LOCO-MP: Built-in Uncertainty Quantification for LOCO Feature Importance

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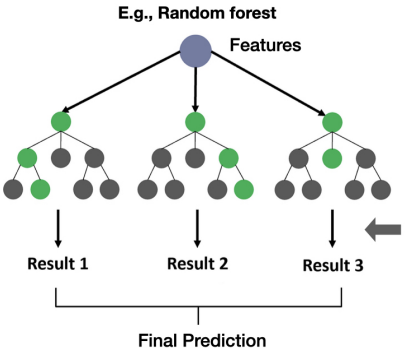
Motivation: Interpretable Machine Learning

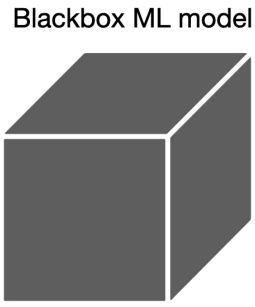
Interpreting Black-box Machine Learning Models

Machine learning is widely applied in **high-stakes applications**:

Can we trust machine learning? Make it interpretable!

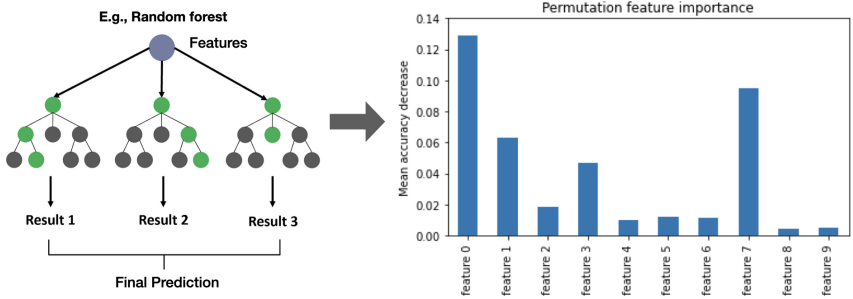
Interpreting Black-box Machine Learning Models





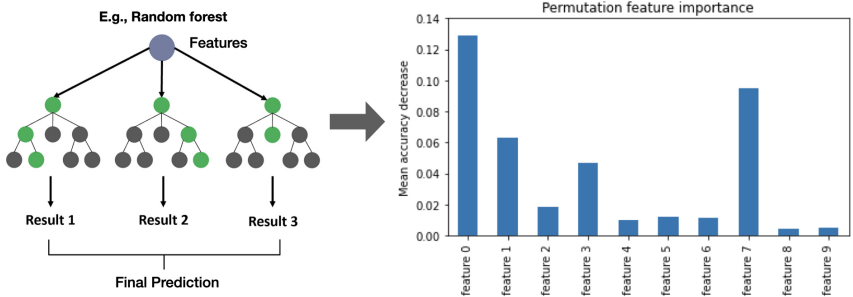
What is this ML system's rationale of rejecting/approving mortgage applications?

Feature importance: How does my model's prediction rely on each feature?



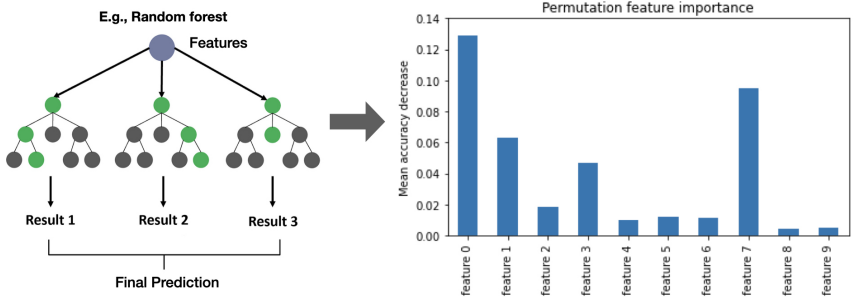
- Model-specific: defined for random forest, linear models, deep learning, etc.
- **Model-agnostic**: feature occlusion [Covert et al., 2021], permutation [König et al., 2021], Shapley values [Sundararajan and Najmi, 2020], etc.

Feature importance: How does my model's prediction rely on each feature?



- We focus on **global** feature importance: explanation **for the whole population** instead of one instance.
- Answers "Which features often drives the decision for most applications?"

Feature importance: How does my model's prediction rely on each feature?



Many model-agnostic, global feature importance metrics exist.

Can we trust feature importance? Uncertainty quantification?

Literature: Feature Importance Inference

- Inference for Lasso [Lee et al., 2016, Van de Geer et al., 2014]
- Conditional independence tests for random forest [Chi et al., 2022]
- Model-agnostic methods: Floodgate [Zhang and Janson, 2020], GCM [Shah and Peters, 2020], VIMP [Williamson et al., 2021]

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Wait a second...

- They all explain population data-generating model, not the ML model itself.
- ML models are only tools
- Impossible without strong assumptions about the data or model [Shah and Peters, 2020]!

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We call this type **population feature importance**

ML Feature Importance

The feature importance we want:

- Property of the model
- Which feature does my ML model rely on for decisions?
- Desired for model diagnostics, auditing, and deployment

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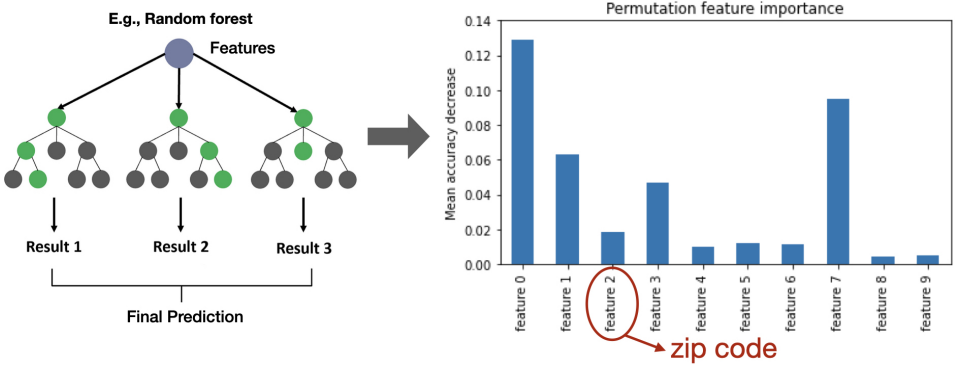
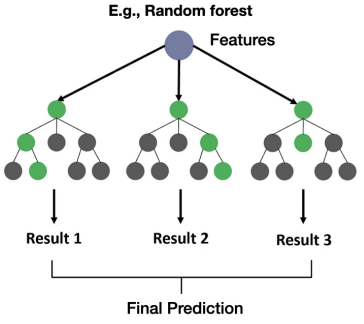
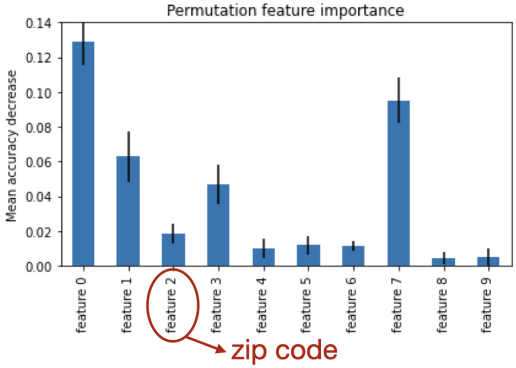


- How much does mortgage decision rely on sensitive features?
- E.g., zip code is a proxy of race?
- Check ML feature importance

ML Feature Importance





UQ for ML feature importance:

- **has important societal consequences but is understudied!**

ML Feature Importance Inference

- Only a few works [Lei et al., 2018, Rinaldo et al., 2019, Watson and Wright, 2021]
- Some require knowing the distribution of features (model-X) [Watson and Wright, 2021]
- The most general, assumption-lean approach is the Leave-one-covariate-out (LOCO) inference [Lei et al., 2018, Rinaldo et al., 2019].
- Practical challenges: statistical & computational cost for inference is substantial.

Uncertainty Quantification for Feature Importance

Prior Work: LOCO Inference

Leave-One-Covariate-Out (LOCO) Inference
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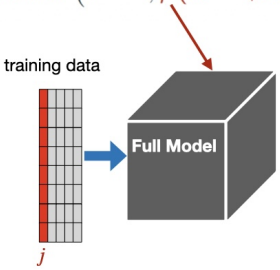
$$\Delta_j^*(\boldsymbol{X}, \boldsymbol{Y}) = \mathbb{E}\left[\text{Error}\left(Y^{\text{test}}, \mu_{-j}(X_{-j}^{\text{test}}; \boldsymbol{X}_{-j}, \boldsymbol{Y})\right) - \text{Error}\left(Y^{\text{test}}, \mu(X^{\text{test}}; \boldsymbol{X}, \boldsymbol{Y})\right) | \boldsymbol{X}, \boldsymbol{Y}\right]$$



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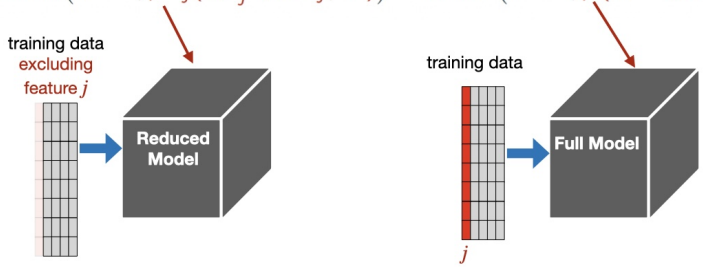

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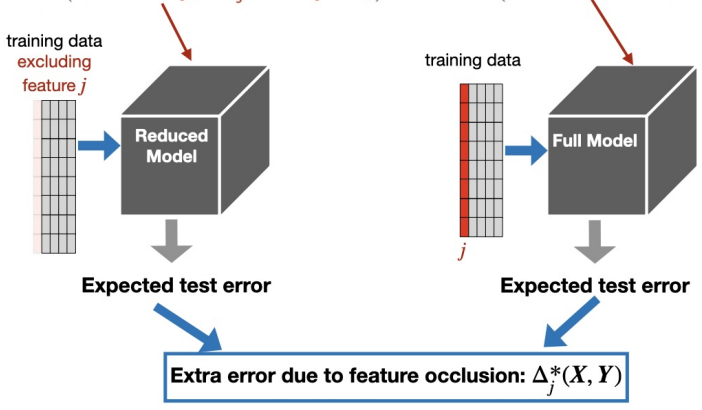

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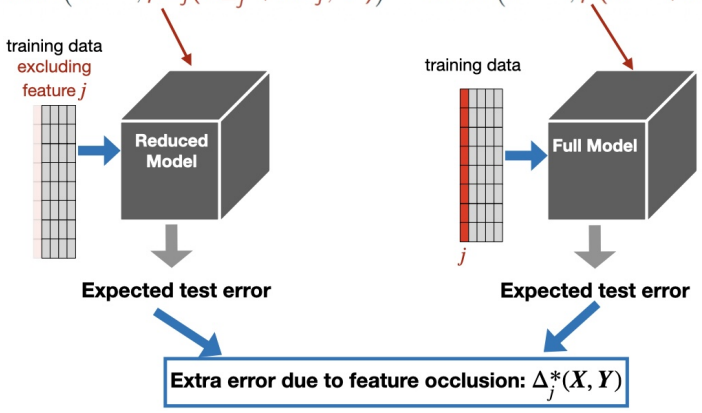

How much does feature j **help or hurt** model μ's predictive performance?

Prior Work: LOCO Inference

LOCO inference approach:

- Splits data; fits full and reduced models to training data
- Feature occlusion scores on test data $\Rightarrow$ confidence intervals

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Advantages

- Model-agnostic (applicability).
- Statistically valid without assuming data distribution/model choice.

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Challenges

- Data splitting loses data efficiency for both training and inference;
- Interpretation is not for the full model & depends on random data splitting
- Model refitting for each feature: prohibitive computation after model training

Prior Work: LOCO Inference

LOCO inference approach:

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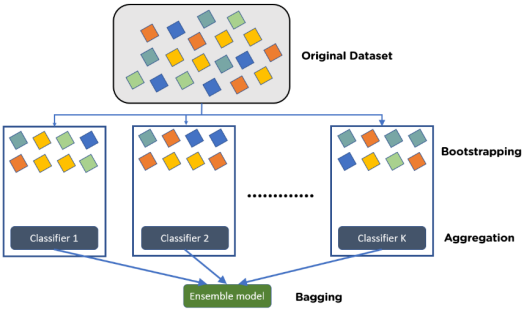
Our Goal

Can we utilize the general LOCO framework to perform ML feature importance inference, while avoiding data splitting and model refitting?

Our Approach: LOCO Inference for an Ensemble Framework

LOCO Inference for Ensemble Learning



Bagging

Picture source: https://www.simplilearn.com/tutorials/machine-learning-tutorial/bagging-in-machine-learning

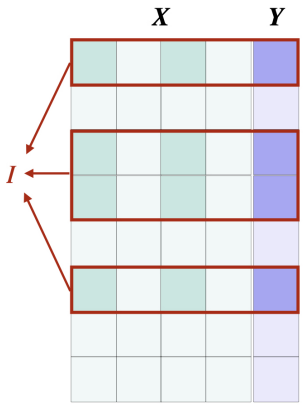
Inspiration: Jacknife+ After Bootstrap [Kim et al., 2020].

- Many ensemble methods are good predictors
- Conformal inference (Jackknife+) for bagging is computationally free with no data-splitting!

Idea: Minipatch Ensembles.

Minipatch Ensemble Learning

Minipatch ensembles: like bagging, but double-subsampling for both observations and features [Yao and Allen, 2020].



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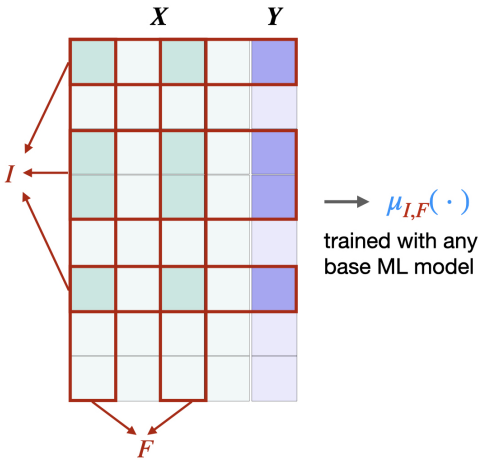

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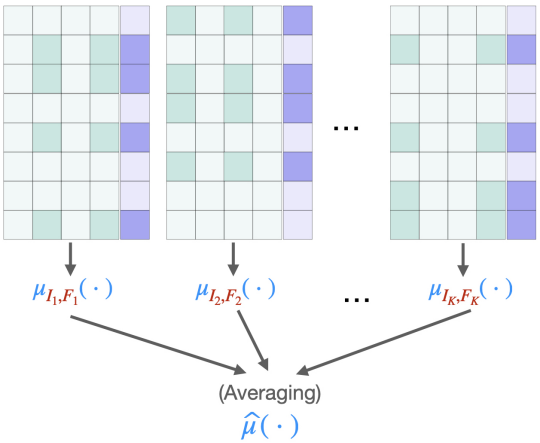
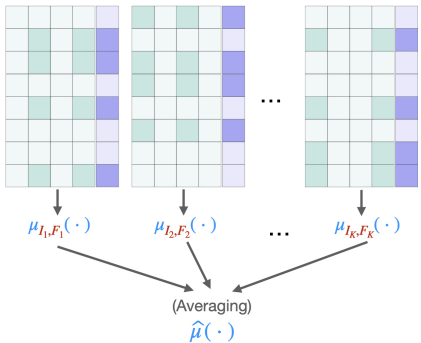


Minipatch Ensemble Learning

Inspiration: Bagging; Random Forests [Louppe and Geurts, 2012]; Stochastic Optimization & Dropout.

Advantages:

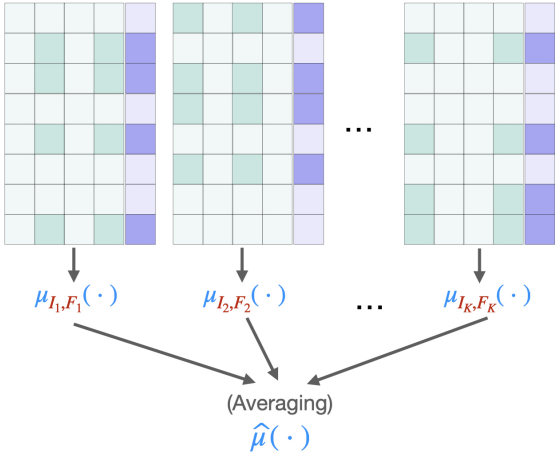
- Fast and easily parallelizable
- Ensemble diversity; **implicit regularization** [LeJeune et al., 2020, Yao et al., 2021]



LOCO Inference for Minipatch Ensembles?

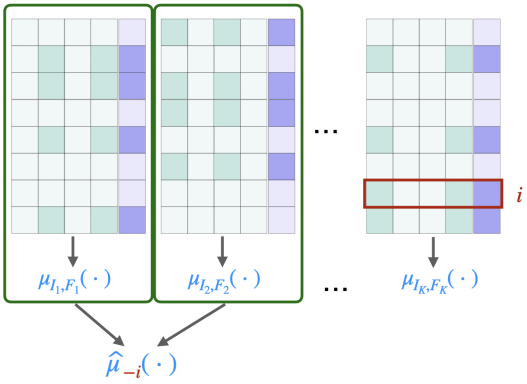
Algorithm: LOCO for Minipatch

- **Step 1**. Fit minipatch learning predictor: $\hat{\mu}$.



Algorithm: LOCO for Minipatch

- **Step 2**. **LOO** (leave-one-observation-out) predictor: $\hat{\mu}_{-i}(X_i)$.
  - Ensemble minipatches without observation i.
  - Compute test error on sample i.



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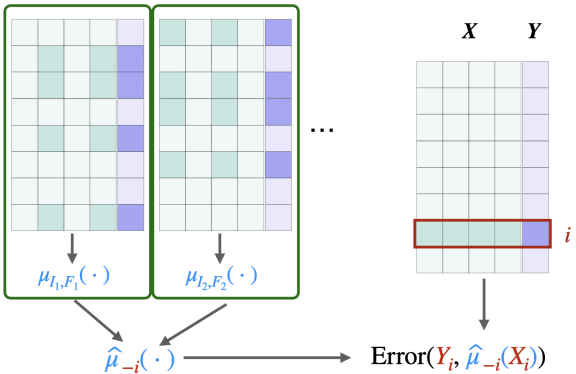

No data-splitting!

Simple model averaging;

Free computationally!

Algorithm: LOCO for Minipatch

- **Step 3**. **LOCO-LOO** predictor: $\hat{\mu}_{-i}^{-j}(X_i)$.
  - Ensemble minipatches without observation i and without feature j.
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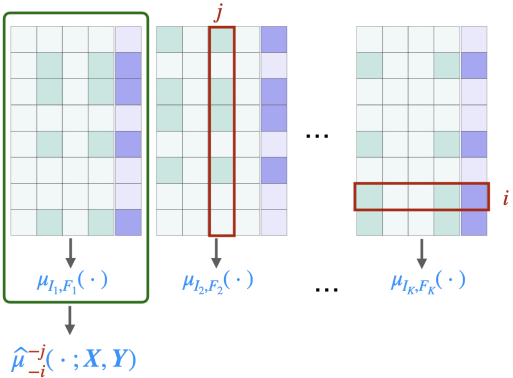

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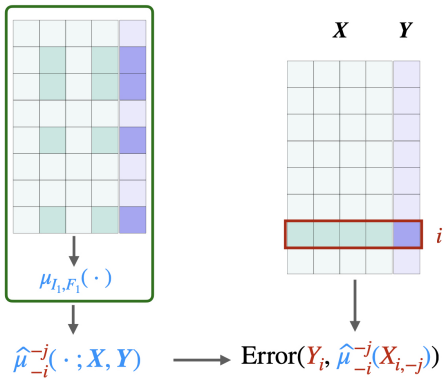

Simple model averaging;
Free computationally!

Algorithm: LOCO for Minipatch

- **Step 4**. Compute feature occlusion scores for observations $1 \leq i \leq N$:

$$\widehat{\Delta}_j(X_i, Y_i) = \text{Error}(Y_i, \hat{\mu}_{-i}^{-j}(X_i)) - \text{Error}(Y_i, \hat{\mu}_{-i}(X_i)).$$

  Importance of feature j for predicting sample i.

- **Step 5**. Construct asymptotically normal interval from $\{\widehat{\Delta}_j(X_i, Y_i)\}_{i=1}^N$:

$$\hat{\mathbb{C}}_j = \left[\bar{\Delta}_j - \frac{z_{\alpha/2}\hat{\sigma}_j}{\sqrt{N}}, \bar{\Delta}_j + \frac{z_{\alpha/2}\hat{\sigma}_j}{\sqrt{N}}\right],$$

  $\bar{\Delta}_j$: mean occlusion score, $\hat{\sigma}_j$: standard deviation.

Algorithm: LOCO for Minipatch

Full Algorithm

- **Step 1**. Fit minipatch learning predictor.
- **Step 2&3**. For each sample i, compute **LOO** and **LOCO-LOO** predictor by simple model averaging.
- **Step 4&5**. Construct the normal confidence interval.

Algorithm: LOCO for Minipatch

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Algorithmic advantages

- No **data-splitting** $\Rightarrow$ all available data is used for training a good predictive model and for powerful inference.
- **No model-refitting** $\Rightarrow$ once predictive model is trained, confidence intervals are computationally free!

Algorithm: LOCO for Minipatch

Algorithmic advantages

- No **data-splitting** $\Rightarrow$ all available data is used for training a good predictive model and for powerful inference.
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- An ensemble framework with **built-in** LOCO inference
- Once a minipatch ensemble is trained, almost no extra cost (data or computation) needed to get its own LOCO confidence intervals!
- As a comparison: *LOCO-Split require extra data set-aside for inference only, and model refitting for each feature of interest*.

Uncertainty Quantification for Feature Importance

Theoretical Guarantees

Theoretical Guarantees

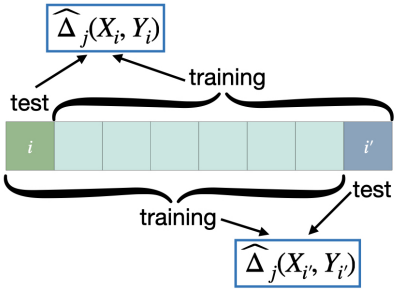
Does LOCO-MP confidence interval have valid coverage?

- Recall: our target $\Delta_j^*(\boldsymbol{X}, \boldsymbol{Y})$ is **a function of the models $\mu_{-j}(\cdot)$, $\mu(\cdot)$, trained by data $(\boldsymbol{X}, \boldsymbol{Y})$**.
- A selective inference problem. Common approaches: data-splitting; characterize statistic distribution conditioning on training (requires assumptions on data and model).
- Our approach: leave-one-observation-out, independent training and testing for each $\hat{\Delta}_j(X_i, Y_i)$.

Theoretical Guarantees

Does LOCO-MP confidence interval have valid coverage?

- However, dependency still exists amongst $\{\widehat{\Delta}_j(X_i, Y_i)\}_{i=1}^N$!
- $\widehat{\Delta}_j(X_i, Y_i)$ and $\widehat{\Delta}_j(X_{i'}, Y_{i'})$ switches i and i' for training and testing; share $N-2$ training samples.



Theoretical Guarantees

A1. $\mathrm{Error}(Y, \hat{Y})$ is Lipschitz w.r.t. prediction $\hat{Y}$.

A2. Average minipatch prediction is bounded (automatically hold for classification).

A3. Small MP: $n = o(\sqrt{N})$; If each base model is stable, this assumption can be further relaxed.

A4. Large number of MPs: $K \gg N \log N$

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Theorem

Suppose samples $(\boldsymbol{X}_i, Y_i)$ are i.i.d., and assumptions A1-A4 hold. Then

$$\lim_{N \to \infty} \mathbb{P}(\Delta_j^* \in \hat{\mathbb{C}}_j) = 1 - \alpha.$$

Valid asymptotic coverage under mild assumptions; applicable to any data distributions and base ML models.

Theoretical Guarantees

- **Algorithmic stability**: prediction is stable against change in one training sample.
- Stability facilitates statistical inference under dependency [Bayle et al., 2020]!

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- **Algorithmic stability**: prediction is stable against change in one training sample.
- Stability facilitates statistical inference under dependency [Bayle et al., 2020]!
- Minipatch ensembles are stable with any base model and any data distribution!
- Independent interest: stability also helps with conformal inference [Liang and Barber, 2023].

Extension: Beyond Tiny Minipatches

For better predictiveness, MP size should be carefully chosen.

- Relax minipatch size assumption: $n = o(\sqrt{N}) \to n << N/\log N$
- Data-driven tuning for minipatch size: train minipatch ensembles with a list of MP sizes; minimize the LOO error (easily computed).

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Inference still valid! As long as we add a buffer to the confidence interval width:

$$\max\left\{\frac{\hat{\sigma}_j}{\sqrt{N}}, c\sqrt{\widehat{\mathrm{stb}}}\frac{n\log N}{N}\right\},$$

$\widehat{\mathrm{stb}}$: an estimate of the base model stability using trained minipatches.

Uncertainty Quantification for Feature Importance

Simulations and Case Studies

Simulation Framework

- Data generation process:
  - Sparse linear model
  - Sparse additive, non-linear model
- $M = 50,\ N = 100, 200, \ldots, 2000.$

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- $m = 0.5M,\ n = N^{0.8},\ K = 10,000.$

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- Data generation process:
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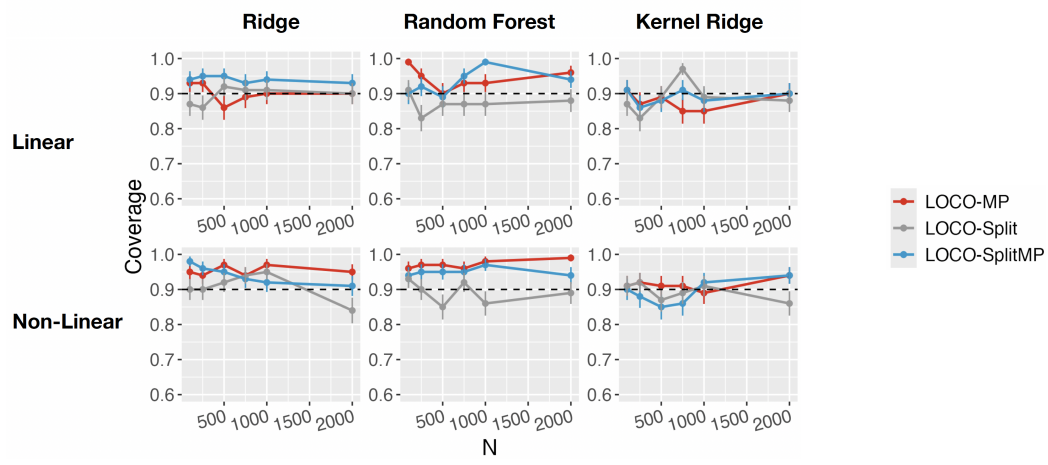
- $M = 50,\ N = 100, 200, \ldots, 2000.$
- Base model: ridge regression, decision tree, kernel ridge regression.
- $m = 0.5M,\ n = N^{0.8},\ K = 10,000.$
- Compare with the original LOCO method via data-splitting, where the trained models are
  - ridge, random forest, kernel ridge (LOCO-Split)
  - minipatch ensembles of these base models (LOCO-SplitMP)

Simulations: Validation of Theory

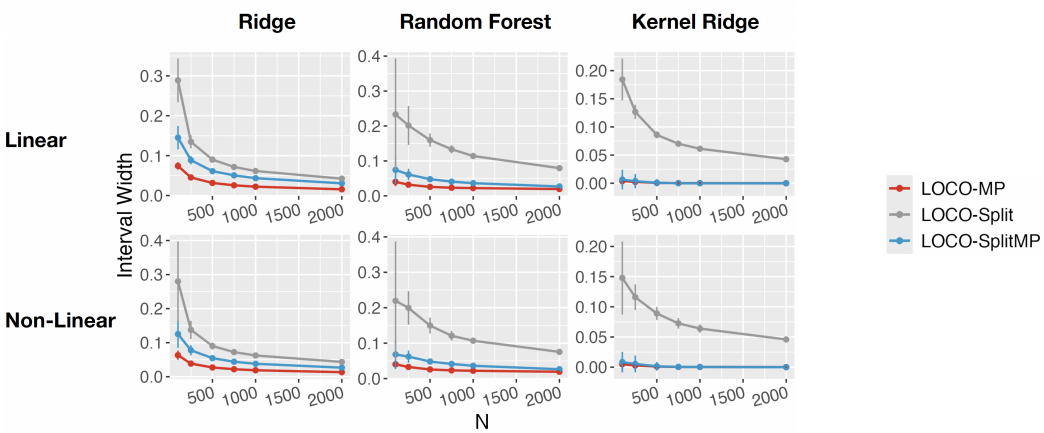
Regression, inference for a signal feature.



Asymptotically valid coverage.

Simulations: Validation of Theory

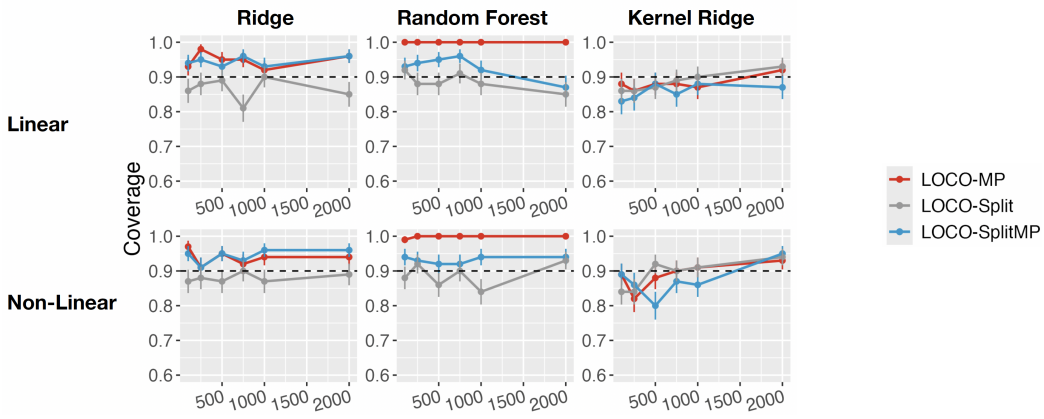
Regression, inference for a signal feature.



Width decreases as N increases; LOCO-MP has the smallest interval width.

Simulations: Validation of Theory

Regression, inference for a noise feature.



Slight over-coverage for random forest due to variance barrier.

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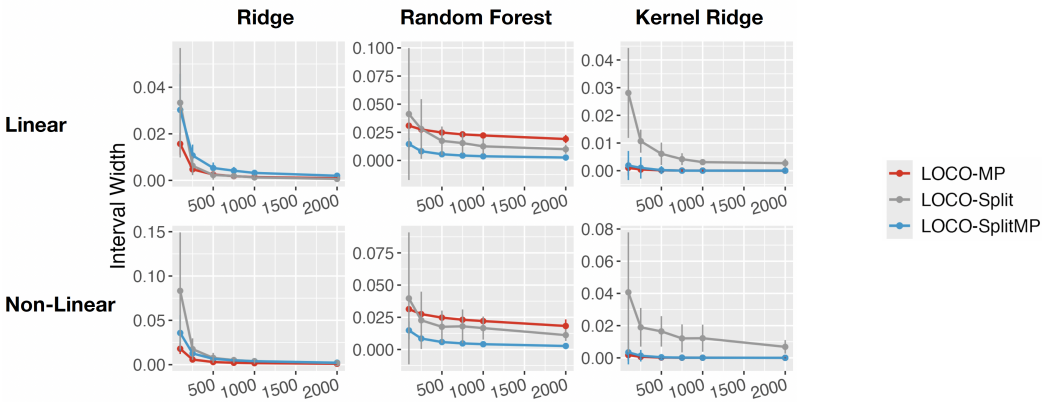
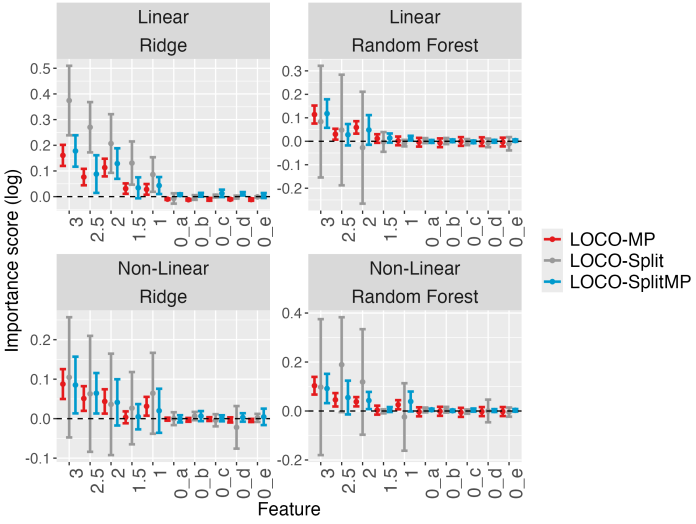
Regression, inference for a noise feature.



Slight over-coverage for random forest due to variance barrier.

Simulation: Comparative Study

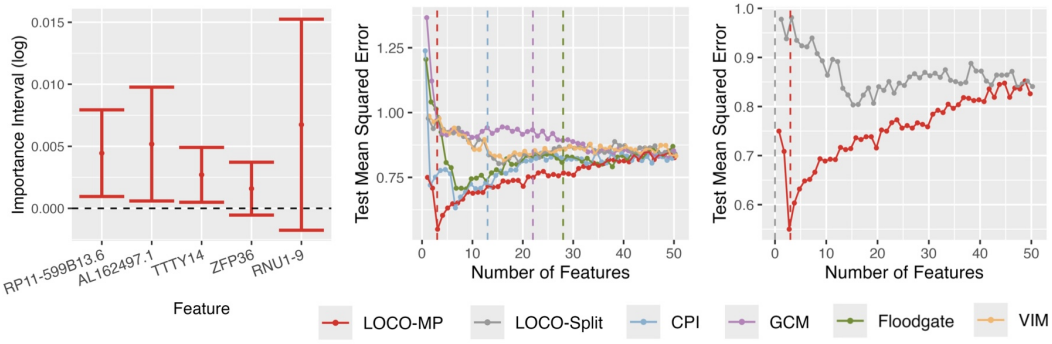
- $N = 200$
- Confidence intervals for features 1-10
- LOCO-Split fails to identify most signal features
- LOCO-MP has shorter intervals than LOCO-SplitMP



Real Data Example

- Religious Orders Study Memory and Aging Project (ROSMAP) data [Bennett et al., 2018]
- Response: cognition scores of 507 patients
- Features: 86 biomarkers with variance $>= 0.5$
- Compare with LOCO-Split, CPI [Watson and Wright, 2021], GCM [Shah and Peters, 2020], Floodgate [Zhang and Janson, 2020], VIM [Williamson et al., 2021]

Real Data Example

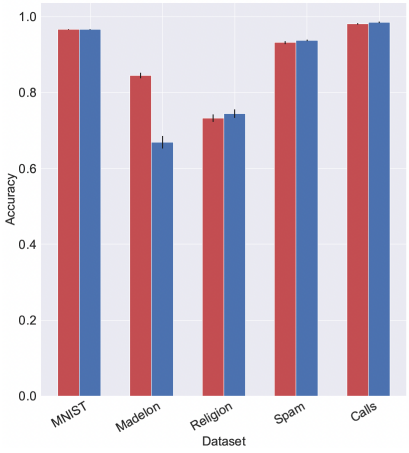


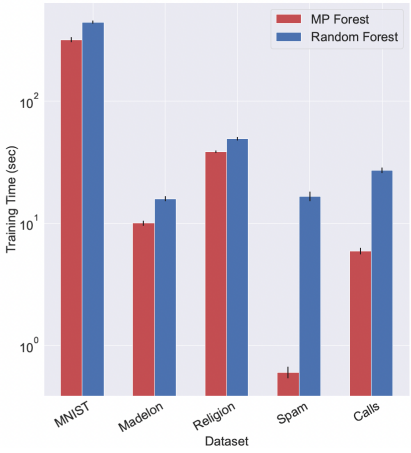
- LOCO-MP identify relevant biomarkers (supported by biomedical literature)
- Fit random forest with top k features and check prediction error on test set (**LOCO-MP selected the most informative features**)

Discussion and Conclusion

What is the Minipatch Learning Predictor?

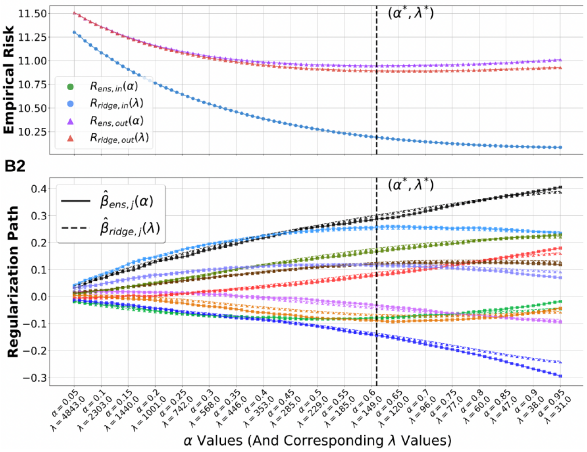
When base models are trees, Minipatch predictor is similar to random forest





What is the Minipatch Learning Predictor?

When base models are linear regression, Minipatch predictor is equivalent to ridge regression [LeJeune et al., 2020, Yao et al., 2021]



Minipatch Feature Importance vs. Population Feature Importance?

Special Case: Linear Model. For independent features,

- Δ_j^* concentrates around $\tilde{\Delta}_j^*$: $\tilde{\Delta}_j^* \asymp 2\gamma \left(\beta_j^{*2} - \frac{\|\beta^*_{\setminus j}\|_2^2}{M-1} \right)$ (with $\gamma = m/M$).
- Under assumptions on the minipatch size and number; valid coverage for $\tilde{\Delta}_j^*$.

Minipatch Feature Importance vs. Population Feature Importance?

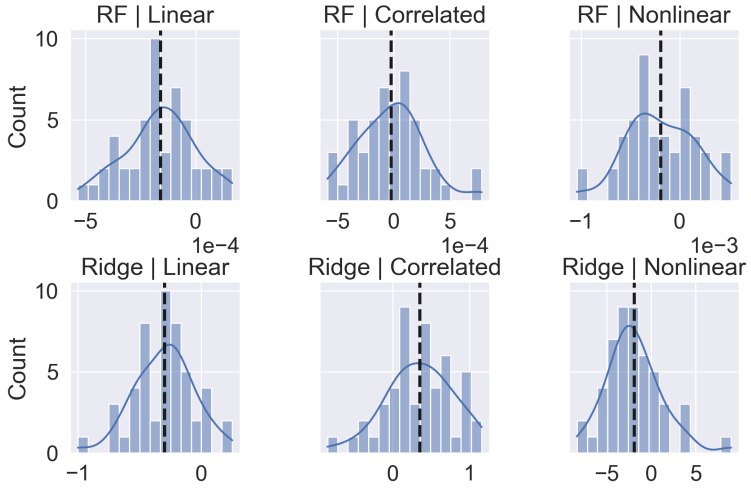
Special Case: Linear Model. For correlated features:

- When x_1 and x_2 have correlation $\rho \to 1$, we prove that $\Delta_1^* \to \Delta_2^*$ and are a function of $(\beta_1^* + \beta_2^*)^2$ for LOCO-MP.

As a comparison: original LOCO inference tends to miss correlated features.

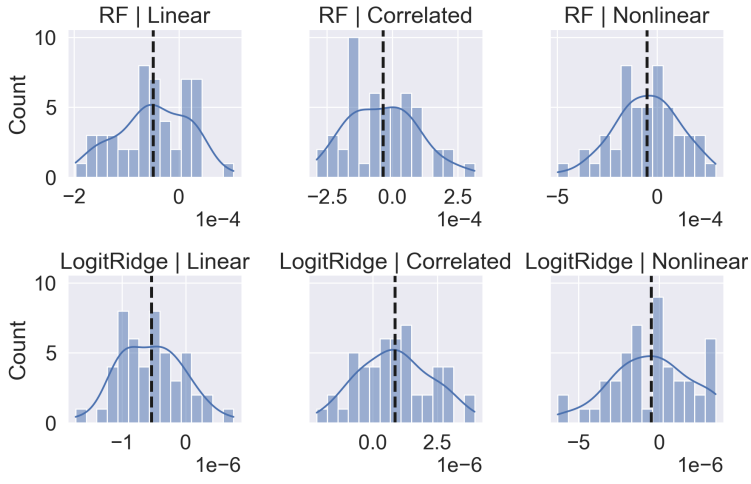
Minipatch Feature Importance vs. Population Feature Importance?

Histograms of the inference target for a noise feature in the regression setting



Minipatch Feature Importance vs. Population Feature Importance?

Histograms of the inference target for a noise feature in the classification setting



Extension to Hypothesis Testing

Recall: our inference target $\Delta_j^*(\boldsymbol{X}, \boldsymbol{Y})$ is a function of the data instead of a population quantity.

- $\mathcal{H}_0 : \Delta_j^*(\boldsymbol{X}, \boldsymbol{Y}) \leq 0$ is random event
- Directly inverting our confidence interval to hypotheis test guarantees:

$$\mathbb{P}(\text{We reject } \mathcal{H}_0 \,\&\, \mathcal{H}_0 \text{ is true}) \leq \alpha.$$

* Different from the conditional Type I error control in selective inference literature.

Conclusion

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  - Statistical efficiency: all data utilized for training & inference
  - Almost model-agnostic (within minipatch framework)
  - Assumption-light

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  - Extension to high-dimensional setting: selective inference for top features?
  - Strengthen the minipatch predictor via adaptive sampling?
  - Beyond tabular data?

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Conclusion

Paper: L. Gan*, **L. Zheng***, G. I. Allen (*: equal contribution), "Model-Agnostic Confidence Intervals for Feature Importance: A Fast and Powerful Approach Using Minipatch Ensembles", https://arxiv.org/abs/2206.02088. *Updated version coming soon!*

Thank you!

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