Machine Learning Interpretability

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Outline

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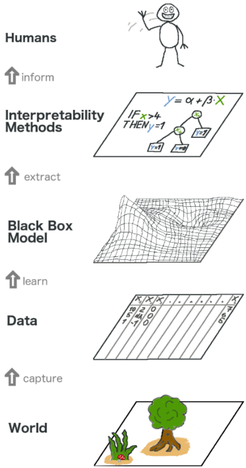
Problem Setting

Problem

- Metrics such as Accuracy, F1-score,...:
  * they are not very informatives and reliable/trustful to take decisions
  * they don't answer the "How" and "Why" questions for the returned prediction
- **Question** : How to get more reliable predictions ? => **machine learning interpretability/explainability** ?



Fundamental definition

ML Explanation definition

- It must be human understandable, what ever his/her background is .
- It should give us an insightful justification for a given prediction
- It is often instance/example based
- the terms "Interpretability" and "Explainability" are used interchangeably in Machine learning

Objectifs

- Build low risk applications (sensitive domains such as health).
- Advanced debugging and therefore performances improvement for ML researchers and engineers.
- Build robust and reliable models.
- AI fairness.

Fundamental definitions

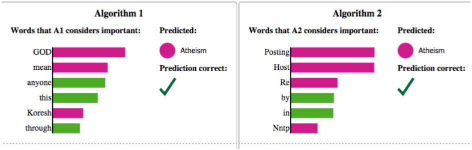
General notions

- There are some AI system that don't require an interpretability !
- We have 2 models (**"ML"** and **"EXplainability"**)
- The features are not necessary the same for both the ML model and the EX model, for instance in NLP we have words embeddings for **ML** and one hot encoding for **EX**

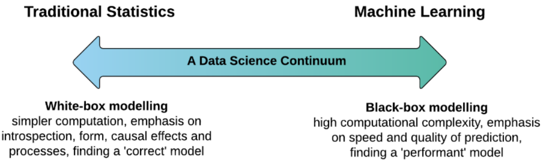
ML models are splitted into 2 categories

- **White box** :Models that are interpretable by essence, but they are less expressive and less performant
- **Black box** : Models that are more performant, more complex, and more expressive, **But** their decisions are impossible to understand, hence the **Explainability**

Fundamental definitions



Source : (LIME paper)



Source : (Applied AI)

Fundamental definitions

Explainability models are splitted into 2 categories

- **Model-Agnostic** : a model that works for all ML models considering it as a "black box"
- **Specific** : a model which explains a specific family of models by definition, for example : "Neural Networks", "Tree-Based", ...

The interpretability scope : Global vs Local

- **Local** : explain a certain prediction for a specific instance
- **Global** : explain the global behaviour of the ML model

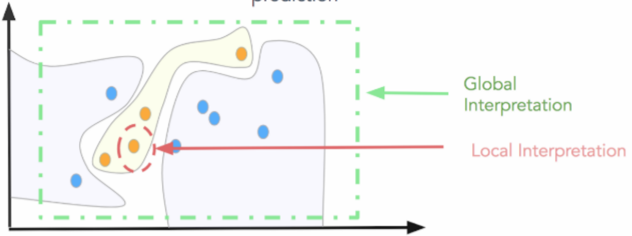
Fundamental definitions

Global Interpretation

Being able to explain the conditional interaction between dependent(*response*) variables and independent(*predictor, or explanatory*) variables based on the complete dataset

Local Interpretation

Being able to explain the conditional interaction between dependent(*response*) variables and independent(*predictor, or explanatory*) variables wrt to a single prediction



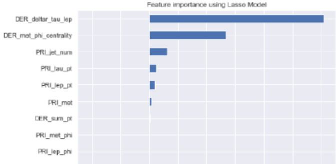
Source : (Datascience.com)

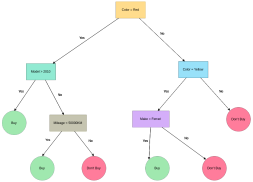
Interpretable models

White box models

the ML model and EX model are both the same model :

- Linear models (**)
- Decision Trees(**)
- Others(*): Decision Rules, Naive Bayes, KNN, ...



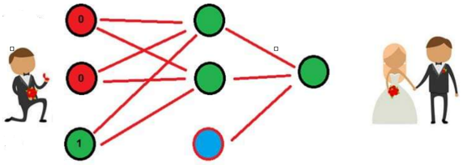


Complex Models

Very performant models but black box

We need a separate model to explain them

- Neural networks
- Bagging, Boosting, Random forests and others



XGBoost
RandomForests
ConvolutionalNets
RecurrentNeuralNetwork
FeedForwardNets
LightGBM
GANs

LIME

LIME (Local Interpretable Model-agnostic Explanations)

Idea : for a specific instance, we approximate the ML model locally

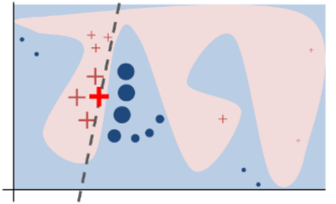
Framework

- an instance $x \in R^d$ and its EX representation $x' \in \{0,1\}^{d'}$
- The ML Model $f : R^d \mapsto R$ and the EX Model $g : \{0,1\}^d \mapsto R$
- Sampled instances $z_i \in R^d$,their representation z_i', and a proximity kernel $\pi_x(z)$
- Optimization problem : $\xi(x) = \arg\min_{g \in G} [\mathcal{L}(f, g, \pi_x) + \Omega(g)]$
- Custom MSE (weighted by a kernel) : $\mathcal{L}(f, g, \pi_x) = \sum_i \pi_x(z_i)(f(z_i) - g(z_i'))^2$

Algorithm 1 Sparse Linear Explanations using LIME

Require: Classifier f, Number of samples N
Require: Instance x, and its interpretable version x'
Require: Similarity kernel π_x, Length of explanation K

$\mathcal{Z} \leftarrow \{\}$
for $i \in \{1, 2, 3, ..., N\}$ **do**
  $z_i' \leftarrow sample\_around(x')$
  $\mathcal{Z} \leftarrow \mathcal{Z} \cup \langle z_i', f(z_i), \pi_x(z_i) \rangle$
end for
$w \leftarrow$ K-Lasso$(\mathcal{Z}, K)$ ▷ with z_i' as features, $f(z)$ as target
return w



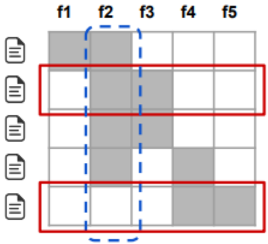
SP-LIME : Global extension of LIME

SP-LIME (Sub-modular Pick LIME)

Idea : locate representative instances and learn a LIME on each of them in order to approximate the model behavior **globally**

Algorithm 2 Submodular pick (SP) algorithm

Require: Instances X, Budget B
  for all $x_i \in X$ **do**
    $\mathcal{W}_i \leftarrow \textbf{explain}(x_i, x'_i)$ ▷ Using Algorithm 1
  end for
  for $j \in \{1 \ldots d'\}$ **do**
    $I_j \leftarrow \sqrt{\sum_{i=1}^{n} |\mathcal{W}_{ij}|}$ ▷ Compute feature importances
  end for
  $V \leftarrow \{\}$
  while $|V| < B$ **do** ▷ Greedy optimization of Eq (4)
    $V \leftarrow V \cup \text{argmax}_i \, c(V \cup \{i\}, \mathcal{W}, I)$
  end while
  return V



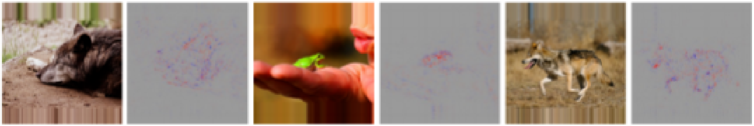
LRP

LRP (Layer-wise Relevance Propagation)

Idea : Backprop the outputs signals to the input layer in Neural Nets

Framework

- *aj* is the neuron *j* output which is defined as the non-linearity g : $a_j = g(\sum_i w_{ij} * a_i + b)$
- an instance x, an ML model f, a layer l, a dimension p, a relevance score R_p^l, as $f(x) \approx \sum_p R_p^{(1)}$ (features contribution is summed)
- features p with $R_p^{(1)} < 0$ contribute negatively to activate the output neuron and reversely ($R_p^{(1)} > 0$)



Source : (LRP with Local Renormalization Layers paper)

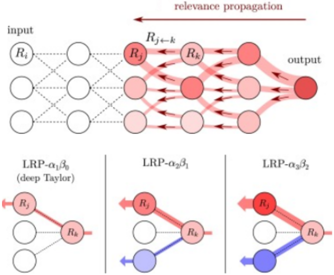
LRP

Details ...

- the relevance score for :
  - the **output** neurons is : $R^{(L)} = f(x)$
  - the **intermediate** neurons (back-prop) : $R_i^{(l)} = \sum_{j \in (l+1)} R_{i \leftarrow j}^{(l,l+1)}$
  - the **input** neurons ($l = 1$) where they are considered as the last intermediate neurons $R_i^{(1)}$
- All the variations of the EX model are based on $R_{i \leftarrow j}^{(l,l+1)}$ formula

Name	Formula	Usage	DTD
LRP-0 [7]	$R_j = \sum_k \frac{a_j w_{jk}}{\sum_{0,j} a_j w_{jk}} R_k$	upper layers	✓
LRP-ϵ [7]	$R_j = \sum_k \frac{a_j w_{jk}}{\epsilon + \sum_{0,j} a_j w_{jk}} R_k$	middle layers	✓
LRP-γ	$R_j = \sum_k \frac{a_j (w_{jk} + \gamma w_{jk}^+)}{\sum_{0,j} a_j (w_{jk} + \gamma w_{jk}^+)} R_k$	lower layers	✓
LRP-$\alpha\beta$ [7]	$R_j = \sum_k \left(\alpha \frac{(a_j w_{jk})^+}{\sum_{0,j} (a_j w_{jk})^+} - \beta \frac{(a_j w_{jk})^-}{\sum_{0,j} (a_j w_{jk})^-} \right) R_k$	lower layers	$\times^\star$
flat [30]	$R_j = \sum_k \frac{1}{\sum_j 1} R_k$	lower layers	$\times$
w^2-rule [36]	$R_i = \sum_j \frac{w_{ij}^2}{\sum_i w_{ij}^2} R_j$	first layer ($\mathbb{R}^d$)	✓
$z^{\mathcal{B}}$-rule [36]	$R_i = \sum_j \frac{x_i w_{ij} - l_i w_{ij}^+ - h_i w_{ij}^-}{\sum_i x_i w_{ij} - l_i w_{ij}^+ - h_i w_{ij}^-} R_j$	first layer (pixels)	✓

(* DTD interpretation only for the case $\alpha = 1, \beta = 0$.)



DeepLIFT

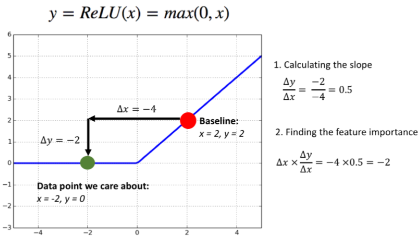
DeepLIFT (Deep Learning Important FeaTures)

Idea : Replace **gradients** by **differences** during the backprop

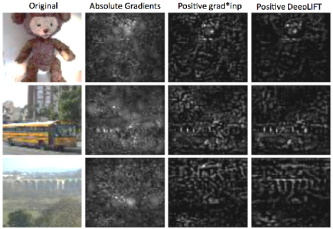
Détails

- Gradients raise 2 major problems : **Saturation, ReLU(virer les Negatifs, Discontinuité)**
- We are not interested in the gradient **(how y changes when x changes infinitesimally)**
- We are interested in the slope **(how y changes when x vary from its reference x_{ref})**
- $gradient = \frac{\partial y}{\partial x} \Rightarrow slope = \frac{y - y_{ref}}{x - x_{ref}} = \frac{\Delta y}{\Delta x}$
- We keep the "Chain rule" : $\frac{\partial y}{\partial x} = \frac{\partial y}{\partial z} * \frac{\partial z}{\partial x} \Rightarrow \frac{\Delta y}{\Delta x} = \frac{\Delta y}{\Delta z} * \frac{\Delta z}{\Delta x}$
- $Feature_i$ Importance : $x_i \times \frac{\partial y}{\partial x_i} \Rightarrow (x_i - x_i^{ref}) \times \frac{\Delta y}{\Delta x_i}$
- **Problem** ? how to get the reference ?
  - inputs neurons : handcrafted by **domain experts** (Ex: MNIST => images initialized with 0)
  - intermediate and outputs neurons, we just need to **forward** the references inputs

DeepLIFT



Source : (Gabriel Tseng Medium Blogs)



Source : (DeepLIFT paper)

SHAP

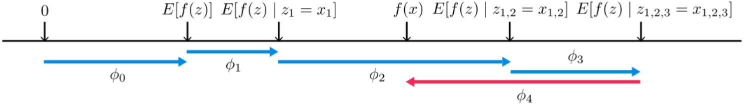
SHAP (SHapley Additive exPlanations)

Idea : Unify all the previous methods and many more under the game theory paradigm

Framework

- la **The shapley value** is a method of attributing individual rewards to players based on their contribution to the total reward .
- Players are **features values**,The total reward for an instance z is : $f(z) - E(f(z))$
- the shapley value is the average marginal contribution of a feature value for all possible coalitions.

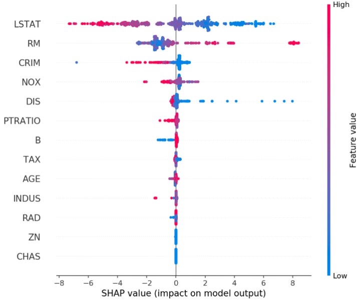
$$\phi_j(val) = \sum_{S \subseteq \{x_1,\ldots,x_p\} \setminus \{x_j\}} \frac{|S|!\,(p-|S|-1)!}{p!} \left(val\left(S \cup \{x_j\}\right) - val(S)\right)$$

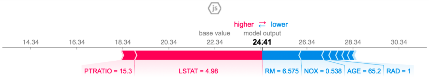


SHAP

SHAP EX Models

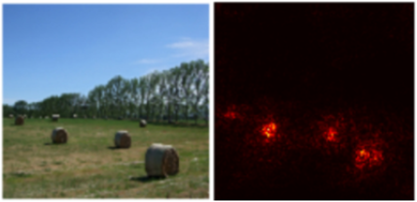
- **KernelSHAP (LIME+Shapley values)** : Lime uses heuristics to seek a kernels , SHAP demonstrates that the best kernel is unique and it is : $\pi_x(z') = \frac{M-1}{\binom{M}{|z'|} * |z'| * (M - |z'|)}$
- **DeepSHAP (DeepLIFT+Shapley values)** : Adapted for Neural Networks
- **TreeSHAP(Decision Tree+Shapley values)**: Adapted for Tree-based models



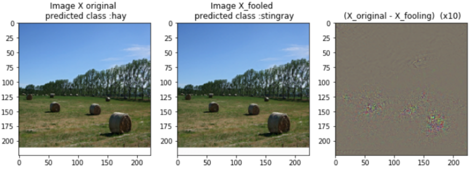


Example-based

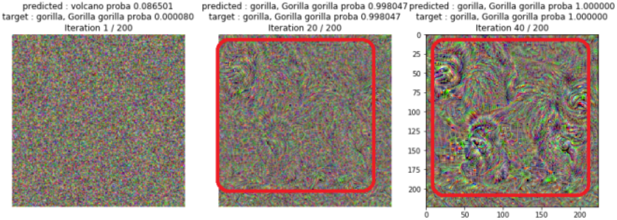
Saliency Maps (hay class)



Adversarial attacks(hay class)



Deep Visualization(Gorilla class)



Comparative summary

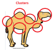
Models	LIME	LRP	DeepLift	Attacks	SHAP
Model-agnostic	✓				✓KernelSHAP
Model-specific		✓	✓	✓	✓DeepSHAP
local approximation	✓	✓	✓	✓	✓KernelSHAP ✓TreeSHAP
global approximation	✓SP-LIME				✓Feature Importance and others
gradient-based				✓	
backprop-based		✓	✓	✓	✓DeepSHAP
perturbation-based	✓				✓KernelSHAP

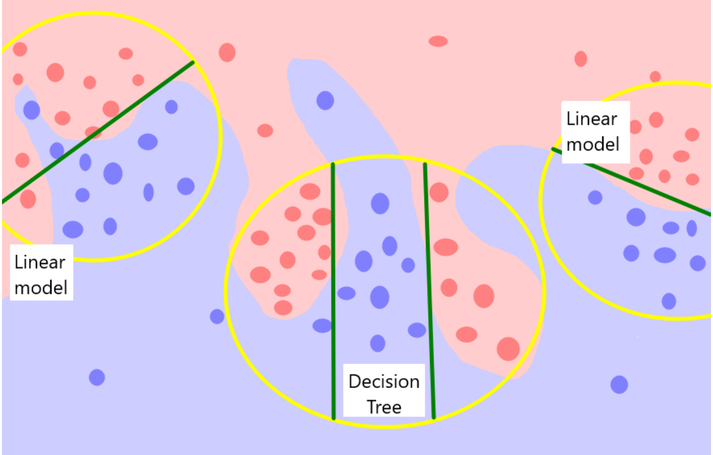
Common problems ...

- The sampling problem that could lead to unrealistic datapoints
- Gradient major problems : saturation, discontinuities, and negative signals backprop
- Explanations variability : for small changes on the same point, interpretability may change drastically

Our model in one slide !

CAMEL (Clustering bAsed Model-agnostic ExpLanations)

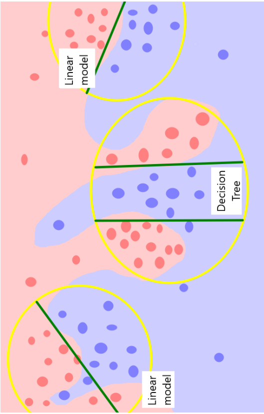




Architecture choisie

Idea and pseudo-algorithm

- No sampling we use only our datapoints, since the model learns a boundary from existing points !
- We apply a clustering algorithms based on the dataset distribution such as K-means or DBSCAN or ... (see clusters in Yellow)
- We learn an interpretable model locally in each cluster with a Kernel SHAP (see Green approximators)
- we could extend it to a global explanation



Evaluation

Protocole

- Dataset : Cervical Cancer (Risk Factors)
- As any other EX model cited previously we will need human volunteers to evaluate the quality of our explanations
- Each instance should be reviewed by different persons
- Then, we could build comparative tables and plots with other models

Hyper parameters to explore

- The clustering algorithm itself
- the number of clusters C
- $TreeDepth$ for Tree-based models and $K - Lasso$ for linear models
- others : for instance **weighted?** datapoints or not etc ...

Conclusion

Important points to keep in mind

- **Interpretability** vs **Performance**
- **Our approach** :

  combine both the global and local scope by essence
  No sampling
  No gradients back propagation
- **Cost** : similar to the other methods ...

Merci pour votre attention

Des questions?

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