

Interpretability methods in AI and a comparison with sensitivity analysis

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Outline

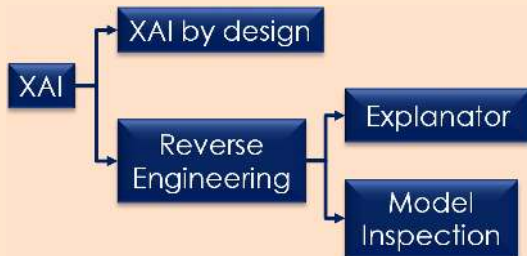
- 1 Introduction
- 2 Feature Importance
 - Pairwise Comparison in Decision
 - Absolute Assessment In Decision
 - In Machine Learning
 - In Sensibility Analysis
- 3 Extension on trees
 - Context
 - axiomatic characterization
- 4 Conclusion

Why shall we explain decisions?

Why is “explaining” important?

- Man-Machine Interaction: Increase acceptance & trust of user
- Trustable AI: Validation and qualification for safety-critical systems

Taxonomy of XAI [Guidotti et al'18]

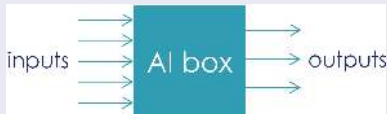


Explanation by Feature Attribution

Aim

Feature Attribution:

- Given an AI box with inputs and outputs,
- identify the input variables that mostly influence the outputs.
- Done by calculating the impact level of each input variable on the outputs.



Scope: numerical functions

- Filter relevant information/motivation to be presented to the user;
- Debugging mode in Machine Learning (inputs = features).

Decision setting

Decision setting

- $N = \{1, \dots, n\}$: index set of attributes/features.
- X_i : set of values representing attribute i (for $i \in N$).
- $X = X_1 \times \dots \times X_n$: set of alternatives/acts.
- $U : X \rightarrow \mathbb{R}$: utility representing preferences of decision maker over X
 - $U(y) > U(x)$: y is preferred to x
- Decision problems:
 - Selection: find the best element in $\mathcal{X} \subseteq X$
 - Ranking: order the elements of $\mathcal{X} \subseteq X$
 - Scoring: assign a score to each element of $\mathcal{X} \subseteq X$
 - Sorting: assign each element of $\mathcal{X} \subseteq X$ to a class \mathcal{C}

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Why shall we explain decisions?

A simple example

Function of 3 binary variables:

$$u(x_1, x_2, x_3) = \max(x_1, x_2, x_3) + 4 \max(x_2, x_3) + 2 \min(x_2, x_3)$$

How to explain the difference between

- $x = (0, 0, 0)$, with $u(x) = 0$
- and $y = (1, 1, 1)$, with $u(y) = 7$?

A simple problem? NO!

- A simple Gradient does not work
 - it is unstable!
- Figures shall have a meaning
- There are interactions among the inputs

Idea

Idea of the approach

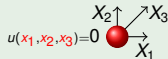
- How to isolate the contribution of each input variable?
- Assess the influence of a criterion in the evaluation of two alternatives x, y
- by looking at alternatives obtained by replacing subsets of values of y with values of x .

A simple example

Function of 3 binary variables, with $x = (0, 0, 0)$ and $y = (1, 1, 1)$:

$$u(x_1, x_2, x_3) = \max(x_1, x_2, x_3) + 4 \max(x_2, x_3) + 2 \min(x_2, x_3)$$

$$\bullet 7 = u(y_1, y_2, y_3)$$


$$u(x_1, x_2, x_3) = 0$$

Idea

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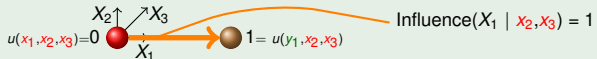
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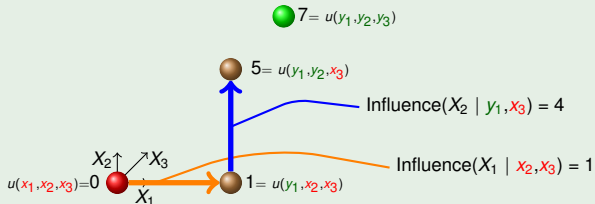
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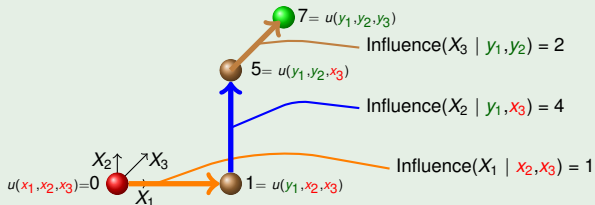
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Idea

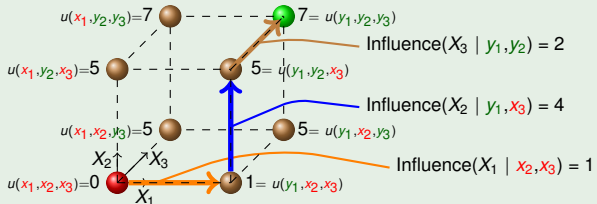
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Idea

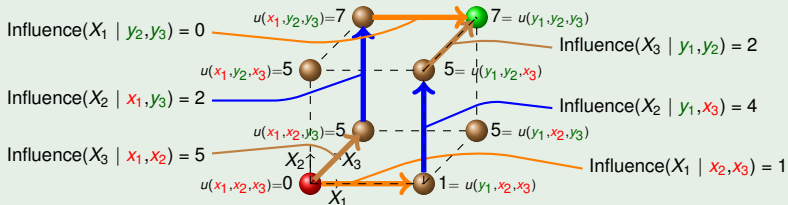
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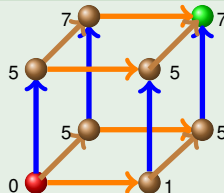
Conversion to Cooperative Game Theory

Feature attribution

	Game Theory	Decision
N	players	attributes
$v : 2^N \rightarrow \mathbb{R}$	game, with $v(\emptyset) = 0$	$v(S) = u(y_S, x_{N \setminus S}) - u(x)$
$\phi \in \mathbb{R}^N$	imputation	feature importance
Efficiency	$\sum_{i \in N} \phi_i = v(N) - v(\emptyset)$	

A simple example

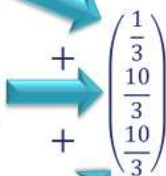
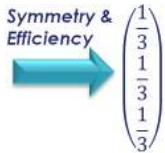
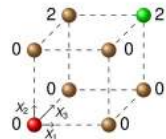
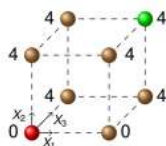
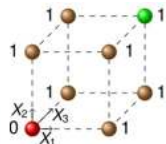
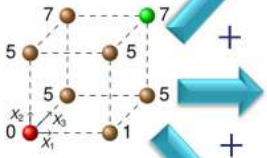
- Approach 1: $\phi_i = \frac{v(N)}{n}$
 $\phi = (7/3, 7/3, 7/3)$
- Approach 2: $\phi_i = v(\{i\}) - \frac{v(N) - \sum_k v(\{k\})}{n}$
 $\phi = (-1/3, 11/3, 11/3)$
- Approach 3: $\phi_i = \frac{1}{2^n - 1} \sum_{S \subseteq N \setminus \{i\}} (v(S \cup \{i\}) - v(S))$
 $\phi = (1/4, 13/4, 13/4)$



Axioms

$$u(x_1, x_2, x_3) = \max(x_1, x_2, x_3) + 4 \max(x_2, x_3) + 2 \min(x_2, x_3)$$

Linearity



Characterization result

Characterization of the Shapley value [Shapley'53]

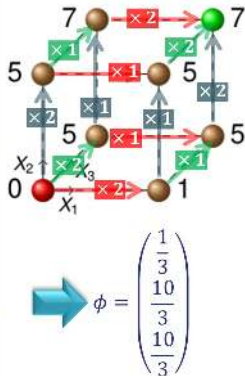
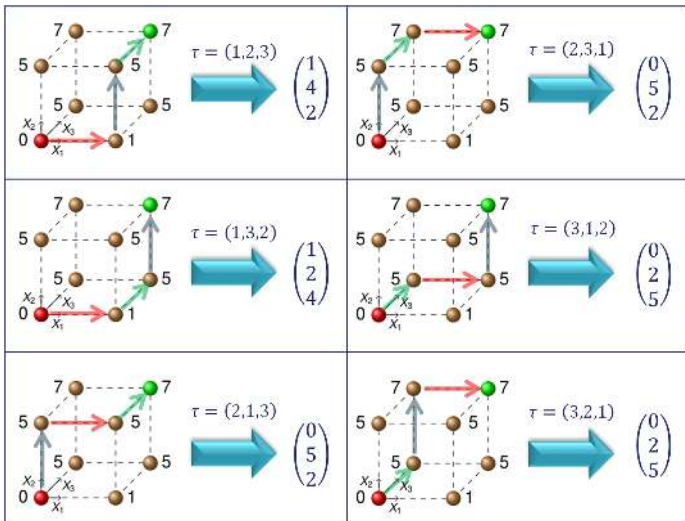
There is only one imputation ϕ which satisfies to the following properties:

- Additivity: $\phi_i(N, v + w) = \phi_i(N, v) + \phi_i(N, w)$,
- Null player: if $v(S \cup \{i\}) = v(S)$ for all $S \subseteq N \setminus \{i\}$, then $\phi_i(N, v) = 0$,
- Symmetry: $\phi_{\pi k}(\pi N, \pi v) = \phi_k(N, v)$ for every permutation π on N ,
- Efficiency: $\sum_{i \in N} \phi_i(N, v) = v(N)$.

It is equal to:

$$\begin{aligned} \phi_i(N, v) = \text{Sh}_i(N, v) &:= \frac{1}{n!} \sum_{\tau \in \Pi(N)} \left[v(\{\tau(1), \dots, i\}) - v(\{\tau(1), \dots, \tau(\tau^{-1}(i) - 1)\}) \right] \\ &= \sum_{S \subseteq N \setminus i} \frac{(n - |S| - 1)! |S|!}{n!} [v(S \cup \{i\}) - v(S)]. \end{aligned}$$

Shapley value



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Absolute Assessment In Decision

Basic Idea

Compare x to a reference r (e.g. expectation from user).

Drowning effect

Function $u(x_1, x_2) = \min(x_1, x_2)$, with $x = (0.2, 0.8)$.

Choice of reference r :

- $r = (0, 0)$ vs. x :

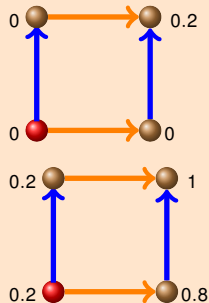
$$\phi_1 = \phi_2 = \frac{1}{2} \min(x_1, x_2) = 0.1$$

Same importance for the two attributes $\forall x_1, x_2!$

- x vs. $r = (1, 1)$:

$$\phi_1 = \frac{1}{2} [1 - x_1 + x_2 - \min(x_1, x_2)] = 0.7$$

$$\phi_2 = \frac{1}{2} [1 - x_2 + x_1 - \min(x_1, x_2)] = 0.1$$



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Feature attribution in Machine Learning

Notation

- \mathcal{D} : distribution of elements $x \in X$.
- $\mathcal{D}^{\text{JM}} = \prod_{i=1}^n \mathcal{D}_i^{\text{JM}}$, $\mathcal{D}_i^{\text{JM}}$ has the same marginal distribution than \mathcal{D} over variable i
- \mathcal{U} : uniform distribution.

How to define the game? [Merrick, Taly'20] [Kumar et al'20]

Feature Attribution:

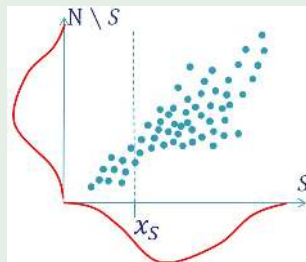
- **Interventional distribution:**
 - KernelSHAP [Lundberg, Lee'17]:

$$v(S) = \mathbb{E}_{R \sim \mathcal{D}} [u(x_S, R_{N \setminus S})] - \mathbb{E}_{R \sim \mathcal{D}} [u(R)]$$
 - QII [Datta et al'16]:

$$v(S) = \mathbb{E}_{R \sim \mathcal{D}^{\text{JM}}} [u(x_S, R_{N \setminus S})] - \mathbb{E}_{R \sim \mathcal{D}^{\text{JM}}} [u(R)]$$
 - IME [Strumbelj et al'10]:

$$v(S) = \mathbb{E}_{R \sim \mathcal{U}} [u(x_S, R_{N \setminus S})] - \mathbb{E}_{R \sim \mathcal{U}} [u(R)]$$
- **Conditional distribution:** SHAP [Lundberg, Lee'17], TreeSHAP [Lundberg et al'18]

$$v(S) = \mathbb{E}_{R \sim \mathcal{D}} [u(x_S, R_{N \setminus S}) | R_S = x_S] - \mathbb{E}_{R \sim \mathcal{D}} [u(R)]$$



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Shapley value in Sensibility Analysis

When variables are independent

- Functional ANOVA of $Y = u(X)$:

$$u(x) = \sum_{A \subseteq N} u_A(x_A), \quad u_A(x_A) = \sum_{B \subseteq A} (-1)^{|A \setminus B|} \mathbb{E}_{N \setminus B}(u | x_B)$$

$$\text{Var}(Y) = \sum_{A \subseteq N} \text{Var}_A(u_A(x_A))$$

- Sobol index $S_A = \frac{\text{Var}_A(u_A(x_A))}{\text{Var}(Y)}$, with $\sum_{A \subseteq N} S_A = 1$.

When variables are dependent [Owen'14]

- $\sum_{A \subseteq N} S_A \neq 1$
- Game (with $v(\emptyset) = 0$ and $v(N) = 1$)

$$v(A) = \frac{\text{Var}_A[\mathbb{E}_{N \setminus A}(Y | X_A)]}{\text{Var}(Y)}$$

- Contribution of variable i in $\text{Var}(Y)$

$$\text{Sh}_i(N, v)$$

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Example of application

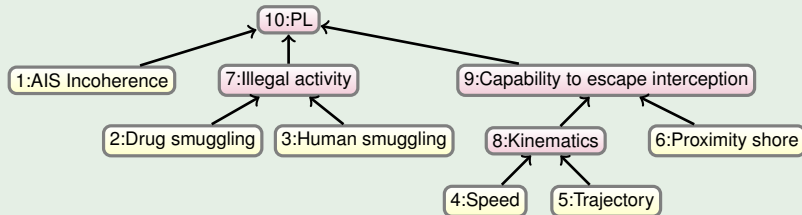
Maritime Patrol

Mission of Maritime Patrol:

- monitor a maritime area,
- and seek for illegal activity.
- \Rightarrow It evaluates in real time a Priority Level (PL) associated to each ship in this area



PL is intrinsically based on multiple criteria:



Hierarchical evaluation

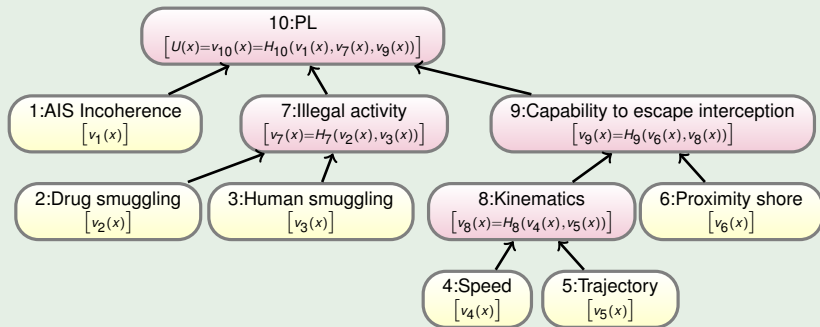
Maritime Patrol

8. Kinematics: $8 \approx 4 \wedge 5$: $v_8(x) = 0.3v_4(x) + 0.7v_4(x) \wedge v_5(x)$

- Complementarity & Speed slightly more important

10. $10 \approx 9 \wedge (1 \vee 7)$: $U(x) = v_{10}(x) = (v_1(x) \vee v_7(x) + v_1(x) \wedge v_9(x) + v_7(x) \wedge v_9(x)) / 3$

- There is suspicion of illegal activity when either 1 or 7 are satisfied;
- We also need to have a risk of missed interception to get high PL;



Why not using the standard Shapley value?

Shapley value approach on trees

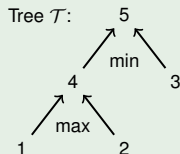
- Use the Shapley value on the leaves
- Use a recursive formulae otherwise: $l_i(x, y) = \sum_{j \in C(i)} l_j(x, y)$

Illustration

Comparison between $x = (0, 0, 0)$ and $y = (1, 1, 1)$.

Use of Shapley value on tree \mathcal{T} :

- $l_1(x, y) = l_2(x, y) = 1/6, l_3(x, y) = 2/3$
- $l_4(x, y) = l_1(x, y) + l_2(x, y) = 1/3$
- $l(x, y) = (1/6, 1/6, 2/3, 1/3, 1)$



Why not using the standard Shapley value?

Shapley value approach on trees

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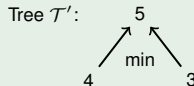
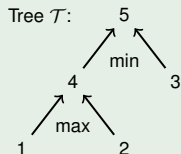
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On subtree \mathcal{T}' :

- On \mathcal{T}' : $l_3(x, y) = l_4(x, y) = 1/2$
- Nodes 1 and 2 shall share equally $l_4(x, y) = 1/2$
- $l(x, y) = (1/4, 1/4, 1/2, 1/2, 1)$



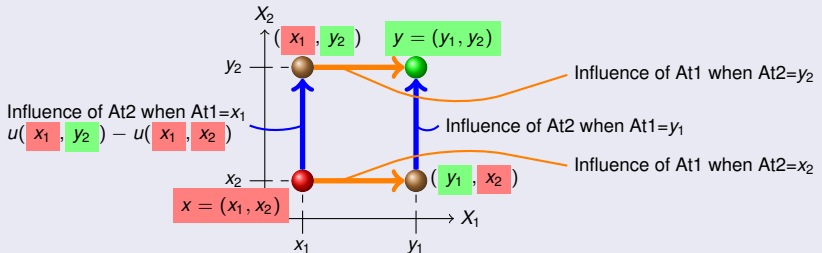
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Axioms

Idea of the approach

- Assess the influence of a criterion in the evaluation of two alternatives x, y
- by looking at alternatives obtained by replacing subsets of values of y with values of x .
- Example with 2 attributes: $x = (x_1, x_2)$, (y_1, x_2) , (x_1, y_2) , and $y = (y_1, y_2)$



Restricted Value (RV)

I_k depends only on the utility u of compound options mixing values of x, y .

Axioms

Null Attribute (NA)

if changing x_k to y_k never changes u , then $I_k = 0$.

Consistency with Restricted Tree (CRT)

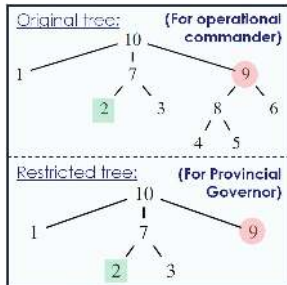
I_2 shall be the same for the original tree or a subtree where 9 becomes a leaf.

Generalized Efficiency (GE)

- General Share: $I_{10} = u(y) - u(x)$
- Decomposability: e.g. $I_9 = I_6 + I_8$

Other axioms

- Additivity (ADD): $I_k(u + u') = I_k(u) + I_k(u')$
- Restricted Equal Treatment (RET): All attributes are treated symmetrically



Are these axioms sufficient to derive I ?

Theorem

There is a unique influence index satisfying **RV**, **NA**, **RET**, **ADD**, **GE** and **CRT**.

Remark

This influence index is an extension of the Shapley value on general trees.

Are these axioms sufficient to derive I?

Extended Shapley/Owen value

In order to distinguish the contribution of each attribute, we move from x to y changing one attribute at a time, following an ordering π on N :

$$x, (y_{\{\pi(1)\}}, x_{-\{\pi(1)\}}), (y_{\{\pi(1), \pi(2)\}}, x_{-\{\pi(1), \pi(2)\}}), \dots, y.$$

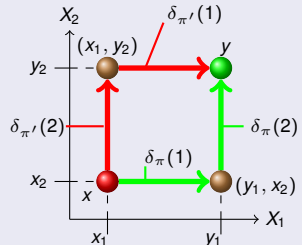
Definition:

$$I_i(x, y, T, u) = \begin{cases} \frac{1}{|\Pi(T)|} \sum_{\pi \in \Pi(T)} \delta_{\pi}(i) & \text{if } i \in N \\ \sum_{k \in \text{Leaf}_T(i)} I_k(x, y, T, u) & \text{else} \end{cases}$$

$$\delta_{\pi}(i) := u(y_{S_{\pi}(i)}, x_{-S_{\pi}(i)}) - u(y_{S_{\pi}(i) \setminus \{i\}}, x_{-S_{\pi}(i) \setminus \{i\}}), \quad S_{\pi}(\pi(k)) := \{\pi(1), \dots, \pi(k)\}$$

Example with 2 attributes:

- Path #1, $\pi = (1, 2)$:
 - for $\pi(1) = 1$: $\delta_{\pi}(1) = U(y_1, x_2) - U(x_1, x_2)$,
 - for $\pi(2) = 2$: $\delta_{\pi}(2) = U(y_1, y_2) - U(y_1, x_2)$
- Path #2, $\pi' = (2, 1)$:
 - for $\pi'(1) = 2$: $\delta_{\pi'}(2) = U(x_1, y_2) - U(x_1, x_2)$,
 - for $\pi'(2) = 1$: $\delta_{\pi'}(1) = U(y_1, y_2) - U(x_1, y_2)$



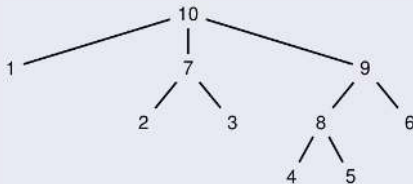
Are these axioms sufficient to derive I ?

What is $\Pi(T)$?

$\Pi(T)$: set of orderings of elements of N for which all elements of a subtree of T are consecutive.

Example:

- $(5, 4, 6, 2, 3, 1) \in \Pi(T)$ (indicating that $\pi(1) = 5, \pi(2) = 4, \pi(3) = 6, \pi(4) = 2, \pi(5) = 3, \pi(6) = 1$)
- $(1, 6, 4, 5, 2, 3) \in \Pi(T)$
- $(1, 2, 3, 4, 5, 6) \in \Pi(T)$
- $(2, 3, 4, 5, 1, 6) \notin \Pi(T)$ since 1 is interleaved between attributes $\{4, 5\}$ and $\{6\}$



Computational complexity

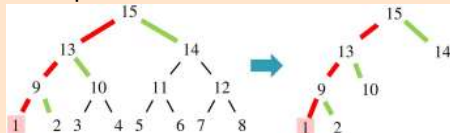
Complexity issue

Computation of I_i is exponential with n

Theorem

CRT implies that index I_i can be equivalently computed by cutting all branches not directly linking the path from node i to the root.

Example with I_1 :



d	p	n	$\log_{10} \Pi(N) $	$\log_{10} \Pi(T) $	$\log_{10} \Pi(T_{i,n}) $
2	2	4	1.38	0.903	0.602
2	3	9	5.559	3.112	1.556
2	4	16	13.320	6.901	2.76
2	5	25	25.19	12.47	4.158
2	6	36	41.57	20.0	5.715
3	2	8	4.605	2.107	0.903
3	3	27	28.036	10.115	2.334
3	4	64	89.1	28.984	4.14
3	5	125	209.27	64.454	6.237
3	6	216	412.0	122.86	8.571
4	2	16	13.3215	4.515	1.204
4	3	81	120.76	31.126	3.112
4	4	256	506.93	117.31	5.520
4	5	625	1477.7	324.35	8.316
4	6	1296	3473.0	740.04	11.429
5	2	32	35.42	9.332	1.505
5	3	243	475.76	94.156	3.89
5	4	1024	2639.7	470.65	6.901
5	5	3125	9566.3	1623.84	10.395
5	6	7776	26879	4443.15	14.286

Outline

- 1 Introduction
- 2 Feature Importance
 - Pairwise Comparison in Decision
 - Absolute Assessment In Decision
 - In Machine Learning
 - In Sensibility Analysis
- 3 Extension on trees
 - Context
 - axiomatic characterization
- 4 Conclusion

Conclusion & Perspectives

Conclusion

- Shapley value is a generic tool to measure variable importance
- Extension to trees: an extended Shapley value taking into account the tree structure

Perspectives

- Further investigations between sensitivity analysis and interpretability

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