Interpretable Machine Learning

Leave One Covariate Out (LOCO)



Figure: Bike Sharing Dataset



LOCO idea: Remove the feature from the dataset, refit the model on the reduced dataset LOCO idea: Bemove the feature from the dataset, refit the model on the reducedete dataset.

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complete dataset $\mathcal{D}_{\mathsf{train}}, \mathcal{D}_{\mathsf{test}} \subseteq \mathcal{D}$, some \mathcal{I} and a model $\hat{t} = \mathcal{I}$

Then LOCO for a feature $j \in \{1, ..., p\}$ can be computed as follows:

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

learn model on dataset D_{train,-i} where feature x_i was removed, i.e.

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

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- learn model on dataset $\mathcal{D}_{train,+}$ where feature x_i was removed. The state x_i was removed. $\hat{t} \stackrel{\downarrow 0}{\rightleftharpoons} \mathcal{I}(\mathcal{D}_{\text{train}}^{(i)} - \hat{f}_{-i}(x_{-i}^{(i)})) - |y^{(i)} - \hat{f}(x^{(i)})| \text{ with } i \in \mathcal{D}_{\text{test}}$
- **2** compute the difference in local L_1 loss for each element in \mathcal{D}_{test} , i.e.

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

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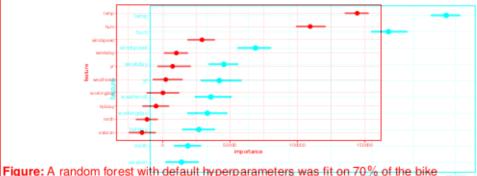
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- Devietd the importance score 4.0CO/the med (Δ/) ctions and aggregations. If we use mean instead of median we can rewrite LOCO as

The method can be generalized to other loss functions and aggregations. If we use mean instead of median we can rewrite COCO as $emp(f_{-j}) = \mathcal{R}_{emp}(f)$.

$$LOCO_j = \mathcal{R}_{emp}(\hat{t}_{-j}) - \mathcal{R}_{emp}(\hat{t}).$$

BIKE SHARING EXAMPLE





sharing data (training set) to optimize MSE. Then LOCO was computed for all features on the dest data. The temperature is the most important feature. Without sharing data (training access to themps the MSE increases by approxult 40,000 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: LOCO estimates the generalization terror of the flearner one a reduced luced dataset \mathcal{D}_{-j} .

Can we get insight into whether the ...

Can we get insight into whether the rediction \hat{y} ?

- feature x/gs.causal for the prediction x2 refit the model (counterexample on the next slide)
 - featin general, no also because we refit the model (counterexample on the next slide)
 in general, no (counterexample on the next slide)
- feature x, contains prediction-relevant information?
 - In general, no (counterexample on the next slide)
 Approximately, it provides insight into whether the learner requires access to x_i
- 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 ith

$$x_1, x_3 \sim N(0, 5)_5$$

•
$$x_{2} = x_{1} + \epsilon_{2}$$
 with $\epsilon_{2} \approx N(0,0,1).1$

•
$$y_y = x_2 + x_3 + \epsilon \text{ with } \epsilon \sim N(0/2), 2)$$

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

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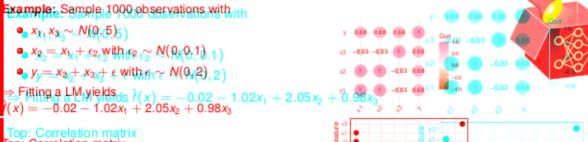
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Top: Correlation matrix

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





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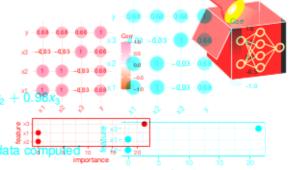
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$$y_y = x_{22} + x_{3x} + \epsilon$$
 with $\epsilon_1 \sim N(0, 2), 2)$

Fitting a LM yields
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⇒ We carried inter(1) from Loco (e.g. Loco 2 20 but coefficient of x2 is 2:05) 2.05)

 \Rightarrow We also can't infer (2), e.g., $cor(x, y) \neq 0.68$ but Loco ≈ 0

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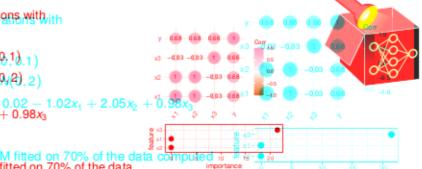
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$$y_y = x_{2} + x_{3} + \text{with}_{1} + \text{with}_{1} + \text{N}(0, 2), 2)$$

Fitting a LM yields
$$\hat{f}(x) = -0.02 - 1.02x_1 + 2.05x_2 + 0.98$$
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⇒ We carried inter(1) from Loco (e.g. Loco 2 20 but coefficient of x2 is 2:05) 2.05)

- \Rightarrow We also can't infer (2) (e.g., $Cor(x, v) \neq 0.68$ but LOCO ≈ 0
- \Rightarrow We can get insight into (3): $\frac{1}{2}$ and x_1 highly correlated with LOCO, $\frac{1}{2}$ LOCO, $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$
 - $\sim x_2$ and x_1 take each others place if one of them is left out (not the case for x_3)

PROS AND CONS

Pross:

- Requires (only?) one refitting step perfeature for evaluation tion
- Easy to implement nt
- Testing framework available in (n (a et al. (2018))



Consts:

- Does not provide insight into a specific model, but rather a dearner one a specific edition dataset
 dataset
 dataset
 dataset
- Model training is larrandom process, so estimates can be noisy (which is problematic for inference about model and data) e

 computationally intensive compared to PFI
- Requires re-fitting the learner for each feature → computationally intensive compared to PFI