Interpretable Machine Learning

Feature Importances 1 Leave One Covariate Out (LOCO)

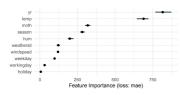


Figure: Bike Sharing Dataset

Learning goals

- Definition of LOCO
- Interpretation of LOCO

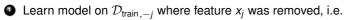


LOCO LEI_2018 TIBSHIRANI_2018

LOCO idea: Remove the feature from data, refit model on reduced data, and measure the loss in performance compared to model fitted on complete data.



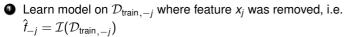
Definition: Given train and test data $\mathcal{D}_{\text{train}}$, $\mathcal{D}_{\text{test}} \subseteq \mathcal{D}$, a learner \mathcal{I} , and model $\hat{f} := \mathcal{I}(\mathcal{D}_{\text{train}})$, the LOCO importance for feat $j \in \{1, \dots, p\}$ is computed by:



$$\hat{f}_{-j} = \mathcal{I}(\mathcal{D}_{\mathsf{train},-j})$$



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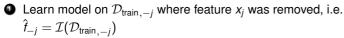


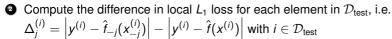


$$\Delta_j^{(i)} = \left| y^{(i)} - \hat{f}_{-j}(x_{-j}^{(i)}) \right| - \left| y^{(i)} - \hat{f}(x^{(i)}) \right| \text{ with } i \in \mathcal{D}_{\mathsf{test}}$$



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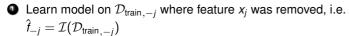


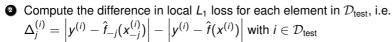


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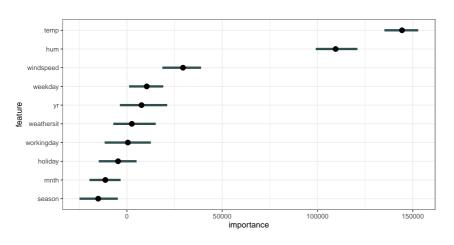
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$$\Delta_i$$
)

The method can be generalized to other loss functions and aggregations. If we use mean instead of median we can rewrite LOCO as

$$\mathsf{LOCO}_j = \mathcal{R}_{\mathsf{emp}}(\hat{f}_{-j}) - \mathcal{R}_{\mathsf{emp}}(\hat{f}).$$



BIKE SHARING EXAMPLE





- Trained random forest (default hyperparams) on 70% of bike sharing data
- Performance measure: mean squared error (MSE)
- Computed LOCO on test set for all features, measuring increase in MSE
- temp was most important: removal increased MSE by approx. 140.000

Interpretation: LOCO estimates the generalization error of the learner on a reduced dataset \mathcal{D}_{-j} .

Can we get insight into whether the ...

- feature x_j is causal for the prediction \hat{y} ?
 - In general, no, also because we refit the model (counterexample on the next slide)
- \bullet feature x_i contains prediction-relevant information?
 - In general, no (counterexample on the next slide)
- \bullet model requires access to x_i to achieve its prediction performance?
 - Approximately, it provides insight into whether the *learner* requires access to x_i



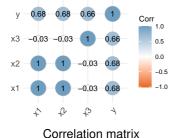
Example: Sample 1000 observations with

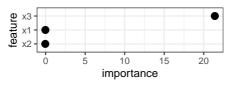
- $x_1, x_3 \sim N(0,5), x_2 = x_1 + \epsilon_2 \text{ with } \epsilon_2 \sim N(0,0.1)$
- $y = x_2 + x_3 + \epsilon$ with $\epsilon \sim N(0, 2)$
- Trained LM: $\hat{f}(x) = -0.02 1.02x_1 + 2.05x_2 + 0.98x_3$



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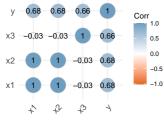


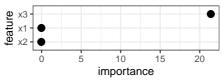
LOCO importance from LM trained on 70% of data, evaluated on remaining 30%



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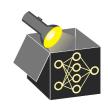




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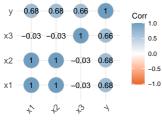
Correlation matrix

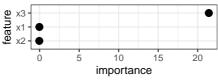
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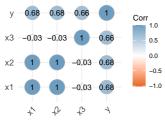
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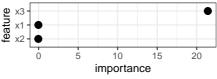
- \Rightarrow We cannot infer (1) from LOCO (e.g. LOCO₂ \approx 0 but coef. of x_2 is 2.05)
- \Rightarrow We also can't infer (2), e.g., $Cor(x_2, y) = 0.68$ but LOCO₂ ≈ 0



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- \Rightarrow We cannot infer (1) from LOCO (e.g. LOCO₂ \approx 0 but coef. of x_2 is 2.05)
- \Rightarrow We also can't infer (2), e.g., $Cor(x_2, y) = 0.68$ but LOCO₂ ≈ 0
- \Rightarrow We can get insight into (3): x_2 , x_1 highly corr. with LOCO₁ = LOCO₂ \approx 0

PROS AND CONS

Pros:

- Requires (only?) one refitting step per feature for evaluation
- Easy to implement
- Testing framework available in → Lei 2018

Cons:

- Provides insight into a learner on specific data, not a specific model
 - + for algorithm-level insight
 - for model-specific insights
- Model training is a random process and LOCO estimates can be noisy
 → Limits inference on model and data, or multiple refittings necessary?
- Requires re-fitting the learner for each feature
 - Computationally intensive compared to PFI

