

Interpretable Machine Learning



Permutation Feature Importance (PFI)

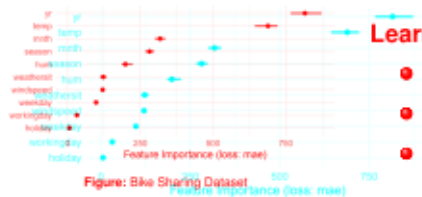


Figure: Bike Sharing Dataset

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Learning goals

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

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- Understanding strengths and weaknesses
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PERMUTATION FEATURE IMPORTANCE (PFI) Brüelmann (2001)

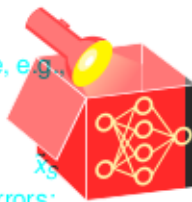
Idea: "Destroy" feat. of interest x_j by perturbing it s.t. it becomes uninformative, e.g., randomly permute obs. in x_j (marginal distribution $\mathbb{P}(x_j)$ stays the same).

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

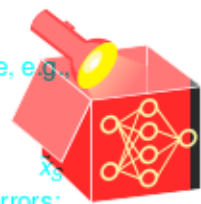
- Measure the error **without permuting feat.** and with **permuted feat. values \tilde{x}_S**
- Repeat permuting the feat. (e.g., m times) and avg. the difference of both errors:

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

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The data \mathcal{D} where x_S is replaced with \tilde{x}_S is denoted as $\tilde{\mathcal{D}}^S$ where $\mathcal{R}_{\text{emp}}(\hat{f}, \tilde{\mathcal{D}}^S) = \frac{1}{n} \sum_{(x,y) \in \tilde{\mathcal{D}}^S} L(\hat{f}(x), y)$
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 Example of permuting feature x_S with $S = \{1\}$ and $m = 6$:

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



	$\tilde{D}_{(k)}^S$						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	
2	1	5	8	5	2	8	5	8	
3	3	6	9	3	6	9	3	6	9

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

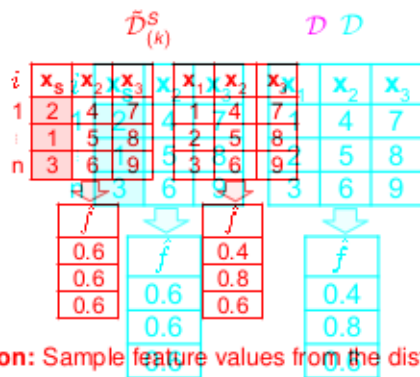
1. **Perturbation:** Sample feature values from the distribution of x_s ($P(X_s)$).

⇒ Randomly permute feature x_s

⇒ Replace original feature with permuted feature \tilde{x}_s and create data \tilde{D}^S containing \tilde{x}_s

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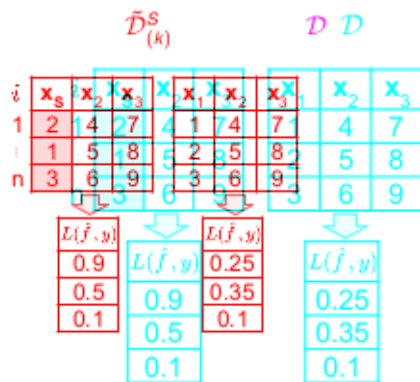
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PERMUTATION FEATURE IMPORTANCE



3. Aggregation:

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



	$\tilde{D}_{(k)}^S$			D			
i	x_{s_1}	x_{s_2}	x_{s_3}	x_{s_1}	x_{s_2}	x_{s_3}	ΔL
1	2	14	27	4	1	74	0.65
2	1	5	18	5	2	85	0.55
3	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

$L(\hat{f}, y)$

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PERMUTATION FEATURE IMPORTANCE

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

i	x_s	x_2	x_3	x_2	x_1	x_2	x_3	x_1	ΔL	x_3	ΔL
1	2	4	27	4	1	4	7	0.65	7	7	0.65
i	1	5	18	5	2	8	5	8	0.15	8	0.2675
n	3	6	9	6	3	6	9	9	0	9	0

= 0.267



3. Aggregation:

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- Compute the loss for each observation in both data sets
- Take the difference of both losses ΔL for each observation
- Average this change in loss across all observations

Note: This is equivalent to computing \mathcal{R}_{emp} on both data sets and taking the difference

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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_s	x_2	x_3	x_1	x_2	x_3	ΔL	x_3	ΔL
1	2	14	27	4	1	74	71	0.65	7
\vdots									
n	3	6	9	3	6	9	9	0	9
	n	3	6	9	3	6	9	0	0

i	x_s	x_2	x_3	x_1	x_2	x_3	ΔL	x_3	ΔL
1	3	4	7	1	4	7	8.5	7	0.85
\vdots									
n	1	6	9	3	6	9	9	0.35	8
	n	2	5	8	2	5	8	0	0
	n	1	6	9	3	6	9	0.35	0.35

$$PFI_s = \frac{1}{2} (0.267 + 0.4)$$

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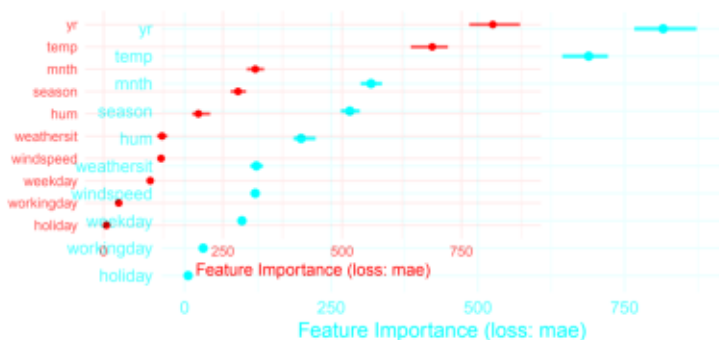
$$= 0.4$$

3. Aggregation:

3. Compute

- Compute the loss for each observation in both data sets
- Take the difference of both losses ΔL for each observation
- Average this change in loss across all observations
- Repeat perturbation and average over multiple repetitions
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EXAMPLE: BIKE SHARING DATASET



Interpretation:

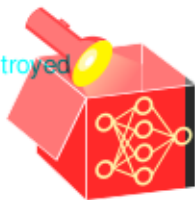
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- Destroying information about yr by permuting it increases mean absolute error of model by 816
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- 5% and 95% quantile of repetitions due multiple permutations are shown as error bars
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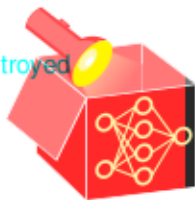
COMMENTS ON PFI

- Interpretation: PFI is the increase of model error when feature's information is destroyed



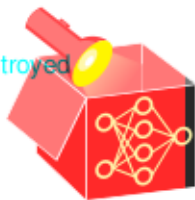
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⇒ Solution: Average results over multiple repetitions



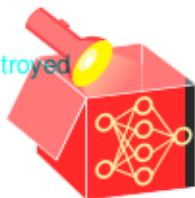
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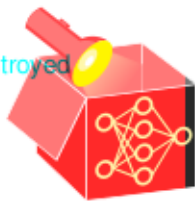


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 - $P(x_j, x_{-j}) \neq P(x_j)P(x_{-j})$ ⇒ Extrapolation issue
 - ⇒ Permutation also destroys information of interactions where permuted feature is involved
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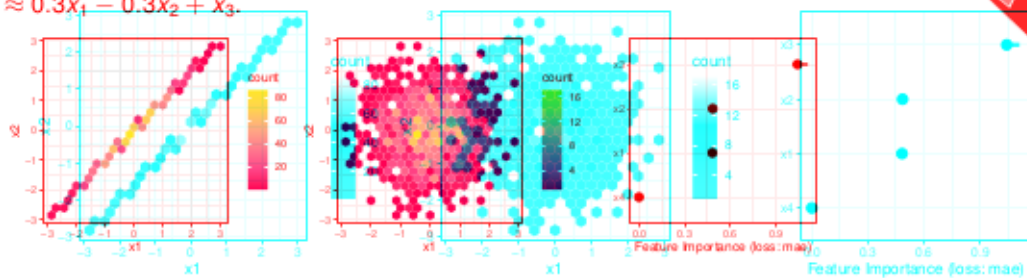
COMMENTS ON PFI-EXTRAPOLATION

Example: Let $y = x_3 + \epsilon_3$ with $\epsilon_3 \sim N(0, 0.1)$ where $x_1 = \epsilon_1$, $x_2 = x_1 + \epsilon_2$ are highly correlated highly correlated ($\epsilon_1 \sim N(0, 1)$, $\epsilon_2 \sim N(0, 0.01)$) and $x_3 = \epsilon_3$ with $\epsilon_3 \sim \epsilon_4$ with $(0, 1)$. All noise terms are independent. Fitting a LM yields $\hat{f}(x) \approx 0.3x_1 - 0.3x_2 + x_3$.



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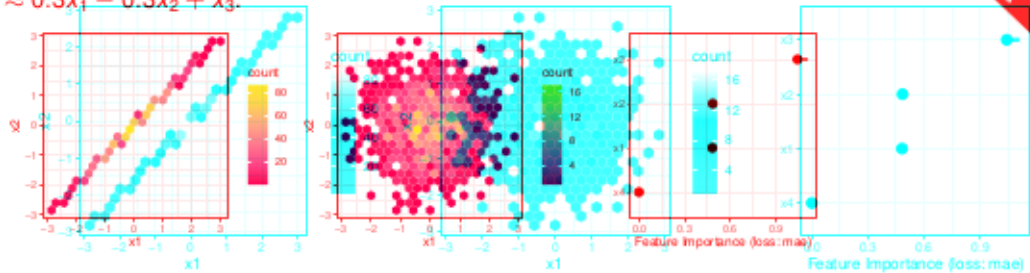


Hexbin plot of x_1, x_2 before permuting x_1 (left), after permuting x_1 (center), and PFI

scores (right)

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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 $P(x) \rightsquigarrow x_1, x_2$ 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

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

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



COMMENTS ON PFI- INTERACTIONS

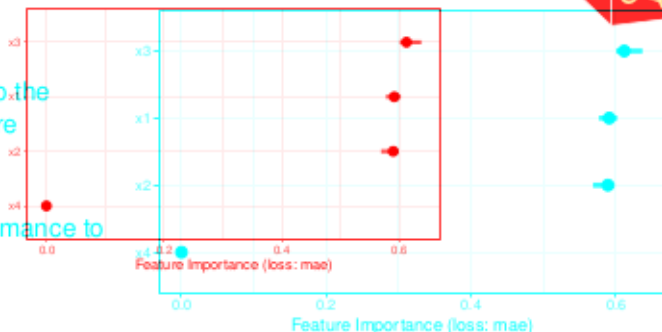
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Fitting a LM yields $\hat{f}(x) \approx x_1 x_2 + x_3$.

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

\Rightarrow 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 $xgboost$ model with default hyperparameters is fit on a small training set of 50 observations. The model overfits heavily.

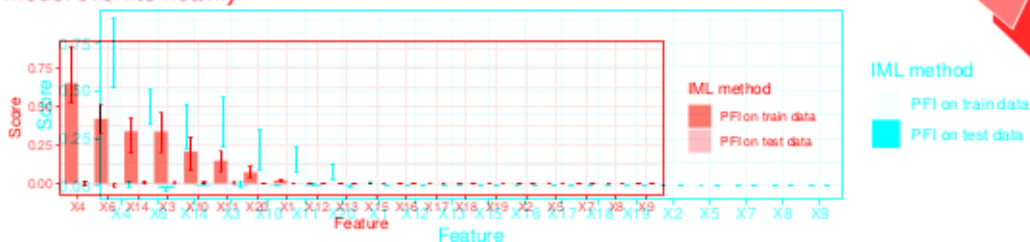


Figure: While PFI on test data considers all features to be irrelevant, PFI on train data exposes the features on which the model overfitted.

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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.

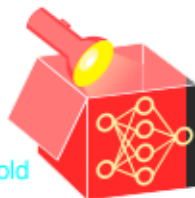
test data.

IMPLICATIONS OF PFI

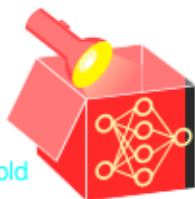
Can we get insight into whether the ...

1 feature x_j is causal for the prediction?

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



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- x_j is not exploited by model (regardless of whether it is useful for y or not) $\Rightarrow PFI_j = 0$

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- As the extrapolation example demonstrates, such insight is not possible $\Rightarrow PFI_j = 0$

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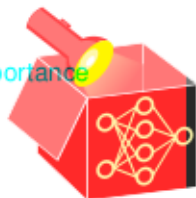
TESTING IMPORTANCE (PIMP) Altmann et al. (2010)

- PIMP was originally introduced for random forest's built-in permutation feature importance

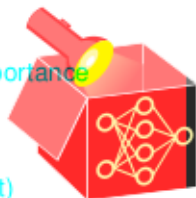


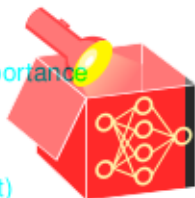
TESTING IMPORTANCE (PIMP) Altmann et al. (2010)

- PIMP was originally introduced for random forest's built-in permutation feature importance
- PIMP investigates whether the PFI score **significantly** differs from 0
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⇒ Useful because PFI can be non-zero due to stochasticity

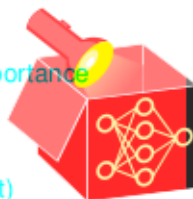


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 - ⇒ Useful because PFI can be non-zero due to stochasticity
- PIMP tests the H_0 -hypothesis: Feature is independent of the target y (unimportant)
 - Sampling under H_0 : Permute target y , retrain model, compute PFI scores (repeat)
 - ⇒ Permuting y breaks relationship to all features
- Sampling under H_1 : 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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 - Compute p-value - the tail probability under H_0 - and use it as a new importance measure
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TESTING IMPORTANCE (PIMP)

PIMP algorithm:

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



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 RF_j^{perm} for each feature j (under H_0)
- 2 Train model with X and unpermuted y

TESTING IMPORTANCE (PIMP)



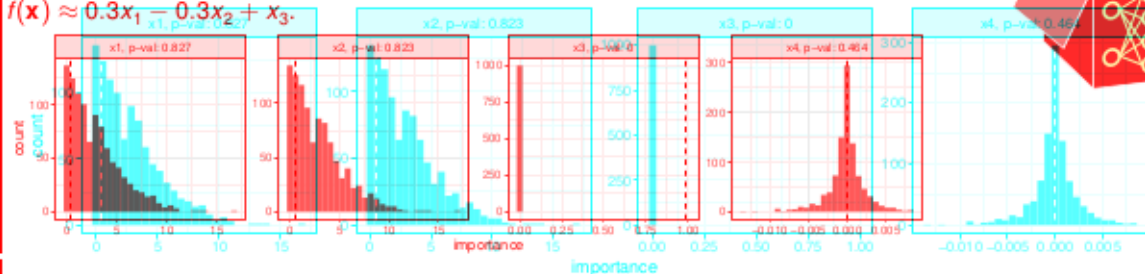
PIMP Algorithm:

- 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)
- 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 choice between Gaussian, lognormal, gamma or non-parametric)
 - Compute feature importance 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 $\epsilon_y \sim N(0, 0.01)$, x_1, x_2 highly correlated but independent of y , x_3 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
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- Results: Although PFI for x_1 and x_2 is nonzero (red), PIMP considers them not significantly relevant (p-value > 0.05)

▶ Romano et al. (2010)

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 - The larger the number of features, the more tests need to be performed by PIMP, the probability that some of the true H_0 -hypothesis is rejected (type-I error) by chance may be large
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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 α/m with m as the number of performed parallel tests

