Interpretable Machine Learning

Leave One Covariate Out (LOCO)

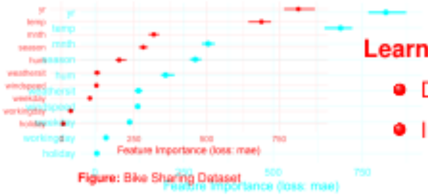

Figure: Bike Sharing Dataset

Learning goals

- Definition of LOCO
- Interpretation of LOCO

LEAVE ONE COVARIATE OUT (LOCO)

▸ Lei et al. (2018) ▸ Tibshirani (2018)

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

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Definition: Given training and test datasets $\mathcal{D}_{\text{train}}, \mathcal{D}_{\text{test}} \subseteq \mathcal{D}$, some $\mathcal{I}$ and a model $\hat{f} = \mathcal{I}(\mathcal{D}_{\text{train}})$. Then LOCO for a feature $j \in \{1, \dots, p\}$ can be computed as follows:

1. learn model on dataset $\mathcal{D}_{\text{train},-j}$ where feature x_j was removed, i.e. $\hat{f}_{-j} = \mathcal{I}(\mathcal{D}_{\text{train},-j})$

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2. compute the difference in local L_1 loss for each element in $\mathcal{D}_{\text{test}}$, i.e. $\Delta_j^{(i)} = \left|y^{(i)} - \hat{f}_{-j}(x_{-j}^{(i)})\right| - \left|y^{(i)} - \hat{f}(x^{(i)})\right|$ with $i \in \mathcal{D}_{\text{test}}$

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

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

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BIKE SHARING EXAMPLE

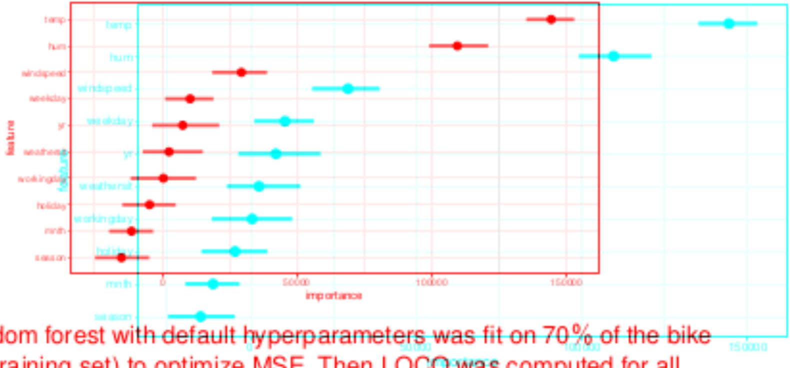

Figure: A random forest with default hyperparameters was fit on 70% of the bike sharing data (training set) to optimize MSE. Then LOCO was computed for all features on the test data. The temperature is the most important feature. Without access to `temp`, the MSE increases by approx. 140,000.

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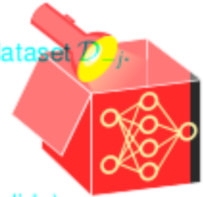
INTERPRETATION OF LOCO



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

Can we get insight into whether the ...

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

Interpretable Machine Learning – 3 / 5

INTERPRETATION OF LOCO

Example: Sample 1000 observations with

- $x_1, x_3 \sim N(0, 5)$
- $x_2 = x_1 + \epsilon_2$ with $\epsilon_2 \sim N(0, 0.1)$
- $y = x_2 + x_3 + \epsilon$ with $\epsilon \sim N(0, 2)$

$\Rightarrow$ Fitting a LM yields $\hat{f}(x) = -0.02 - 1.02x_1 + 2.05x_2 + 0.98x_3$

Interpretable Machine Learning – 4 / 5

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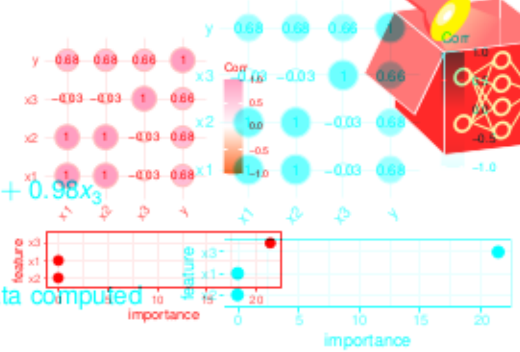

Top: Correlation matrix

Bottom: LOCO importance of LM fitted on 70% of the data computed on 30% remaining observations

Interpretable Machine Learning – 4 / 5

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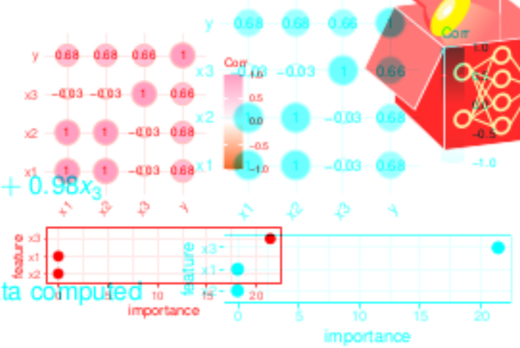

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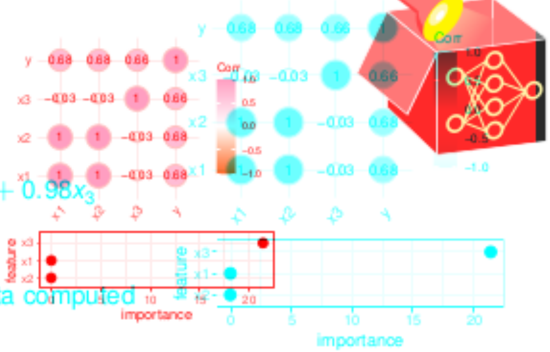

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$\Rightarrow$ We also can't infer (2), e.g., $Cor(x_2, y) = 0.68$ but $LOCO_2 \approx 0$

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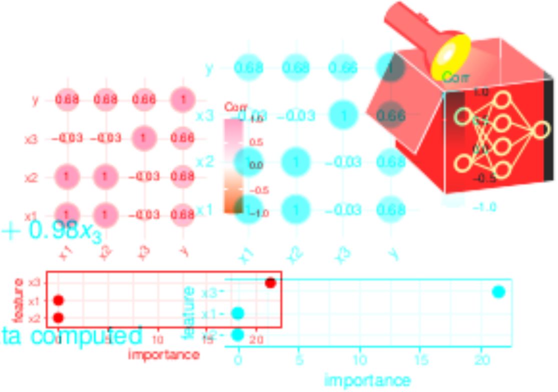

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$\Rightarrow$ We cannot infer (1) from LOCO (e.g. $\text{LOCO}_2 \approx 0$ but coefficient of x_2 is 2.05)
$\Rightarrow$ We also can't infer (2), e.g., $Cor(x_2, y) = 0.68$ but $\text{LOCO}_2 \approx 0$
$\Rightarrow$ We can get insight into (3): x_2 and x_1 highly correlated with $\text{LOCO}_1 = \text{LOCO}_2 \approx 0$
$\rightsquigarrow$ x_2 and x_1 take each others place if one of them is left out (not the case for x_3)

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PROS AND CONS

Pros:

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

Cons:

- Does not provide insight into a specific model, but rather a learner on a specific dataset
- Model training is a random process, so estimates can be noisy (which is problematic for inference about model and data)
- Requires re-fitting the learner for each feature → computationally intensive compared to PFI