Interpretable Machine Learning

Feature Importance

Leave One Covariate Out (LOCO)

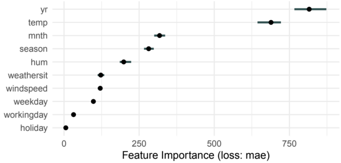
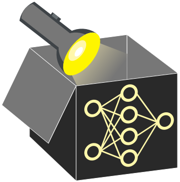


Figure: Bike Sharing Dataset

Learning goals

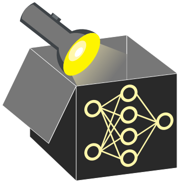
- Definition of LOCO
- Interpretation of LOCO

LOCO ▸ "Lei et al." 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.

LOCO ▸ "Lei et al." 2018 ▸ "Tibshirani" 2018

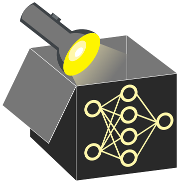


LOCO idea: Remove the feature from data, refit model on reduced data, and measure the loss in performance compared to model fitted on complete data.

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:

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

LOCO ▸ "Lei et al." 2018 ▸ "Tibshirani" 2018

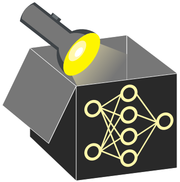


LOCO idea: Remove the feature from data, refit model on reduced data, and measure the loss in performance compared to model fitted on complete data.

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 $j \in \{1, \ldots, p\}$ is computed by:

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

LOCO ▸ "Lei et al." 2018 ▸ "Tibshirani" 2018



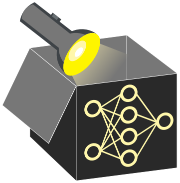
LOCO idea: Remove the feature from data, refit model on reduced data, and measure the loss in performance compared to model fitted on complete data.

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 $j \in \{1, \ldots, p\}$ is computed by:

1. Learn model on $\mathcal{D}_{\text{train},-j}$ where feature x_j was removed, i.e. $\hat{f}_{-j} = \mathcal{I}(\mathcal{D}_{\text{train},-j})$
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 $i \in \mathcal{D}_{\text{test}}$
3. Compute importance score by $\text{LOCO}_j = \text{med}\left(\Delta_j\right)$

LOCO

▸ "Lei et al." 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.

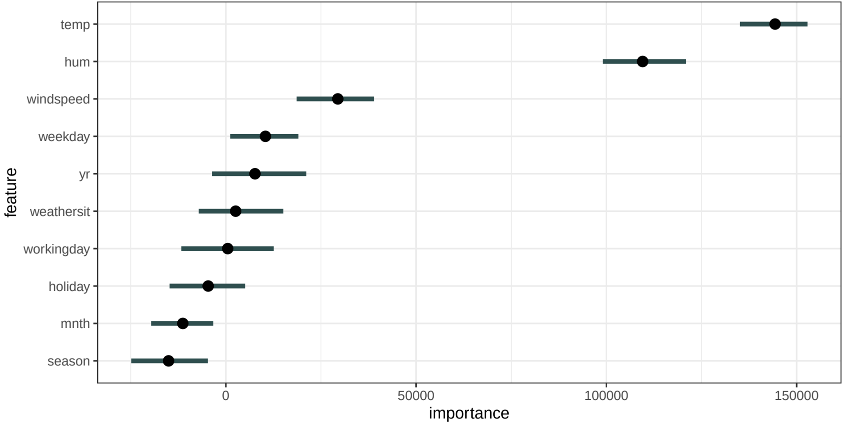
Definition: Given train and test data $\mathcal{D}_{\text{train}}, \mathcal{D}_{\text{test}} \subseteq \mathcal{D}$, a learner $\mathcal{I}$, and model $\hat{f} := \mathcal{I}(\mathcal{D}_{\text{train}})$, the LOCO importance for feat $j \in \{1, \ldots, p\}$ is computed by:

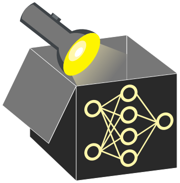
1. Learn model on $\mathcal{D}_{\text{train},-j}$ where feature x_j was removed, i.e. $\hat{f}_{-j} = \mathcal{I}(\mathcal{D}_{\text{train},-j})$
2. Compute the difference in local L_1 loss for each element in $\mathcal{D}_{\text{test}}$, i.e. $\Delta_j^{(i)} = \left|y^{(i)} - \hat{f}_{-j}(x_{-j}^{(i)})\right| - \left|y^{(i)} - \hat{f}(x^{(i)})\right|$ with $i \in \mathcal{D}_{\text{test}}$
3. Compute importance score by $\text{LOCO}_j = \text{med}\left(\Delta_j\right)$

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

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

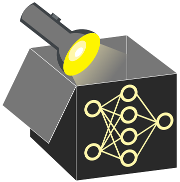
BIKE SHARING EXAMPLE





- 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 OF LOCO

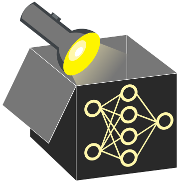


Interpretation: LOCO estimates the generalization error of the learner on a reduced dataset $\mathcal{D}_{-j}$.

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

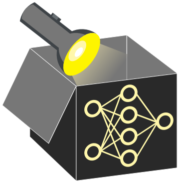
INTERPRETATION OF LOCO



Example: Sample 1000 observations with

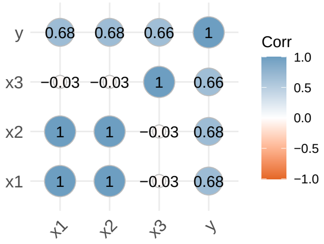
- $x_1, x_3 \sim N(0, 5)$, $x_2 = x_1 + \epsilon_2$ with $\epsilon_2 \sim N(0, 0.1)$
- $y = x_2 + x_3 + \epsilon$ with $\epsilon \sim N(0, 2)$
- Trained LM: $\hat{f}(x) = -0.02 - 1.02x_1 + 2.05x_2 + 0.98x_3$

INTERPRETATION OF LOCO

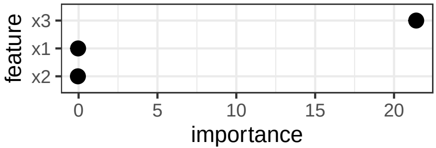


Example: Sample 1000 observations with

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



Correlation matrix

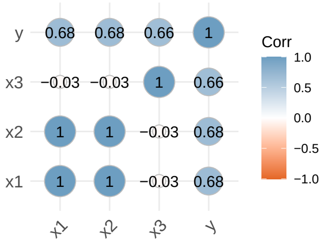


LOCO importance from LM trained on 70% of data, evaluated on remaining 30%

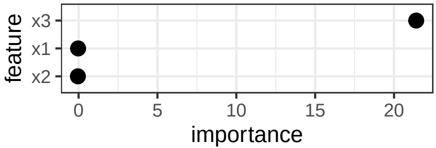
INTERPRETATION OF LOCO

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

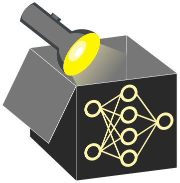


Correlation matrix

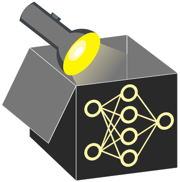


LOCO importance from LM trained on 70% of data, evaluated on remaining 30%

$\Rightarrow$ We cannot infer (1) from LOCO (e.g. $\text{LOCO}_2 \approx 0$ but coef. of x_2 is 2.05)

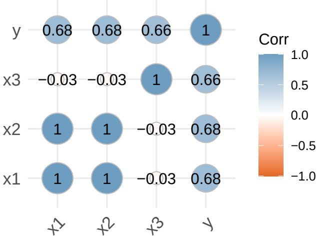


INTERPRETATION OF LOCO

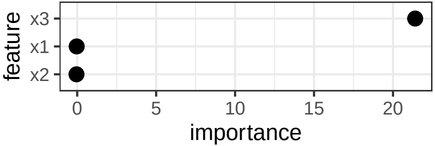


Example: Sample 1000 observations with

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



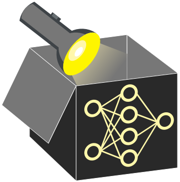
Correlation matrix



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

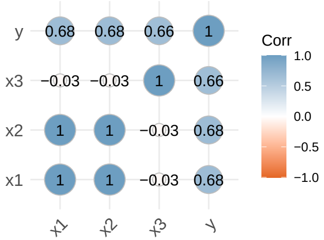
$\Rightarrow$ We cannot infer (1) from LOCO (e.g. $\text{LOCO}_2 \approx 0$ but coef. of x_2 is 2.05)
$\Rightarrow$ We also can't infer (2), e.g., $Cor(x_2, y) = 0.68$ but $\text{LOCO}_2 \approx 0$

INTERPRETATION OF LOCO

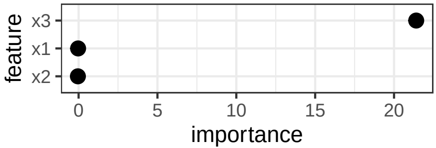


Example: Sample 1000 observations with

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



Correlation matrix



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

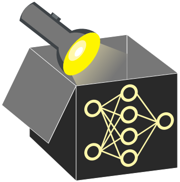
$\Rightarrow$ We cannot infer (1) from LOCO (e.g. $\text{LOCO}_2 \approx 0$ but coef. of x_2 is 2.05)

$\Rightarrow$ We also can't infer (2), e.g., $Cor(x_2, y) = 0.68$ but $\text{LOCO}_2 \approx 0$

$\Rightarrow$ We can get insight into (3): x_2, x_1 highly corr. 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 (unlike x_3)

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:

- 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
  $\rightsquigarrow$ Limits inference on model and data, or multiple refittings necessary?
- Requires re-fitting the learner for each feature
  $\rightsquigarrow$ Computationally intensive compared to PFI