# Explainability in Machine Learning

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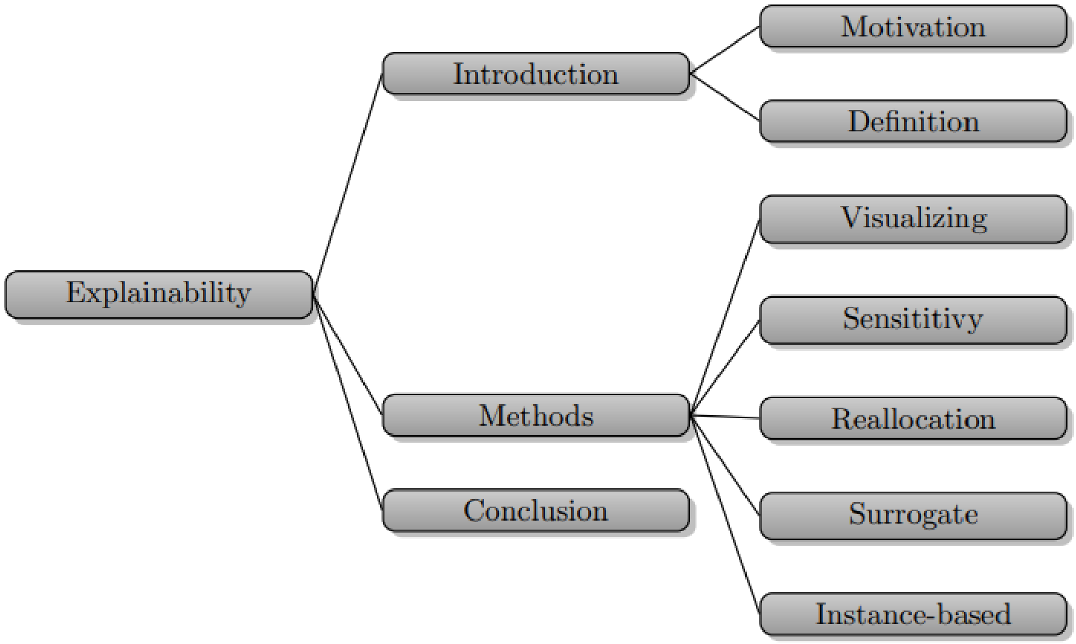
# Outline

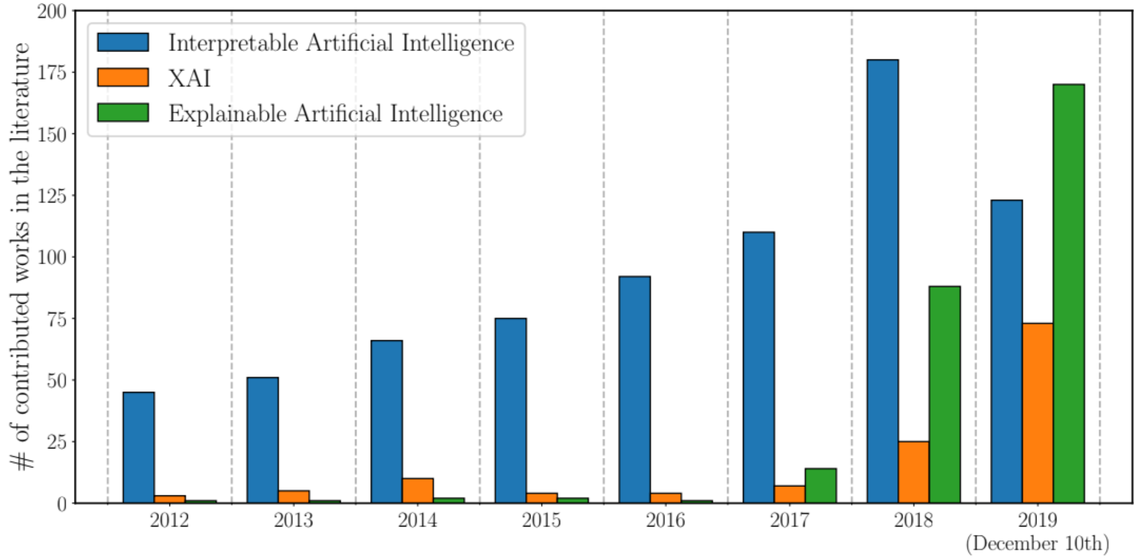
1. Introduction
2. Visualizing
3. Sensitivity
4. Reallocation
5. Surrogate
6. Instance - based
7. Conclusion



# Introduction

## State of Art

- **Molnar, Christoph “*Interpretable Machine Learning*”, 2020.**
- **Guidotti, Riccardo et al. ”*A Survey of Methods for Explaining Black Box Models*”, 2018.**
- **Arrieta Alejandro, “*Explainable Artificial Intelligence (XAI): Concepts, Taxonomies, Opportunities and Challenges toward Responsible AI*”, 2019.**
- **Adadi, Amina et al. “*Peeking inside the black-box: A survey on Explainable Artificial Intelligence (XAI)*" , 2018**




*The term explainability denotes the **ability to translate** something e.g. a **model**, a piece of the model, or a prediction of the model in an **understandable manner to human***

# Motivation

*“The human wants something that mectric doesn’t”*

Incompleteness in the problem formalization:


- Mismatch goal-objective



- Safety for high risk application

- Ethics, non-discriminative, right of explanation

- Knowledge discovering / Feature Engineering


- **Lipton, Zachary C "The mythos of model interpretability" 2018,**
- **Ribeiro, Marco Tulio et al. " Why should i trust you? Explaining the predictions of any classifier“, 2016.**
- **Doshi-Velez, Finale et al. "Towards a rigorous science of interpretable machine learning.“ , 2017.**

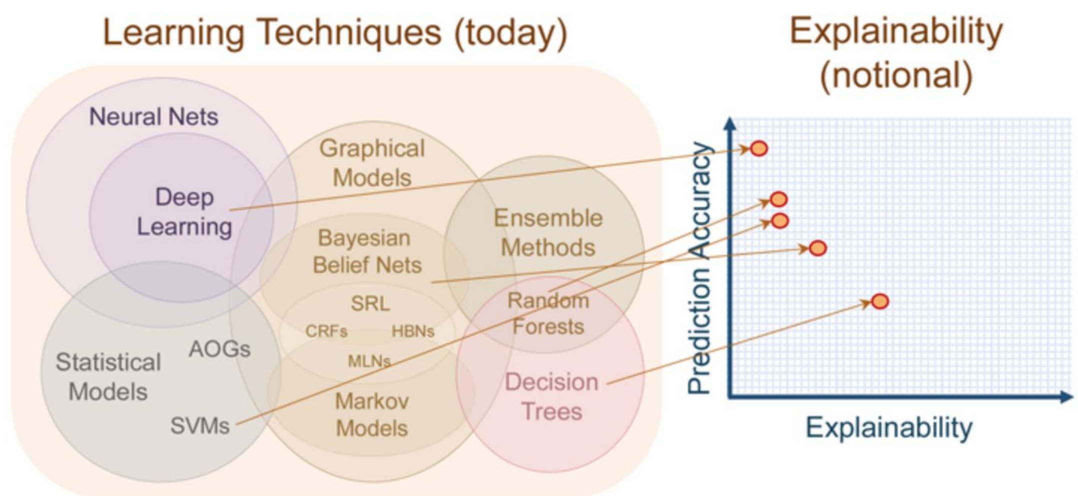
# White/Gray/Black box



- Linear regression
- Rule based

- Decision Tree
- Logistic Regression
- Linear SVM

- Ensemble Methods
- Neural Network
- SVM




**Explainability techniques**

| | |
|---|---|
| Global | Local |
| Model agnostic | Model Specific |

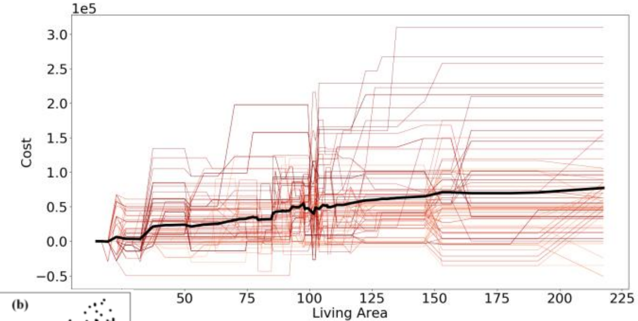
Tabular | Text | Image

- **Gunning, David " Explainable Artificial Intelligence (XAI).“ , DARPA, 2016.**

# Visualizing

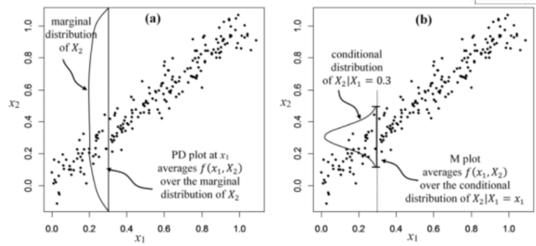
- Individual Conditional Expectation (ICE)

$$ICE^{(n)}(\boldsymbol{x}_S) = \hat{f}([\boldsymbol{x}_S, \boldsymbol{x}^{(n)}_{D/S}])$$



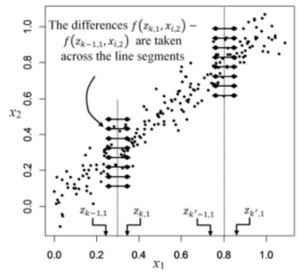

- Partial Dependence Plot (PDP)

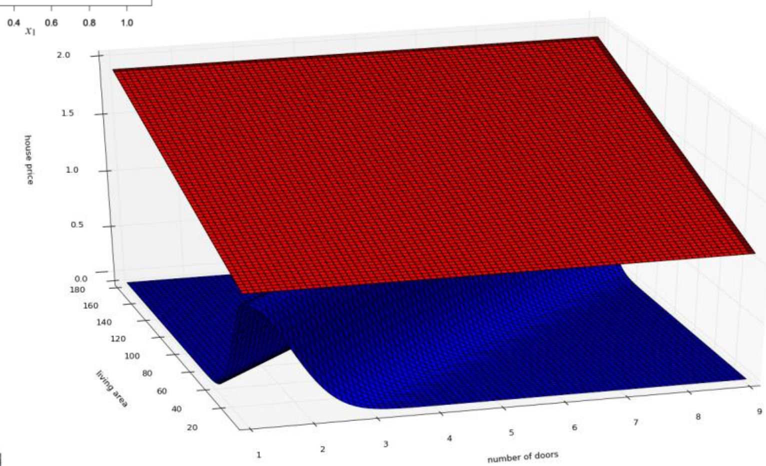
$$f_S(\boldsymbol{x}_S) = \mathbb{E}_{\boldsymbol{x}_C}[\hat{f}(\boldsymbol{x}_S, \boldsymbol{x}_C)] = \int_{\boldsymbol{x}_C} f(\boldsymbol{x}_S, \boldsymbol{x}_C) d\mathbb{P}\boldsymbol{x}_C$$




- M plots

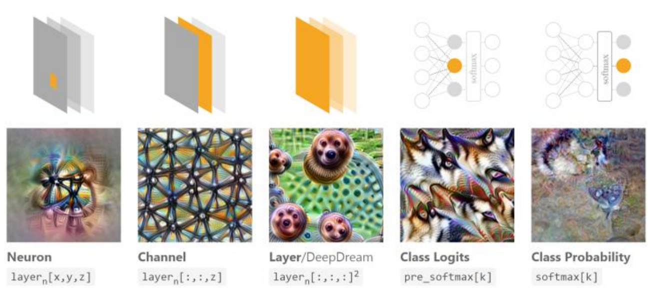
$$f_S(\boldsymbol{x}_S) = \mathbb{E}_{\boldsymbol{x}}[f(\boldsymbol{x})|\boldsymbol{x}_S] = \int_{\boldsymbol{x}} f(\boldsymbol{x}) d\mathbb{P}(\boldsymbol{x}_C|\boldsymbol{x}_S)$$




- Accumulated local effects (ALE)

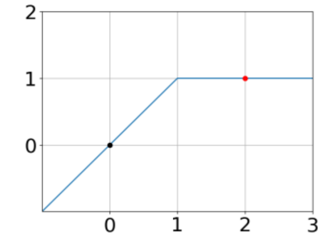
- Feature Visualization

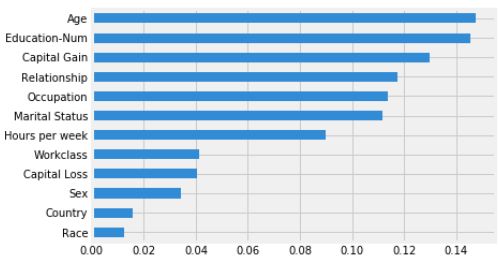



- Apley, Daniel et al. “Visualizing the Effects of Predictor Variables in Black Box Supervised Learning Models”, 2019.
- Goldstein, Alex et al. " Peeking Inside the Black Box: Visualizing Statistical Learning with Plots of Individual Conditional Expectation " , 2014.

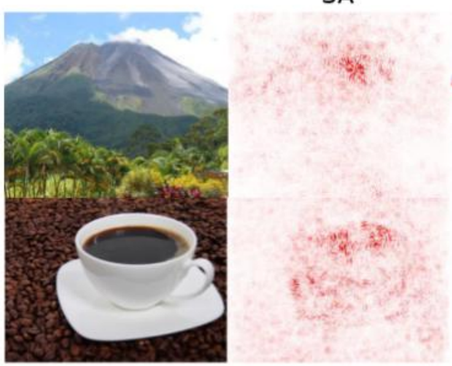
# Sensitivity

- Perturbation-based $\boxed{L}$
  - Permuted feature importance $$F_i = L(Y, f(X_{\text{permuted}, i})) - L(Y, f(X))$$
- Gradient-based $\boxed{f}$
  - Activation Maximization (maximization penalized)
  - Gradient Norm
  - Integrated Gradients (IG)
  - Deep Learning Important FeaTures (Deep Lift)

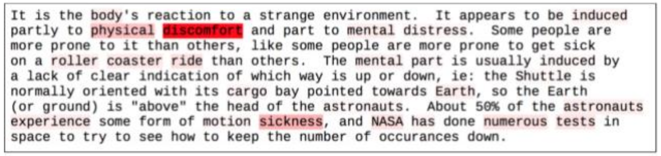



SA



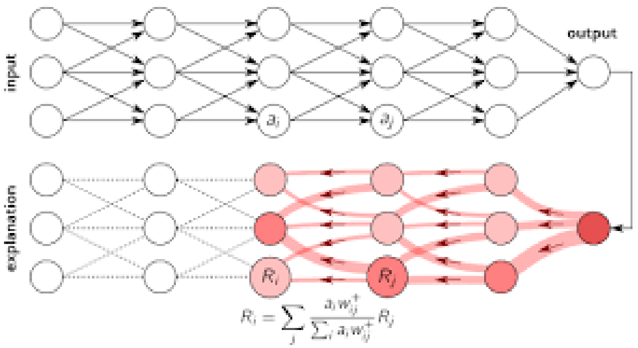
SA



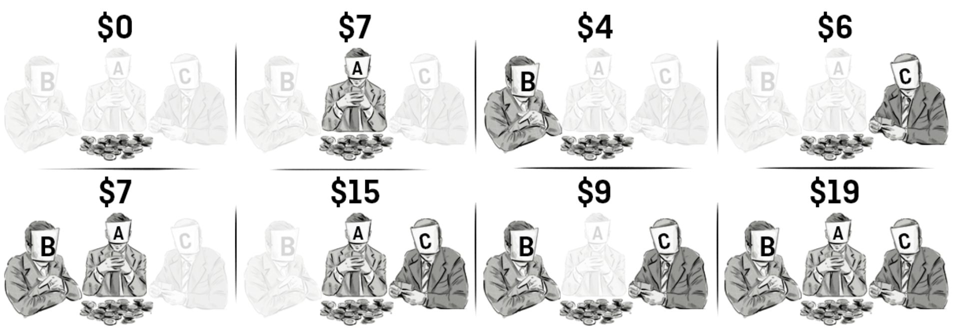

- **Samek , Wojciech et al. Explainabile Artificial Intelligence: understanding, visualizing and interpreting deep learning models**
- **Shrikumar , Avanti et al. Learning Important Features Through Propagating Activation Differences, 2019**
- **Sundararajan, Mukund et al. “Axiomatic Attribution for Deep Networks”, 2017**

# Reallocation (1)

- Layer-wise relevance propagation (LRP)




- Shapley Value




$$v(S \cup \{i\}) - v(S)$$

- ○ Players: $D$
- ○ Overall Payoff: $v(D)$
- ○ Characteristic function: $\nu : \mathcal{P}(D) \rightarrow \mathbb{R}$

$$\sum_{S \subseteq D/\{i\}\ with |S|=k} \frac{v(S \cup \{i\}) - v(S)}{\frac{|D-1|!}{k!(|D|-1-k)!}}$$

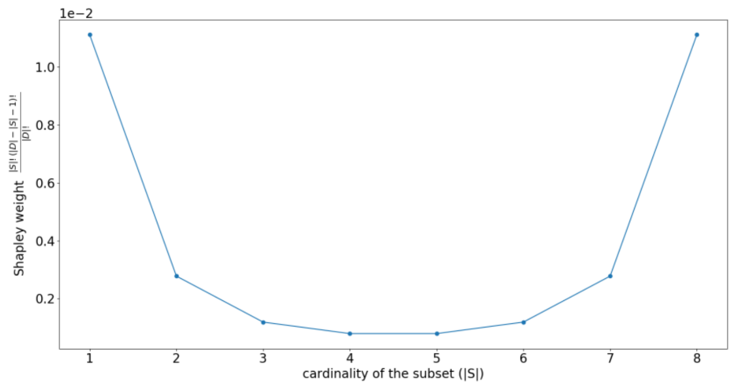
$$\sum_{k \in K} \left( \sum_{S \subseteq D/\{i\} with |S|=k} \frac{(v(S \cup \{i\}) - v(S))}{\frac{|D-1|!}{k!(|D|-1-k)!}} \right) \frac{1}{|D|}$$



- **Mantovan, Gregoire et al. "Methods for interpreting and understanding deep neural networks", 2018**

# Reallocation (2)

$$I_i(v) = \sum_{S\subseteq D/\{i\}} \frac{|S|!(|D|-|S|-1)!}{|D|!}\left(v(S\cup\{i\}) - v(S)\right)$$



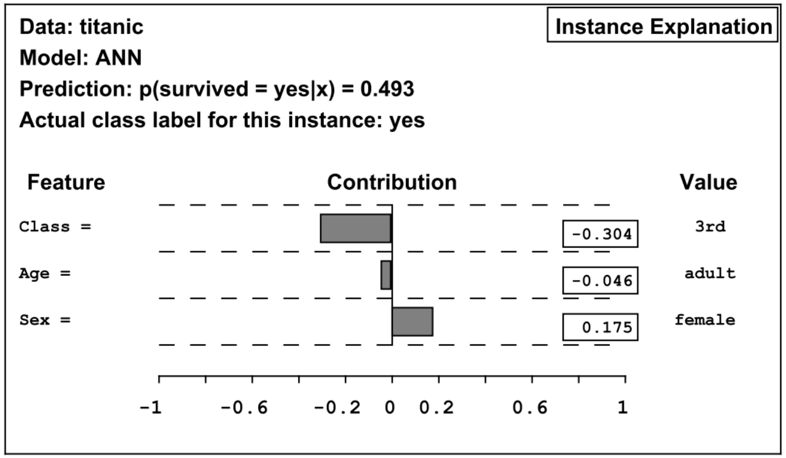

Efficency property

$$\sum_{i\in D} I_i(v) = v(D)$$

- Players -> Features of a particular instance
- Overall Payoff (prediction gain) -> $\hat{f}(\boldsymbol{x}) - \mathbb{E}_X[\hat{f}(X)]$
- Characteristic function $v(Q) = \mathbb{E}_{D/Q}[\hat{f}(D/Q)|Q] - \mathbb{E}_D[\hat{f}(D)]$

$$I_i(\boldsymbol{x}, v) = \frac{1}{|D|!}\sum_{\mathcal{O}\in\pi(|D|)}\left(v(Pre^i(\mathcal{O})\cup\{i\}) - v(Pre^i(\mathcal{O}))\right)$$

$$I_i(v) = \frac{1}{|D|!}\sum_{\mathcal{O}\in\pi(|D|)}\sum_{\boldsymbol{w}\in\mathcal{X}} p(\boldsymbol{w})\left(\hat{f}(\boldsymbol{w}_{[\forall i\in Pre^i(\mathcal{O})\cup\{i\}:\, w_i=x_i]}) - (\hat{f}(\boldsymbol{w}_{[\forall i\in Pre^i(\mathcal{O}):\, w_i=x_i]})\right)$$




- **Strumbelj, Erik et al. “Explaining prediction models and individual predictions with feature contributions”, 2014**

# Surrogate (1)

- Local Interpretable Model-Agnostic Explanations (LIME)





$$\zeta(x) = arg \min_{g \in G} \mathcal{L}(f, g, \pi_{\boldsymbol{x}}) + \Omega(g)$$

$$\mathcal{L}(f, g, \pi_{\boldsymbol{x}}) = \sum_{\boldsymbol{z}, \boldsymbol{z}' \in Z} \pi_{\boldsymbol{x}}(\boldsymbol{z}) \left(f(\boldsymbol{z}) - g(\boldsymbol{z}')\right)^2$$

x

| F 1 | F 2 | F 3 | F 4 |
|---|---|---|---|
| 0.2 | 0.8 | 0.1 | 0.9 |

z

| F 1 | F 2 | F 3 | F 4 |
|---|---|---|---|
| 0.2 | 0.8 | 0.5 | 0.9 |

| F 1 | F 2 | F 3 | F 4 |
|---|---|---|---|
| 0.2 | 0.5 | 0.5 | 0.9 |

| F 1 | F 2 | F 3 | F 4 |
|---|---|---|---|
| 0.2 | 0.8 | 0.5 | 0.5 |

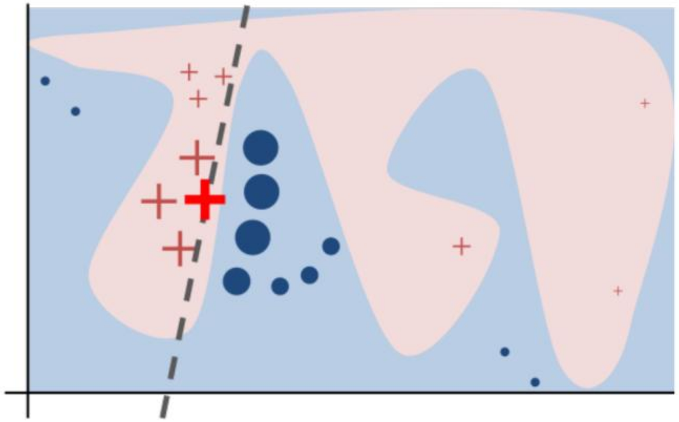
z’

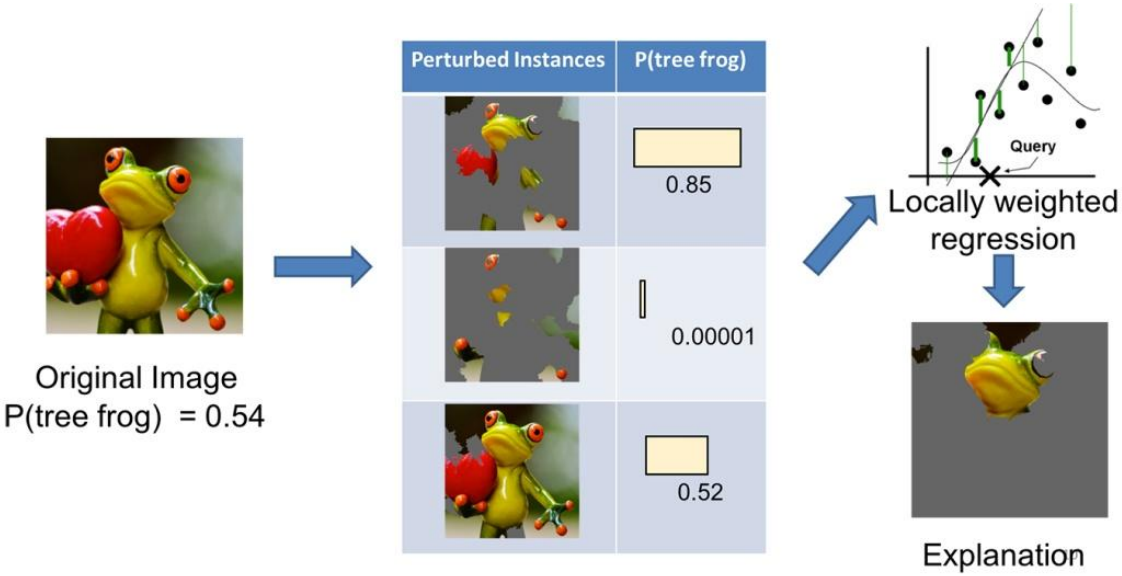
| F 1 | F 2 | F 3 | F 4 |
|---|---|---|---|
| 1 | 1 | 0 | 1 |

| F 1 | F 2 | F 3 | F 4 |
|---|---|---|---|
| 1 | 0 | 0 | 1 |

| F 1 | F 2 | F 3 | F 4 |
|---|---|---|---|
| 1 | 1 | 0 | 0 |

# Surrogate (2)






https://www.oreilly.com/content/introduction-to-local-interpretable-model-agnostic-explanations-lime

- Trepan: tree based surrogate models

- **Craven, Market al. "Extracting Tree-Structured Representations of Trained Networks "**

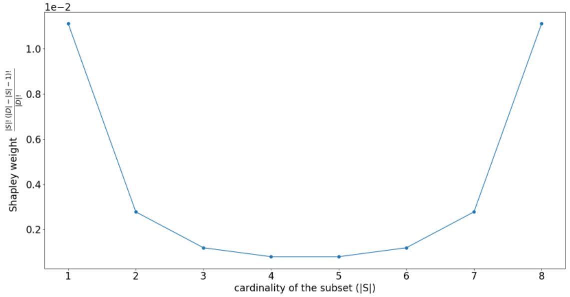
# Surrogate (3)

- SHAP





$$\min_{\boldsymbol{x}} \sum_{S\subset D} k(S)\left(v(S)-\sum_{i\in S}x_i\right)^2$$




| | $v(S)$ | $\sum_{i\in S} x_i$ |
|---|---|---|
| F1 | 2 | 3 |
| F2 | 3 | 3 |
| F3 | 1 | 2 |
| F1 + F2 | 7 | 6 |
| F1 + F3 | 6 | 5 |
| F2 + F3 | 6 | 5 |
| F1 + F2 + F3 | 8 | 8 |

Shapley Values


- **Lundberg, Scott et al. "A unified approach to interpreting model predictions", 2017**
- **Charnes, A et al. "Extremal principle solutions of games in characteristic function form: core, Chebychev and Shapley value generalizations", 1988**

# Instance-Based

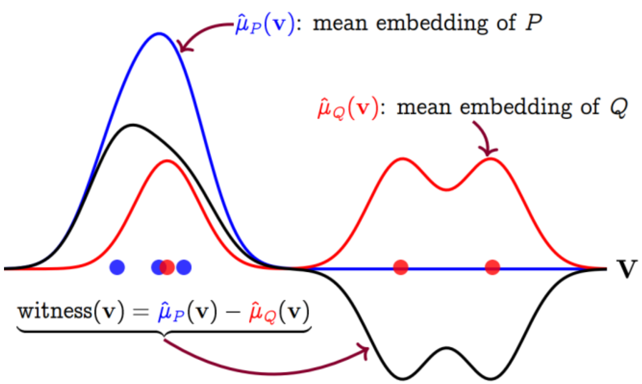
- Counterfactual explaination

$$L(\boldsymbol{x}, \boldsymbol{x}', y_c, \lambda) = \lambda \cdot (\hat{f}(\boldsymbol{x}') - y_c)^2 + d(\boldsymbol{x}, \boldsymbol{x}')$$

$$\arg\min_{\boldsymbol{x}'}$$

- Prototype selection

$$MMD(F, P, Q) = \sup_{f \in \mathcal{F}} (\mathbb{E}_{X \sim P}[f(X)] - \mathbb{E}_{Y \sim Q}[f(Y)])$$



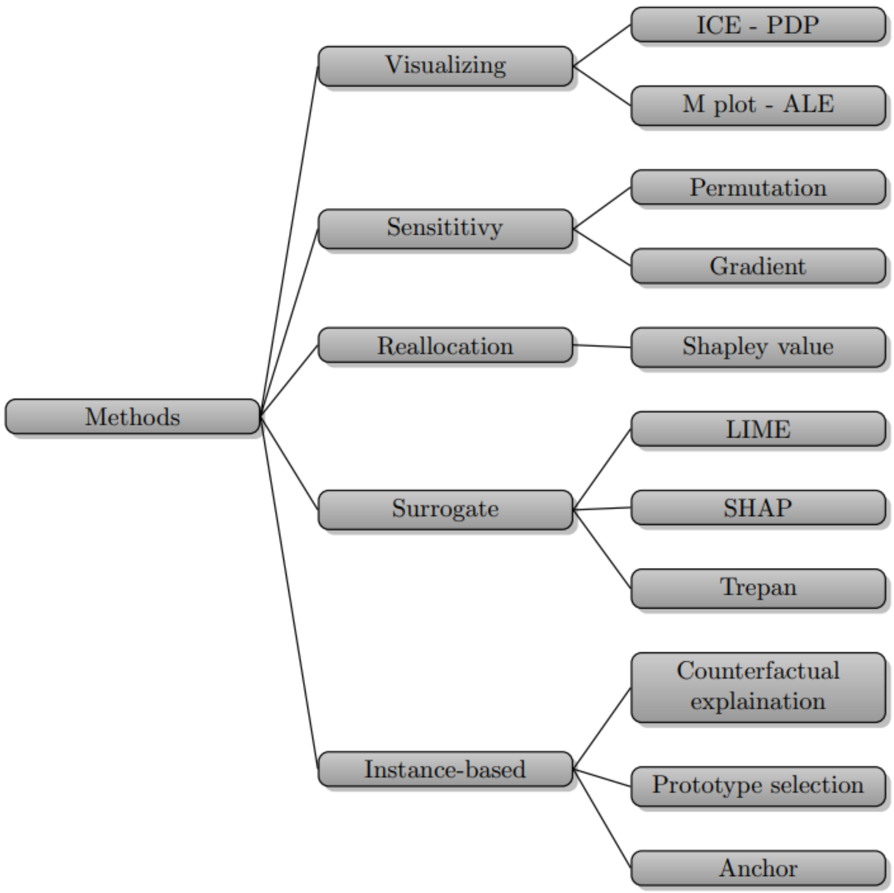


- Anchor

- **Been, Kim et al. "Examples are not Enough, Learn to Criticize! Criticism for Interpretability", 2016**
- **Zhu , Xiaojin et al. "Machine Teaching: An Inverse Problem to Machine Learning and an Approach Toward Optimal Education", 2015**

# Conclusion

- Evolving, broad, etherogeneous field;
- Visualizing / Sensitivity /Local Linearize / Game theory;
- Explainability by design;
- Logic constraints with feature importances.



# Thanks for your attention

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