

# Interpretable Machine Learning

## Permutation Feature Importance (PFI)

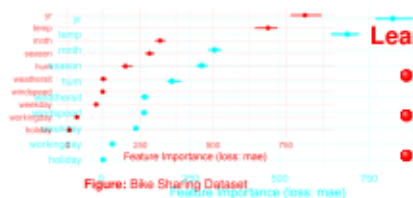


Figure: Bike Sharing Dataset

### Learning goals

- Understand how PFI is computed
- Understanding strengths and weaknesses
- Testing Importance

# PERMUTATION FEATURE IMPORTANCE (PFI) ► Breiman (2001)

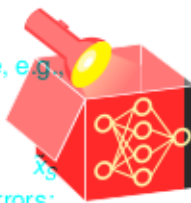
**Idea:** "Destroy" feat. of interest  $x_j$  by perturbing it, it becomes uninformative, e.g., randomly permute obs. in  $x_j$  (marginal distribution  $\mathbb{P}(x_j)$  stays the same).

PFI for features  $x_S$  using test data  $\mathcal{D}$ :

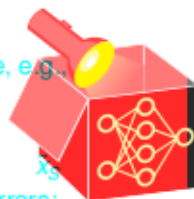
- Measure the error **without permuting feat.** and with **permuted feat. values  $\tilde{x}_S$**
- Repeat permuting the feat. (e.g.,  $m$  times) and **avg. the difference of both errors:**

$$\widehat{PFI}_S = \frac{1}{m} \sum_{k=1}^m \widehat{PFI}_S = \frac{1}{m} \sum_{k=1}^m (\mathcal{R}_{\text{emp}}(\hat{f}, \mathcal{D}_{(k)}) - \mathcal{R}_{\text{emp}}(\hat{f}, \mathcal{D})) \text{ where } \mathcal{R}_{\text{emp}}(\hat{f}, \mathcal{D}) = \frac{1}{n} \sum_{(x,y) \in \mathcal{D}} L(\hat{f}(x), y)$$

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# PERMUTATION FEATURE IMPORTANCE (PFI) Brüdermann (2001):1



**Idea:** "Destroy" feat. of interest  $x_S$  by perturbing it s.t. it becomes uninformative, e.g., randomly permute obs. in  $x_S$  (marginal distribution  $P(x_S)$  stays the same).

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$$\widehat{PFI}_S = \frac{1}{m} \sum_{k=1}^m \widehat{PFI}_S^{(k)} = \frac{1}{m} \left( \sum_{k=1}^m \mathcal{R}_{\text{emp}}(\hat{f}, \tilde{\mathcal{D}}_k^S) - \mathcal{R}_{\text{emp}}(\hat{f}, \mathcal{D}) \right) \text{ where } \mathcal{R}_{\text{emp}}(\hat{f}, \mathcal{D}) = \frac{1}{n} \sum_{(x,y) \in \mathcal{D}} L(\hat{f}(x), y)$$

The data  $\mathcal{D}$  where  $x_S$  is replaced with  $\tilde{x}_S^S$  is denoted as  $\tilde{\mathcal{D}}^S$ .  
Example of permuting feature  $x_S$  with  $S = \{1\}$  and  $m = 6$ :

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Example of permuting feature  $x_S$  with  $S = \{1\}$  and  $m = 6$ :

$\mathcal{D}$			$\tilde{\mathcal{D}}_{(1)}^S$			$\tilde{\mathcal{D}}_{(2)}^S$			$\tilde{\mathcal{D}}_{(3)}^S$			$\tilde{\mathcal{D}}_{(4)}^S$			$\tilde{\mathcal{D}}_{(5)}^S$			$\tilde{\mathcal{D}}_{(6)}^S$		
$x_1$	$x_2$	$x_3$	$x_1$	$x_2$	$x_3$	$x_1$	$x_2$	$x_3$	$x_1$	$x_2$	$x_3$	$x_1$	$x_2$	$x_3$	$x_1$	$x_2$	$x_3$	$x_1$	$x_2$	$x_3$
1	4	7	1	4	7	2	5	8	1	4	7	3	4	7	1	4	7	3	4	7
2	5	8	2	5	8	1	4	7	2	5	8	1	4	7	2	5	8	2	5	8
3	6	9	3	6	9	2	5	8	3	6	9	2	5	8	3	6	9	3	6	9

Note: The  $S$  in  $x_S$  refers to a Subset of features for which we are interested in their effect on the prediction.

Here: We calculate the feature importance for one feature at a time  $|S| = 1$ .

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# PERMUTATION FEATURE IMPORTANCE



$\tilde{\mathcal{D}}^S_{(k)}$        $\mathcal{D}$

$i$	$x_s$	$x_2$	$x_3$	$x_1$	$x_2$	$x_3$	$x_1$	$x_2$	$x_3$
1	2	4	7	4	1	7	4	7	1
2	1	5	8	5	2	8	5	8	2
3	3	6	9	3	6	9	3	6	9

**1. Perturbation:** Sample feature values from the distribution of  $x_s$  ( $P(X_s)$ ).

⇒ Randomly permute feature  $x_s$

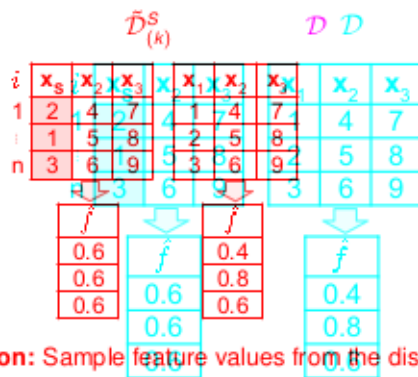
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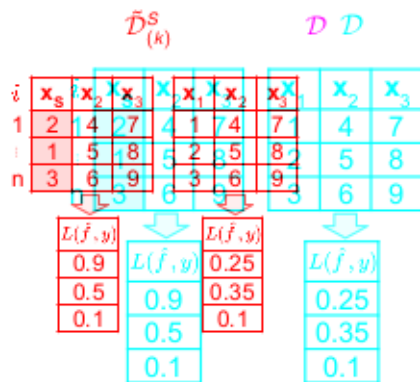
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- Compute the loss for each observation in both data sets
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# PERMUTATION FEATURE IMPORTANCE



$\tilde{\mathcal{D}}_{(k)}^S$        $\mathcal{D}$

	$x_{s_1}$	$x_{s_2}$	$x_{s_3}$	$x_{s_4}$	$x_{s_5}$	$x_{s_6}$	$x_{s_7}$	$x_{s_8}$	$x_{s_9}$	$\Delta L$
1	2	1	4	2	7	4	1	7	4	0.65
2	1	5	1	8	5	2	8	5	8	0.55
3	3	6	9	3	6	9	3	6	9	0

$L(\hat{f}, y)$		$L(\hat{f}, y)$
0.9	$L(\hat{f}, y)$	0.25
0.5	-	0.35
0.1		0.1

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# PERMUTATION FEATURE IMPORTANCE

$$\mathcal{R}_{\text{emp}}(\hat{f}(\tilde{D}_{(k)}^S)) - \mathcal{R}_{\text{emp}}(\hat{f}_p(\hat{D})|D)$$

i	$x_1$	$x_2$	$x_3$	$x_1$	$x_2$	$x_3$	$\Delta L$	$x_3$	$\Delta L$
1	2	1	4	2	1	4	0.65	7	0.65
2	1	5	1	5	2	8	0.15	8	0.267
3	3	6	9	3	6	9	0	9	0

$$= 0.267$$



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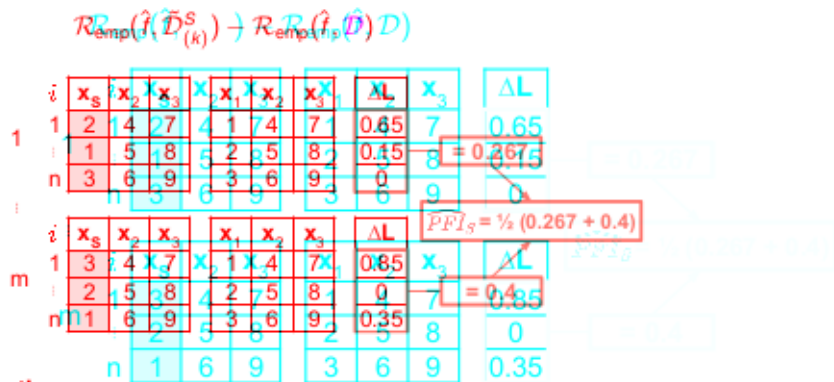
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- Compute the loss for each observation in both data sets
- Take the difference of both losses  $\Delta L$  for each observation
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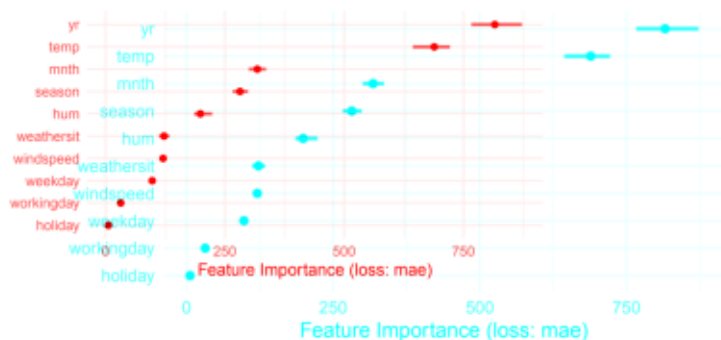
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## EXAMPLE: BIKE SHARING DATASET



### Interpretation:

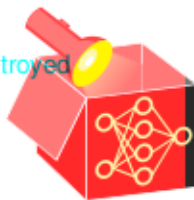
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- 5% and 95% quantile of repetitions due multiple permutations are shown as error bars
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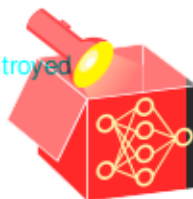
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- Interpretation: PFI is the increase of model error when feature's information is destroyed



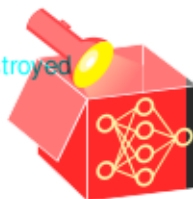
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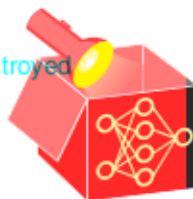
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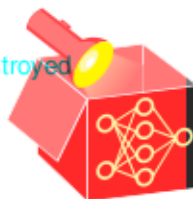
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## COMMENTS ON PFI-EXTRAPOLATION

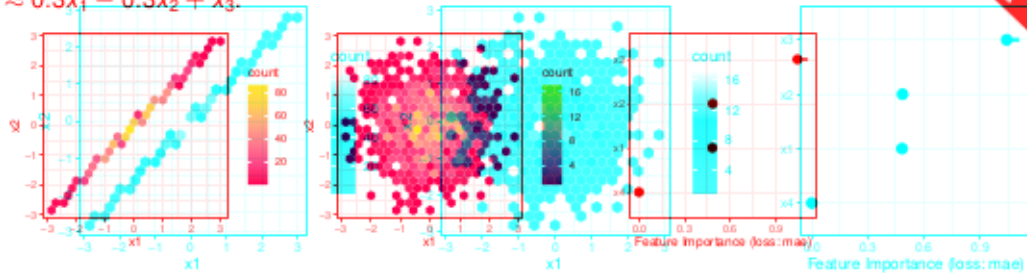
**Example:** Let  $y = x_3 + \epsilon_1$  with  $\epsilon_1 \sim N(0, 0.1)$  where  $x_1 := \epsilon_1$ ,  $x_2 := x_1 + \epsilon_2$  are highly correlated ( $\epsilon_1 \sim N(0, 1)$ ,  $\epsilon_2 \sim N(0, 0.01)$ ) and  $x_3 := \epsilon_3$  with  $\epsilon_3 \sim (0, 1)$ . All noise terms are independent. Fitting a LM yields  $\hat{f}(\mathbf{x}) \approx 0.3x_1 - 0.3x_2 + x_3$ .





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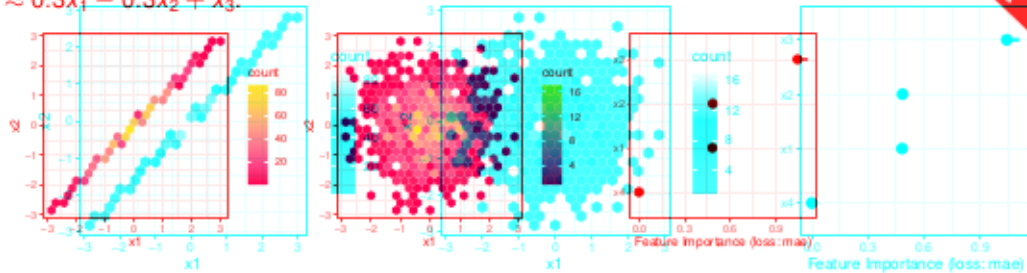


Hexbin plot of  $x_1, x_2$  before permuting  $x_1$  (left), after permuting  $x_1$  (center), and PFI

scores (right)

# COMMENTS ON PFI - EXTRAPOLATION

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Hexbin plot of  $x_1, x_2$  before permuting  $x_1$  (left), after permuting  $x_1$  (center), and PFI scores (right)  $\Rightarrow x_1$  and  $x_2$  should be irrelevant for the prediction  $\hat{f}(x)$  for

$\{x : P(x) > 0\}$  as  $0.3x_1 - 0.3x_2 \approx 0$   
 $\Rightarrow$  PFI evaluates model on unrealistic obs. outside  $P(x) \sim x$   $\rightarrow x_1, x_2$  are considered relevant (PFI > 0)

## COMMENTS ON PFI-INTERACTIONS

**Example:** Let  $x_1, x_2, \dots, x_4$  be independently and uniformly sampled from  $\{-1, 1\}$  and

$$y := x_1 x_2 + x_3 + \epsilon_y \text{ with } \epsilon_y \sim N(0, 1), y \sim N(0, 1)$$

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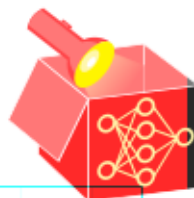
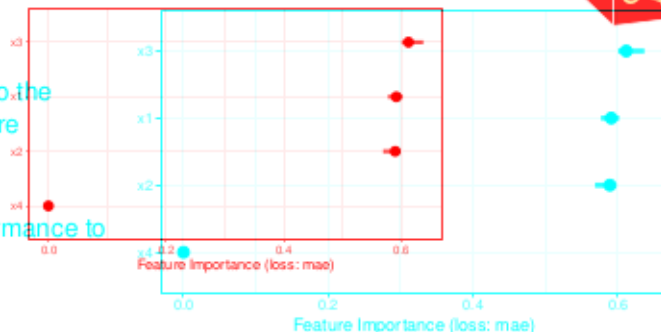
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Fitting a LM yields  $\hat{f}(x) \approx x_1 x_2 + x_3$ .

Although  $x_3$  alone contributes as much to the prediction as  $x_1$  and  $x_2$  jointly, all three are considered equally relevant.

⇒ PFI does not fairly attribute the performance to the individual features.



## COMMENTS ON PFI-TEST VS. TRAINING DATA

**Example:**  $x_1, x_1, \dots, x_{20}, y$  are independently sampled from  $U(-10, 10)$ . An  $xgb$  boost model with default hyperparameters is fit on a small training set of 50 observations. The model overfits heavily.



**Figure:** While PFI on test data considers all features to be irrelevant, PFI on train data exposes the features on which the model overfitted.

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**Figure:** While PFI on test data considers all features to be irrelevant, PFI on train data exposes the features on which the model overfitted.

Why? PFI can only be nonzero if the permutation breaks a dependence in the data. Spurious correlations help the model perform well on train data but are not present in the test data.  
⇒ If you are interested in which features help the model to generalize, apply PFI on test data.

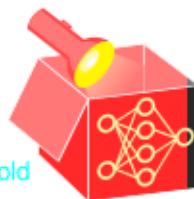
test data.

# IMPLICATIONS OF PFI

Can we get insight into whether the ...

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- $PFI_j \neq 0 \Rightarrow$  model relies on  $x_j$
- As the training vs. test data example demonstrates, the converse does not hold



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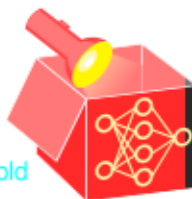
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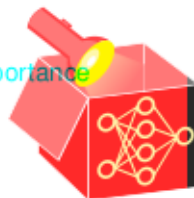
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# TESTING IMPORTANCE (PIMP)

Altman et al. (2010)

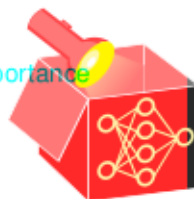
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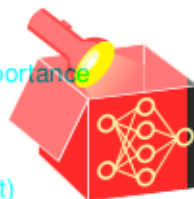
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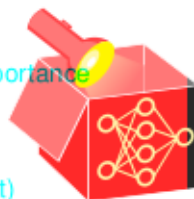


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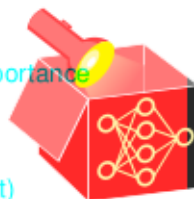
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  - Sampling under  $H_0$ : Permute target  $y$ , retrain model, compute PFI scores (repeat)
    - ⇒ Permuting  $y$  breaks relationship to all features
- Sampling under  $H_0$ : Permute target  $y$ , retrain model, compute PFI scores under  $H_0$  (repeat)
  - ⇒ Permuting  $y$  breaks relationship to all features
  - ⇒ By computing PFI scores again, we obtain distribution of PFI scores under  $H_0$



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  - (repeat)
  - Compute p-value - the tail probability under  $H_0$  - and use it as a new importance measure
    - ⇒ Permuting  $y$  breaks relationship to all features
    - ⇒ By computing PFI scores again, we obtain distribution of PFI scores under  $H_0$
- Compute p-value - the tail probability under  $H_0$  - and use it as a new importance measure

# TESTING IMPORTANCE (PIMP)

PIMP algorithm:

- 1 For  $m \in \{1, \dots, n_{\text{repetitions}}\}$ :
  - Permute response vector  $y$
  - Retrain model with data  $X$  and permuted  $y$
  - Compute feature importance  $PFI_j^m$  for each feature  $j$  (under  $H_0$ )



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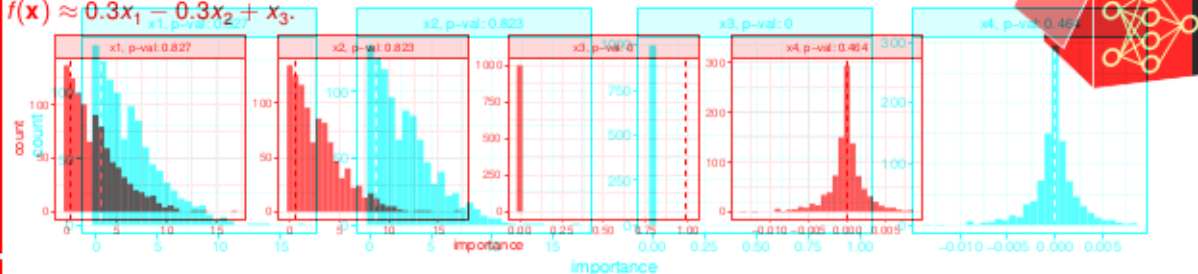
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- 2 Train model with  $X$  and unpermuted  $y$
- 3 For each feature  $j \in \{1, \dots, p\}$ :
  - Fit probability distribution of the feature importance values  $PFI_j^m, m \in \{1, \dots, n_{\text{repetitions}}\}$  ( $m \in \{1, \dots, n_{\text{repetitions}}\}$  choice between Gaussian, lognormal, gamma or non-parametric)
  - Compute feature importance  $PFI_j$  for the model without permutation of  $y$  (under  $H_1$ )
  - Compute the p-value of  $PFI_j$  for the model without permutation of  $y$  (under  $H_1$ )
  - Retrieve the p-value of  $PFI_j$  based on the fitted distribution

# PIMP FOR EXTRAPOLATION EXAMPLE

Recall:  $y = x_3 + \epsilon_y$  with  $\epsilon_y \sim N(0, 0.1)$ .  $x_1, x_2$  highly correlated but independent of  $y$ ,  $x_4$  is independent of  $y$  and all other variables. Fitting a LM yields  $\hat{f}(x) \approx 0.3x_1 - 0.3x_2 + x_3$ .

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- Histograms:  $H_0$  distribution of PFI scores after permuting  $y$  (1000 repetitions)
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- Red: PFI score estimated on unpermuted  $y$  (under  $H_1$ )  $\rightsquigarrow$  compare against  $H_0$  distribution
- Red: PFI score estimated on unpermuted  $y$  (under  $H_1$ )  $\rightsquigarrow$  compare against  $H_0$  distribution
- Results: Although PFI for  $x_1$  and  $x_2$  is nonzero (red), PIMP considers them not significantly relevant (p-value  $> 0.05$ )

# DIGRESSION: MULTIPLE TESTING PROBLEM

► Romano et al. (2010)

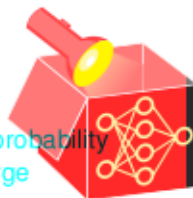
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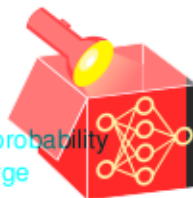
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- One classical method to control the FWE is the **Bonferroni correction** which rejects a null hypothesis if its p-value is smaller than  $\alpha/m$  with  $m$  as the number of performed parallel tests

