_i) - \frac{1}{K}\mathbb{E}\left[\mathbb{I}(i \notin I_k)\mathbb{I}(j \notin F_k)\hat{\mu}_{I_k,F_k}(X_i) | \boldsymbol{X}, \boldsymbol{Y}\right],$$

for $i = 1, \ldots, N$. Then conditioning on data set $(\boldsymbol{X}, \boldsymbol{Y})$, $\{Z_k\}_{k=1}^K$ is a sequence of independent random vectors of mean zero. By the boundedness of $\|\hat{\mu}_{I,F}(X_i)\|_2$, the spectral norm of Z_k satisfies $\|Z_k\|_2 \leq \frac{2B\sqrt{N}}{K}$, and

$$\max\left\{\left\|\sum_k \mathbb{E}(Z_k Z_k^\top)\right\|, \left\|\sum_k \mathbb{E}(Z_k^\top Z_k)\right\|\right\} \leq \frac{4B^2 N}{K},$$

where $\|\cdot\|$ represents the spectral norm. Now we can write out III as follows:

$$\text{III} = \frac{LNM}{\sigma_j\sqrt{N}(N-n)(M-m)}\sum_{i=1}^N\left\|\frac{1}{K}\sum_{k=1}^K(Z_k)_{((i-1)d+1):id}\right\|_2$$
$$\leq \frac{L}{\sigma_j(1-\beta)^2}\left\|\frac{1}{K}\sum_{k=1}^K Z_k\right\|_2.$$

Viewing Z_k as an $Nd \times 1$ matrix, we can then apply the matrix Bernstein inequality [See Theorem 6.1.1 in 66] and obtain the following probabilistic bound:

$$\mathcal{P}(|\text{III}| > \epsilon) \leq \mathcal{P}\left(\left\|\frac{1}{K}\sum_{k=1}^K Z_k\right\|_2 > \frac{\epsilon\sigma_j(1-\beta)^2}{L}\right)$$
$$\leq (dN+1)\exp\left\{\frac{\epsilon^2\sigma_j^2(1-\beta)^4/L^2}{8B^2N/K + 4B\sqrt{N}\epsilon\sigma_j(1-\beta)^2/(3LK)}\right\}$$
$$\leq C\exp\left\{\log N - \min\left\{\frac{\epsilon^2\sigma_j^2(1-\beta)^4 K}{16L^2B^2N}, \frac{3\epsilon\sigma_j(1-\beta)^2 K}{8LB\sqrt{N}}\right\}\right\}.$$

Since we have assumed $K \gg (\frac{L^2B^2N}{\sigma_j^2} + \frac{LB\sqrt{N}}{\sigma_j} + 1)\log N$, there exists $N_0 > 0$ such that for all $N \geq N_0$, $K(N) \geq \max\left\{\frac{32L^2B^2N\log N}{\epsilon^2(1-\beta)^4\sigma_j^2}, \frac{16LB\sqrt{N}\log N}{3\epsilon(1-\beta)^2\sigma_j}\right\}$, which implies

$$\mathcal{P}(|\text{III}| > \epsilon) \leq C\exp\left\{\log N - \min\left\{\frac{\epsilon^2\sigma_j^2(1-\beta)^4 K}{16L^2B^2N}, \frac{3\epsilon\sigma_j(1-\beta)^2 K}{8LB\sqrt{N}}\right\}\right\}$$
$$\leq C\exp\left\{-\log N\right\}.$$

Therefore, for any $\epsilon > 0$, $\lim_{N \to \infty} \mathcal{P}(|\text{III}| > \epsilon) = 0$.

4. By redefining

$$(Z_k)_{((i-1)d+1):id} = \frac{1}{K}\mathbb{I}(i \notin I_k)\hat{\mu}_{I_k,F_k}(X_i) - \frac{1}{K}\mathbb{E}[\mathbb{I}(i \notin I_k)\hat{\mu}_{I_k,F_k}(X_i)],$$

and following almost the same argument as above, we can also show that for any $\epsilon > 0$, $\lim_{N\to\infty}\mathcal{P}(|\text{IV}| > \epsilon) = 0$.

Therefore, combing all the convergence in probability results for I, II, III, and IV, we have $\epsilon_j^{(1)} \xrightarrow{p} 0$.

A.4.2 Bounding $\varepsilon_j^{(2)}$

First note that

$$
|\varepsilon_j^{(2)}| \le \frac{1}{\sigma_j\sqrt{N}}\sum_{i=1}^{N}\left|\mathbb{E}_{(X,Y)}\{\text{Error}(Y,\mu_{-i}^{*-j}(X)) - \text{Error}(Y,\mu^{*-j}(X))\}\right|
$$
$$
+ \left|\mathbb{E}_{(X,Y)}\{\text{Error}(Y,\mu_{-i}^{*}(X)) - \text{Error}(Y,\mu^{*}(X))\}\right|
$$
$$
\le \frac{L}{\sigma_j\sqrt{N}}\sum_{i=1}^{N}\mathbb{E}_X\|\mu_{-i}^{*-j}(X) - \mu^{*-j}(X)\|_2 + \mathbb{E}_X\|\mu_{-i}^{*}(X) - \mu^{*}(X)\|_2.
$$

Recall the definition of $\mu_{-i}^{*-j}(X)$, $\mu^{*-j}(X)$, $\mu_{-i}^{*}(X)$, $\mu^{*}(X)$, and $\hat{\mu}_{I,F}(X)$ in the beginning of Section A. Then we can write

$$
\mu_{-i}^{*-j}(X) = \frac{1}{\binom{N-1}{n}\binom{M-1}{m}}\sum_{\substack{I\subset[N],|I|=n,\\F\subset[M],|F|=m}}\mathbb{I}(i \notin I)\mathbb{I}(j \notin F)\hat{\mu}_{I,F}(X),
$$

$$
\mu^{*-j}(X) = \frac{1}{\binom{N}{n}\binom{M-1}{m}}\sum_{\substack{I\subset[N],|I|=n,\\F\subset[M],|F|=m}}\mathbb{I}(j \notin F)\hat{\mu}_{I,F}(X)
$$
$$
= \frac{N-n}{N}\mu_{-i}^{*-j}(X) + \frac{n}{N}\frac{1}{\binom{N-1}{n-1}\binom{M-1}{m}}\sum_{\substack{I\subset[N],|I|=n,\\F\subset[M],|F|=m}}\mathbb{I}(i \in I)\mathbb{I}(j \notin F)\hat{\mu}_{I,F}(X);
$$

$$
\mu_{-i}^{*}(X) = \frac{1}{\binom{N-1}{n}\binom{M}{m}}\sum_{\substack{I\subset[N],|I|=n,\\F\subset[M],|F|=m}}\mathbb{I}(i \notin I)\hat{\mu}_{I,F}(X),
$$

$$
\mu^{*}(X) = \frac{1}{\binom{N}{n}\binom{M}{m}}\sum_{\substack{I\subset[N],|I|=n,\\F\subset[M],|F|=m}}\hat{\mu}_{I,F}(X)
$$
$$
= \frac{N-n}{N}\mu_{-i}^{*}(X) + \frac{n}{N}\frac{1}{\binom{N-1}{n-1}\binom{M}{m}}\sum_{\substack{I\subset[N],|I|=n,\\F\subset[M],|F|=m}}\mathbb{I}(i \in I)\hat{\mu}_{I,F}(X),
$$

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and hence

$$\|\mu_{-i}^{*-j}(X) - \mu^{*-j}(X)\|_2 = \frac{n}{N}\|\frac{1}{\binom{N-1}{n-1}\binom{M-1}{m}}\sum_{\substack{I\subset[N],|I|=n,\\F\subset[M],|F|=m}}\mathbb{I}(i\in I)\mathbb{I}(j\notin F)[\mu_{-i}^{*-j}(X) - \hat{\mu}_{I,F}(X)]\|_2$$
$$\leq \frac{Bn}{N},$$

where we have applied the fact that $\|\hat{\mu}_{I,F}(X) - \mu_{-i}^{*-j}(X)\|_2 \leq B$ which is directly implied by Assumption 2. Similarly,

$$\|\mu_{-i}^{*}(X) - \mu^{*}(X)\|_2 = \frac{n}{N}\|\frac{1}{\binom{N-1}{n-1}\binom{M}{m}}\sum_{\substack{I\subset[N],|I|=n,\\F\subset[M],|F|=m}}\mathbb{I}(i\in I)[\mu_{-i}^{*}(X) - \hat{\mu}_{I,F}(X)]\|_2$$
$$\leq \frac{Bn}{N}.$$

Therefore, $|\varepsilon_j^{(2)}| \leq \frac{2LBn}{\sigma_j\sqrt{N}}$. By Assumption 3, $|\varepsilon_j^{(2)}| \xrightarrow{p} 0$.

A.4.3 Bounding $\varepsilon_j^{(3)}$

Recall the definition of $\tilde{h}_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i})$, $h_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i})$, and $h_j(X_i, Y_i)$ in the beginning of Section A. Then we can write

$$\varepsilon_{i,j}^{(2)} = h_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}) - \mathbb{E}[h_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i})|\boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}] - h_j(X_i, Y_i) + \mathbb{E}[h_j(X_i, Y_i)].$$

Define

$$\bar{h}_j(X_i, Y_i) = \mathbb{E}_{\boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}}[h_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i})|X_i, Y_i], \tag{10}$$

and $h_j'(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}) = h_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}) - \mathbb{E}[h_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i})|\boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}]$, then we can further decompose $\varepsilon_{i,j}^{(2)}$ as follows:

$$\varepsilon_{i,j}^{(2)} = h_j'(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}) - \mathbb{E}[h_j'(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i})|X_i, Y_i]$$
$$+ \bar{h}_j(X_i, Y_i) - h_j(X_i, Y_i) + \mathbb{E}[h_j(X_i, Y_i)] - \mathbb{E}[\bar{h}_j(X_i, Y_i)].$$

Denote $h_j'(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}) - \mathbb{E}[h_j'(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i})|X_i, Y_i]$ by E_i, and we will first deal with E_i in the following by leveraging a asymptotic linearity result established in [10], and then show an upper bound for $|\bar{h}_j(X_i, Y_i) - h_j(X_i, Y_i) + \mathbb{E}[h_j(X_i, Y_i)] - \mathbb{E}[\bar{h}_j(X_i, Y_i)]|$.

Bounding E_i In fact, $h_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i})$ can be viewed as a leave-one-out test value, which is a special case of the cross-validation test error in [10]. We would like to apply Theorem 2 in [10] with $h_n'(Z_i, Z_{B_j})$ substituted by $h_j'(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i})$. Let (X_{N+1}, Y_{N+1}) be a sample from

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$\mathcal{P}$ which is independent from $(\boldsymbol{X}, \boldsymbol{Y})$, and denote by $(\boldsymbol{X}_{\backslash i,:}^{\backslash l}, \boldsymbol{Y}_{\backslash i}^{\backslash l})$ the $N-1$ training set with sample i excluded, and sample l replaced by (X_{N+1}, Y_{N+1}). One key quantity in [10] called the loss stability of $h_j(\cdot, \cdot; \cdot, \cdot)$ can be written out as

$$\gamma_{loss}(h_j) = \frac{1}{N-1} \sum_{l \neq i} \mathbb{E}[(h_j'(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}) - h_j'(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}^{\backslash l}, \boldsymbol{Y}_{\backslash i}^{\backslash l}))^2].$$

The consistency for $\frac{1}{\sigma_j \sqrt{N}} \sum_{i=1}^{N} E_i$ hinges on an upper bound for $\gamma_{loss}(h_j)$. To bound $\gamma_{loss}(h_j)$, note that

$$|h_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}) - h_j(X_i, Y_i; \boldsymbol{X}_{\backslash i,:}^{\backslash l}, \boldsymbol{Y}_{\backslash i}^{\backslash l})|$$
$$\leq L \|\mu(X_{i,\backslash j}; \boldsymbol{X}_{\backslash i,\backslash j}, \boldsymbol{Y}_{\backslash i}) - \mu(X_{i,\backslash j}; \boldsymbol{X}_{\backslash i,\backslash j}^{\backslash l}, \boldsymbol{Y}_{\backslash i}^{\backslash l})\|_2 + L \|\mu(X_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}) - \mu(X_i; \boldsymbol{X}_{\backslash i,:}^{\backslash l}, \boldsymbol{Y}_{\backslash i}^{\backslash l})\|_2.$$

Let $I^{\backslash l} = \begin{cases} I, & l \notin I \\ \{i \neq l : i \in I\} \cup \{N+1\}, & l \in I \end{cases}$ denote the index set with l replaced by $N+1$, then

$$\|\mu(X_{i,\backslash j}; \boldsymbol{X}_{\backslash i,\backslash j}, \boldsymbol{Y}_{\backslash i}) - \mu(X_{i,\backslash j}; \boldsymbol{X}_{\backslash i,\backslash j}^{\backslash l}, \boldsymbol{Y}_{\backslash i}^{\backslash l})\|_2$$
$$\leq \frac{1}{\binom{N-1}{n}\binom{M-1}{m}} \sum_{\substack{I \subset [N], |I|=n, \\ F \subset [M], |F|=m}} \mathbb{I}(i \notin I) \mathbb{I}(j \notin F) \mathbb{I}(l \in I) \|\hat{\mu}_{I,F}(X_i) - \hat{\mu}_{I^{\backslash l},F}(X_i)\|_2$$
$$\leq \frac{Bn}{N-1},$$

where we have applied Assumption 2 on the last line. Similarly, one has

$$\|\mu(X_i; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}) - \mu(X_i; \boldsymbol{X}_{\backslash i,:}^{\backslash l}, \boldsymbol{Y}_{\backslash i}^{\backslash l})\|_2 \leq \frac{Bn}{N-1},$$

which further implies

$$\gamma_{loss}(h_j) \leq \frac{16L^2 B^2 n^2}{(N-1)^2}.$$

Therefore, applying Theorem 2 in [10] leads to

$$\text{Var}\left(\frac{1}{\sigma_j \sqrt{N}} \sum_{i=1}^{N} E_i\right) \leq \frac{24 L^2 B^2 n^2}{\sigma_j^2 (N-1)}. \tag{11}$$

Since $\mathbb{E}(E_i) = 0$ and $n = o(\frac{\sigma_j \sqrt{N}}{LB})$, (11) suggests $\frac{1}{\sigma_j \sqrt{N}} \sum_{i=1}^{N} E_i \xrightarrow{L_2} 0$ which then implies $\frac{1}{\sigma_j \sqrt{N}} \sum_{i=1}^{N} E_i \xrightarrow{p} 0$.

Bounding $\bar{h}_j(X_i, Y_i) - h_j(X_i, Y_i)$ For bounding $\bar{h}_j(X_i, Y_i) - h_j(X_i, Y_i)$, note that for any (X, Y),

$$|\bar{h}_j(X, Y) - h_j(X, Y)| = \mathbb{E}\left[h_j(X, Y; \boldsymbol{X}_{\backslash i,:}, \boldsymbol{Y}_{\backslash i}) - h_j(X, Y; \boldsymbol{X}, \boldsymbol{Y}) | X, Y\right]$$

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$$\leq L\mathbb{E}[\|\mu_{-i}^{*-j}(X) - \mu^{*-j}(X)\|_2|X] + L\mathbb{E}[\|\mu_{-i}^{*}(X) - \mu^{*}(X)\|_2|X]$$

$$\leq \frac{2LBn}{N},$$

where the last line is due to the arguments in Section A.4.2. Therefore,

$$\frac{1}{\sigma_j\sqrt{N}} \sum_{i=1}^{N} \left|\bar{h}_j(X_i, Y_i) - h_j(X_i, Y_i) + \mathbb{E}[h_j(X_i, Y_i)] - \mathbb{E}[\bar{h}_j(X_i, Y_i)]\right| \leq \frac{4LBn}{\sigma_j\sqrt{N}} \to 0.$$

Combining the convergence in probability results for both

$$\frac{1}{\sigma_j\sqrt{N}} \sum_{i=1}^{N} \left|\bar{h}_j(X_i, Y_i) - h_j(X_i, Y_i) + \mathbb{E}[h_j(X_i, Y_i)] - \mathbb{E}[\bar{h}_j(X_i, Y_i)]\right|$$

and $\frac{1}{\sigma_j\sqrt{N}} \sum_{i=1}^{N} E_i$, we have $\varepsilon_j^{(3)} \xrightarrow{p} 0$.

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