DATA MINING 2
Explainability

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Definitions

- To ***interpret*** means to give or provide the meaning or to explain and present in understandable terms some concepts.

- In AI, and in data mining and machine learning, interpretability is the ***ability to explain*** or to provide the meaning ***in understandable terms to a human***.

- https://www.merriam-webster.com/
- Finale Doshi-Velez and Been Kim. 2017. ***Towards a rigorous science of interpretable machine learning***. arXiv:1702.08608v2.

What is a Black Box Model?

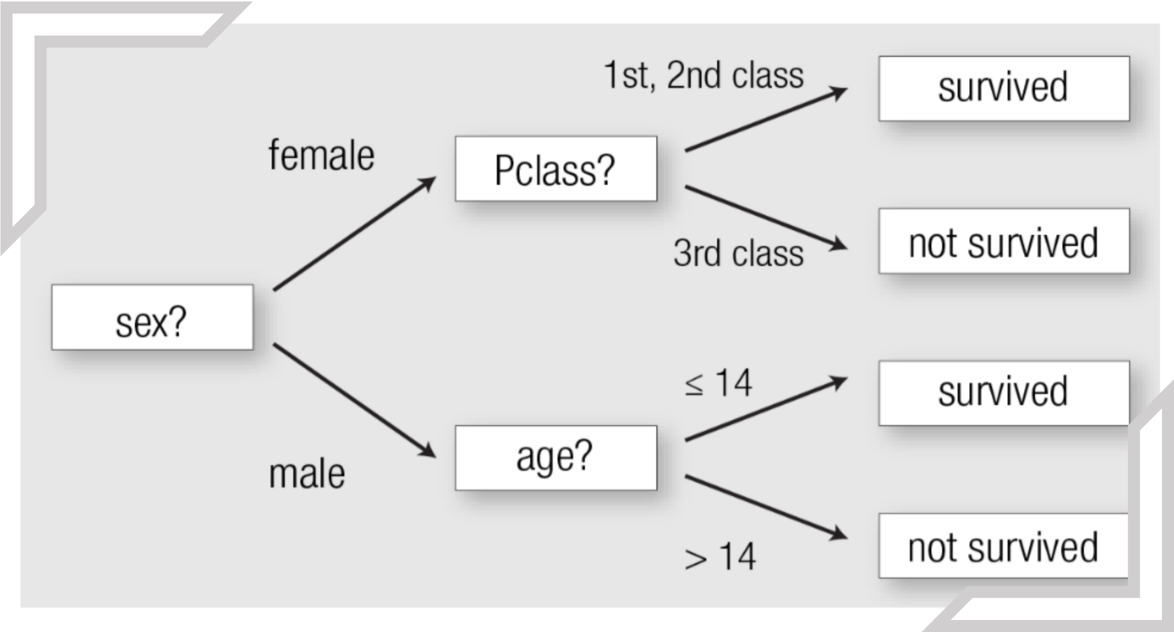
A ***black box*** is a model, whose internals are either unknown to the observer or they are known but uninterpretable by humans.

Example:

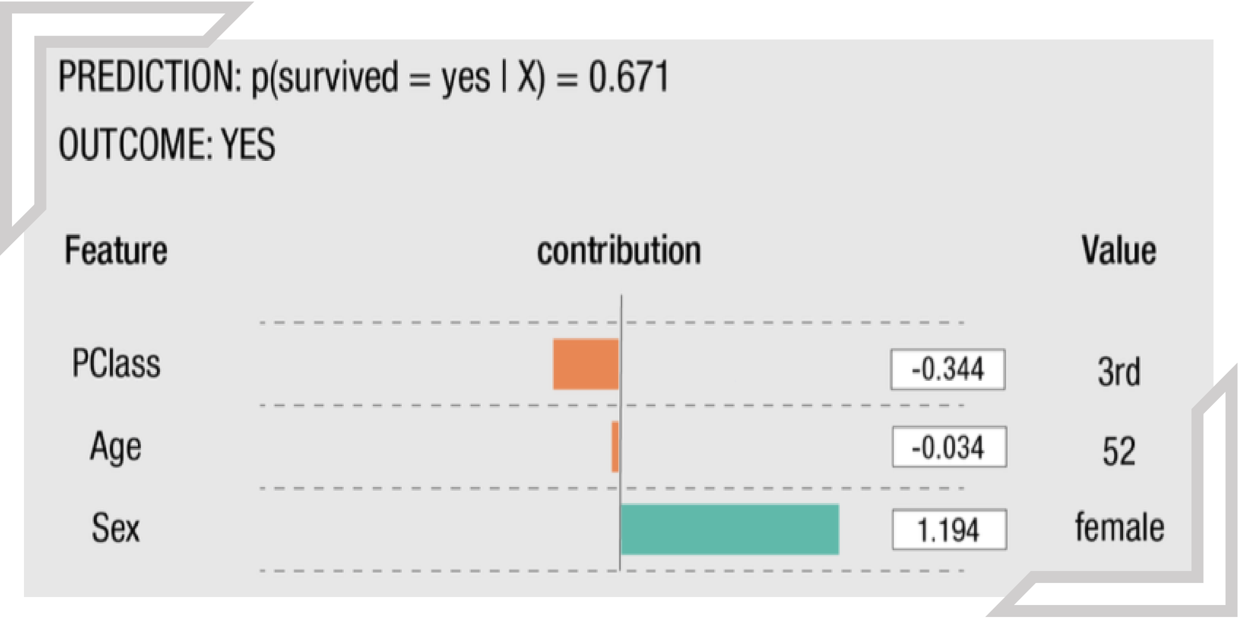
- DNN
- SVM
- Ensemble

- Guidotti, R., Monreale, A., Ruggieri, S., Turini, F., Giannotti, F., & Pedreschi, D. (2018). ***A survey of methods for explaining black box models***. *ACM Computing Surveys (CSUR)*, *51*(5), 93.

Interpretable Models



Decision Tree



Linear Model

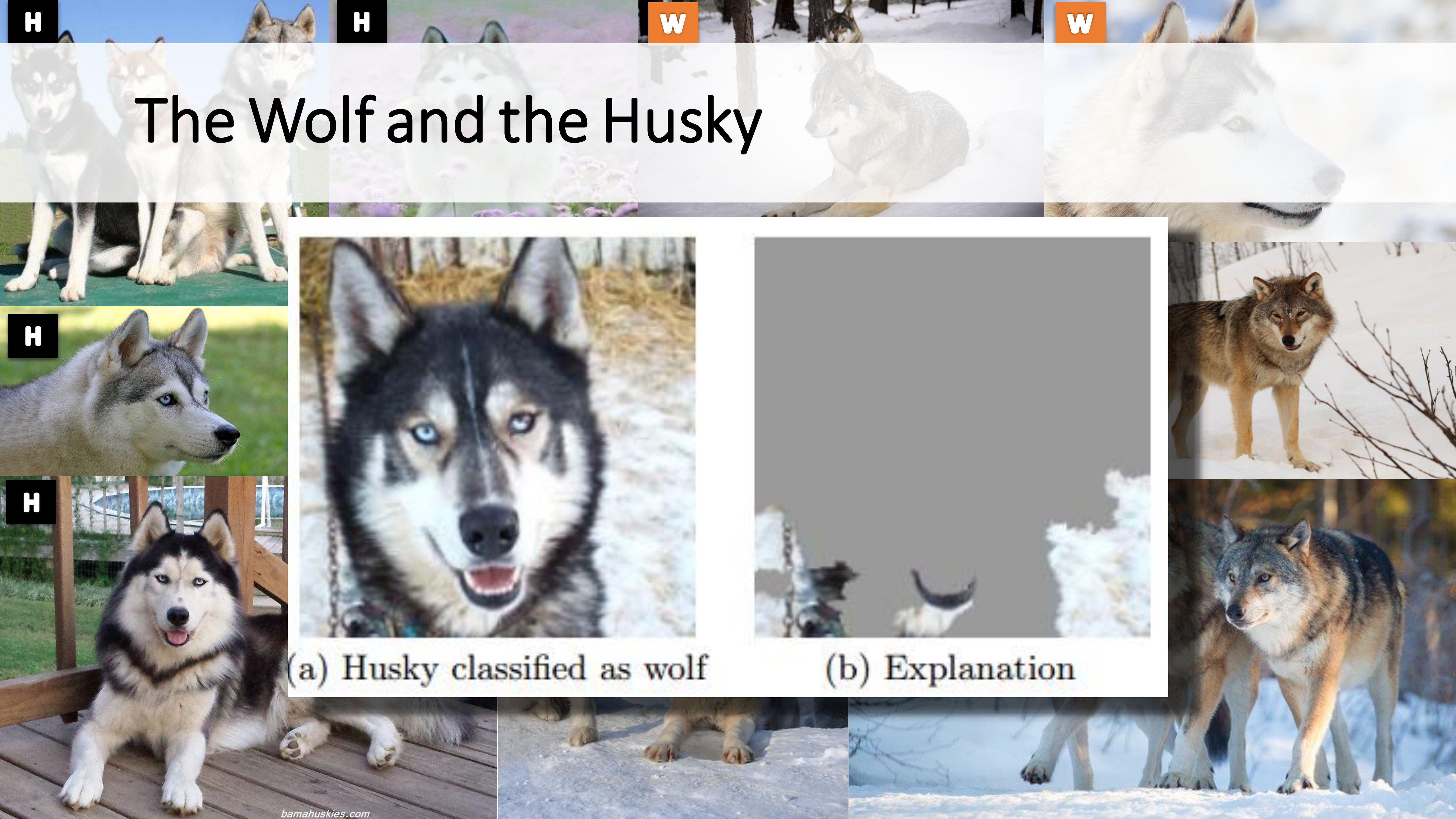
$$\text{if } condition_1 \wedge condition_2 \wedge condition_3 \text{ then } outcome$$

Rules

Motivations For Explanation Methods

COMPAS Recidivism

The Wolf and the Husky



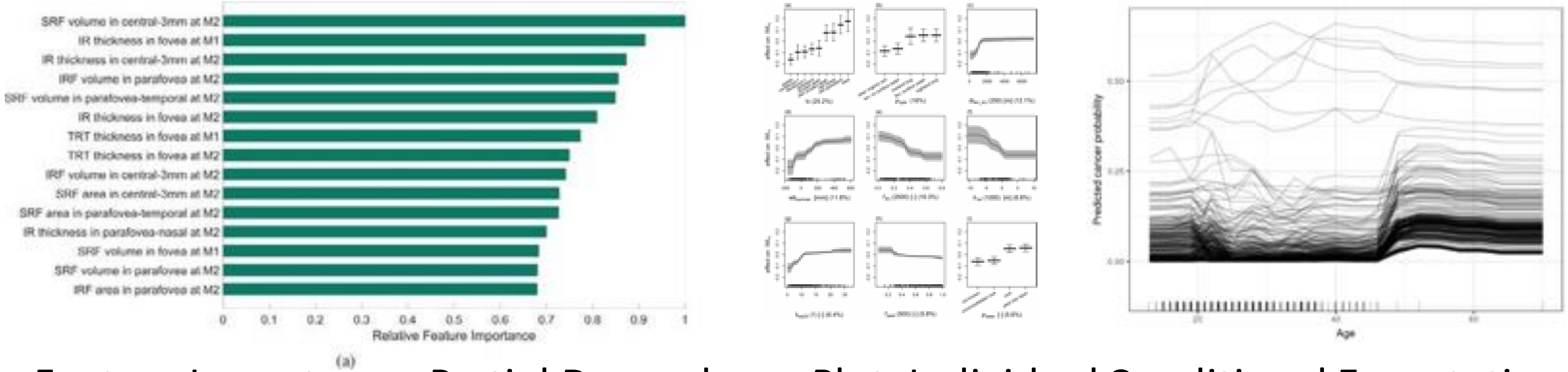
(a) Husky classified as wolf (b) Explanation

Right of Explanation

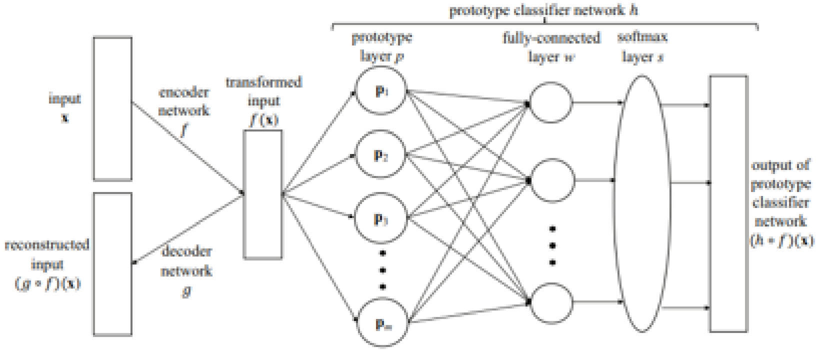
Since 25 May 2018, GDPR establishes a right for all individuals to obtain "meaningful explanations of the logic involved" when "automated (algorithmic) individual decision-making", including profiling, takes place.

Explanation in different AI fields

- Machine Learning

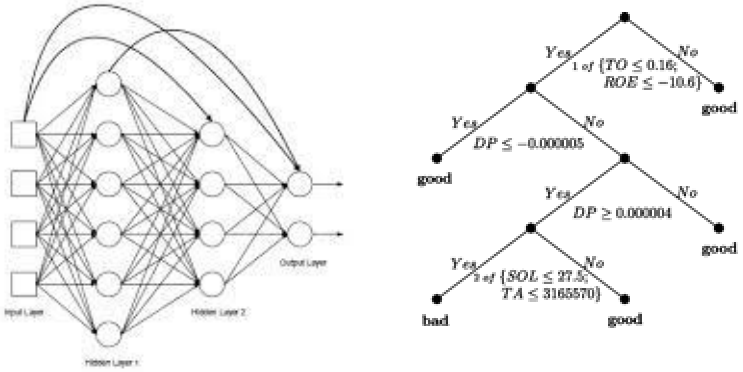


Feature Importance, Partial Dependence Plot, Individual Conditional Expectation



Auto-encoder

Oscar Li, Hao Liu, Chaofan Chen, Cynthia Rudin: Deep Learning for Case-Based Reasoning Through Prototypes: A Neural Network That Explains Its Predictions. AAAI 2018: 3530-3537

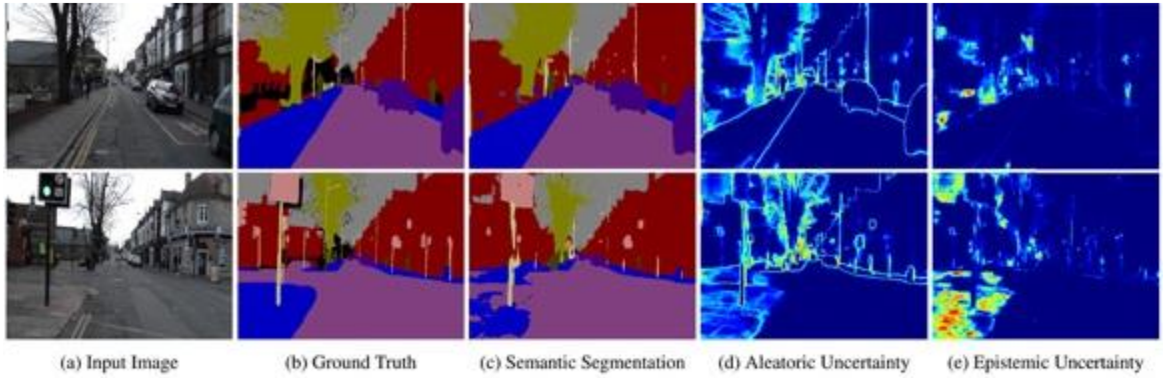


Surogate Model

Mark Craven, Jude W. Shavlik: Extracting Tree-Structured Representations of Trained Networks. NIPS 1995: 24-30

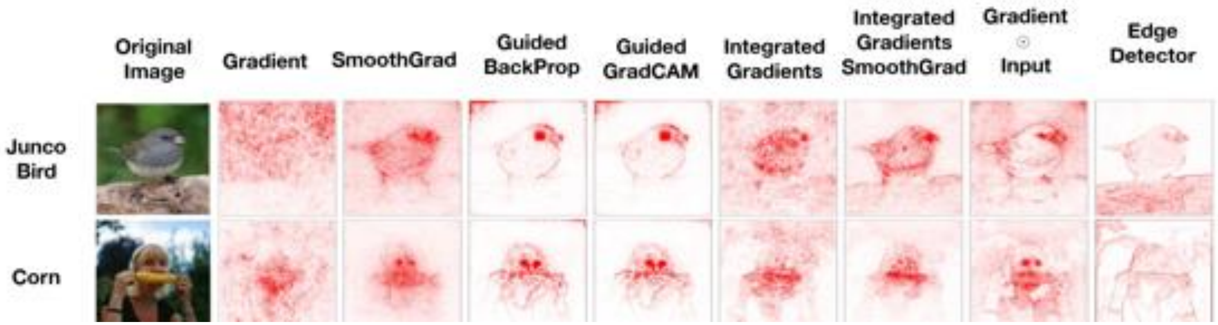
Explanation in different AI fields

- Machine Learning
- Computer Vision



Uncertainty Map

Alex Kendall, Yarin Gal: What Uncertainties Do We Need in Bayesian Deep Learning for Computer Vision? NIPS 2017: 5580-5590

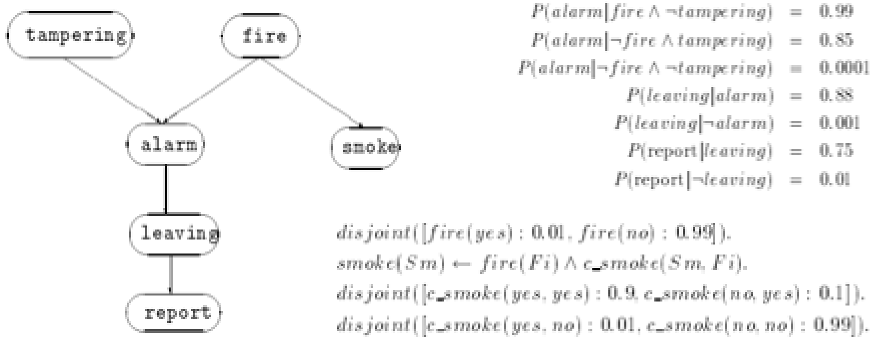


Saliency Map

Julius Adebayo, Justin Gilmer, Michael Muelly, Ian J. Goodfellow, Moritz Hardt, Been Kim: Sanity Checks for Saliency Maps. NeurIPS 2018: 9525-9536

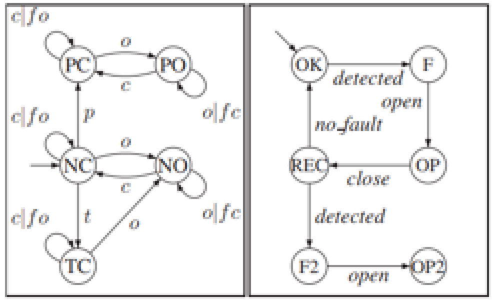
Explanation in different AI fields

- Machine Learning
- Computer Vision
- Knowledge Representation and Reasoning



Abduction Reasoning (in Bayesian Network)

David Poole: Probabilistic Horn Abduction and Bayesian Networks. Artif. Intell. 64(1): 81-129 (1993)

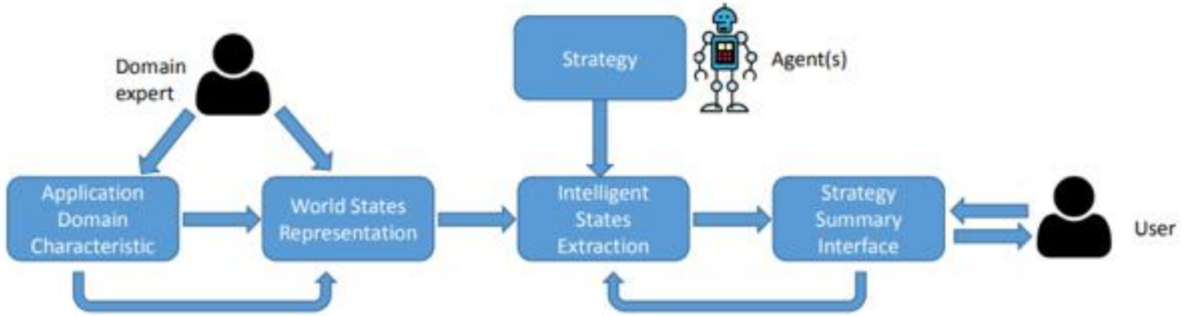


Diagnosis Inference

Alban Grastien, Patrik Haslum, Sylvie Thiébaux: Conflict-Based Diagnosis of Discrete Event Systems: Theory and Practice. KR 2012

Explanation in different AI fields

- Machine Learning
- Computer Vision
- Knowledge Representation and Reasoning
- Multi-agent Systems



Agent Strategy Summarization

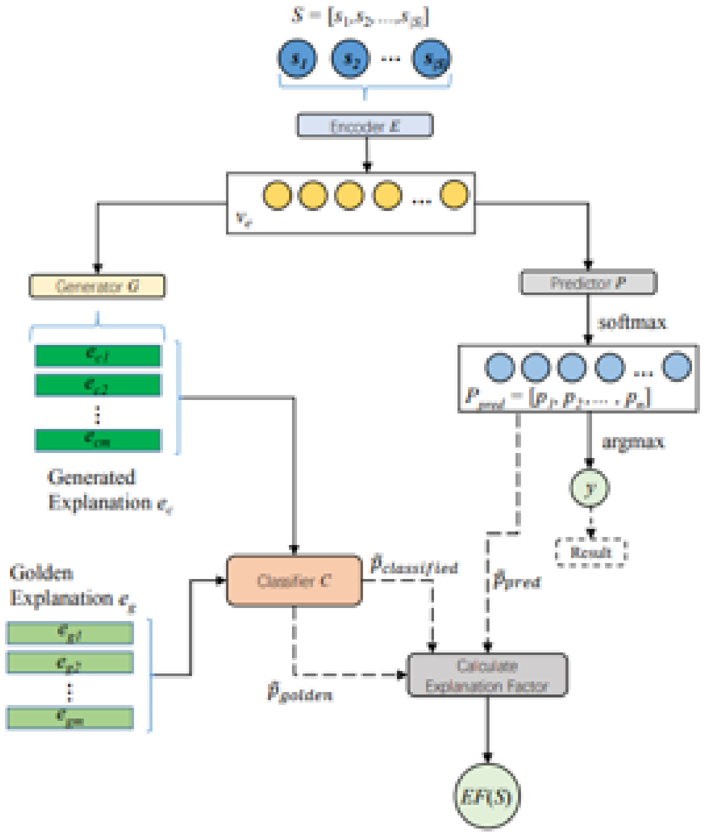
Ofra Amir, Finale Doshi-Velez, David Sarne: Agent Strategy Summarization. AAMAS 2018: 1203-1207

Explainable Agents

Joost Broekens, Maaike Harbers, Koen V. Hindriks, Karel van den Bosch, Catholijn M. Jonker, John-Jules Ch. Meyer: Do You Get It? User-Evaluated Explainable BDI Agents. MATES 2010: 28-39

Explanation in different AI fields

- Machine Learning
- Computer Vision
- Knowledge Representation and Reasoning
- Multi-agent Systems
- NLP

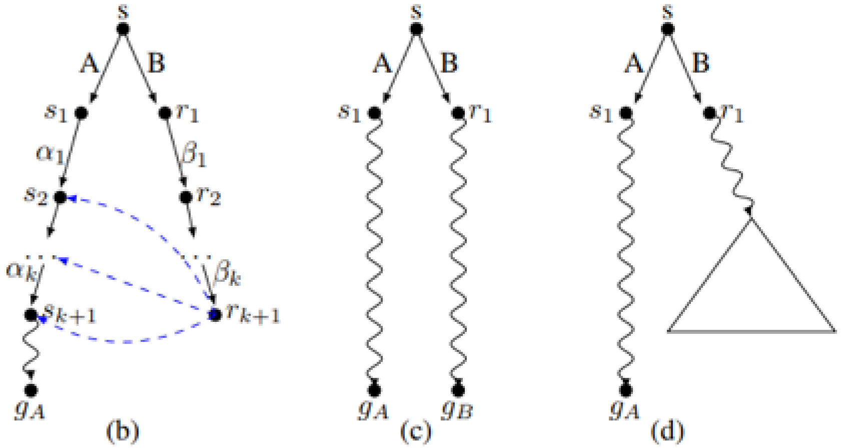


Explainable NLP

Hui Liu, Qingyu Yin, William Yang Wang: Towards Explainable NLP: A Generative Explanation Framework for Text Classification. CoRR abs/1811.00196 (2018)

Explanation in different AI fields

- Machine Learning
- Computer Vision
- Knowledge Representation and Reasoning
- Multi-agent Systems
- NLP
- Planning and Scheduling



Human-in-the-loop Planning

Maria Fox, Derek Long, Daniele Magazzeni: Explainable Planning. CoRR abs/1709.10256 (2017)

Explanation in different AI fields

- Machine Learning
- Computer Vision
- Knowledge Representation and Reasoning
- Multi-agent Systems
- NLP
- Planning and Scheduling
- Robotics

Robot: I have decided to turn left.

Human: Why did you do that?

Robot: I believe that the correct action is to turn left
BECAUSE:
I'm being asked to go forward
AND This area in front of me was 20 cm higher than me *highlights area*
AND the area to the left has maximum protrusions of less than 5 cm *highlights area*
AND I'm tilted to the right by more than 5 degrees.
Here is a display of the path through the tree that lead to this decision. *displays tree*

Human: How confident are you in this decision?

Robot: The distribution of actions that reached this leaf node is shown in this histogram. *displays histogram* This action is predicted to be correct 67% of the time.

Human: Where did the threshold for the area in front come from?

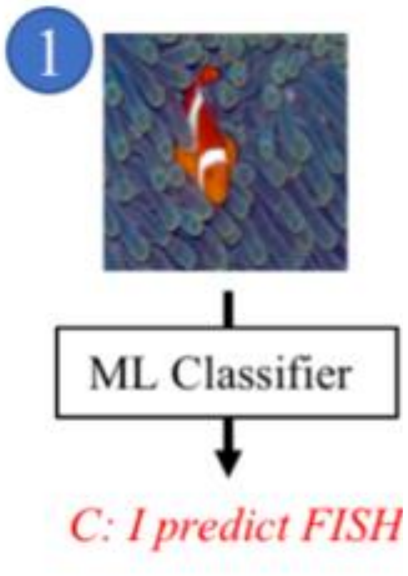
Robot: Here is the histogram of all training examples that reached this leaf. 80% of examples where this area was above 20 cm predicted the appropriate action to be "drive forward".

From Decision Tree to human-friendly information

Raymond Ka-Man Sheh: "Why Did You Do That?" Explainable Intelligent Robots. AAAI Workshops 2017

Explanation as *Machine-Human Conversation*

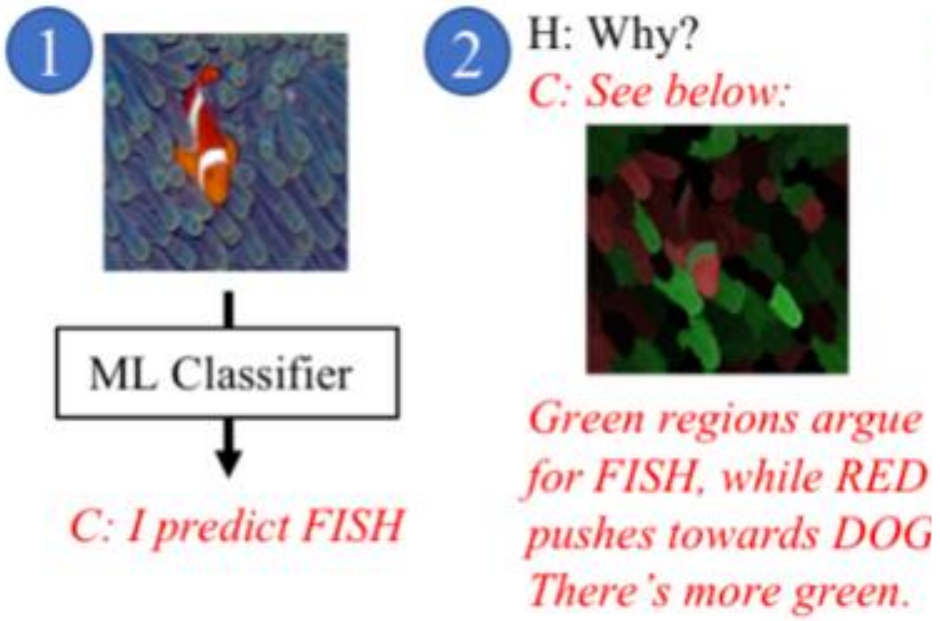
[Weld and Bansal 2018]



- Humans may have follow-up questions
- Explanations cannot answer all users' concerns

Explanation as *Machine-Human Conversation*

[Weld and Bansal 2018]



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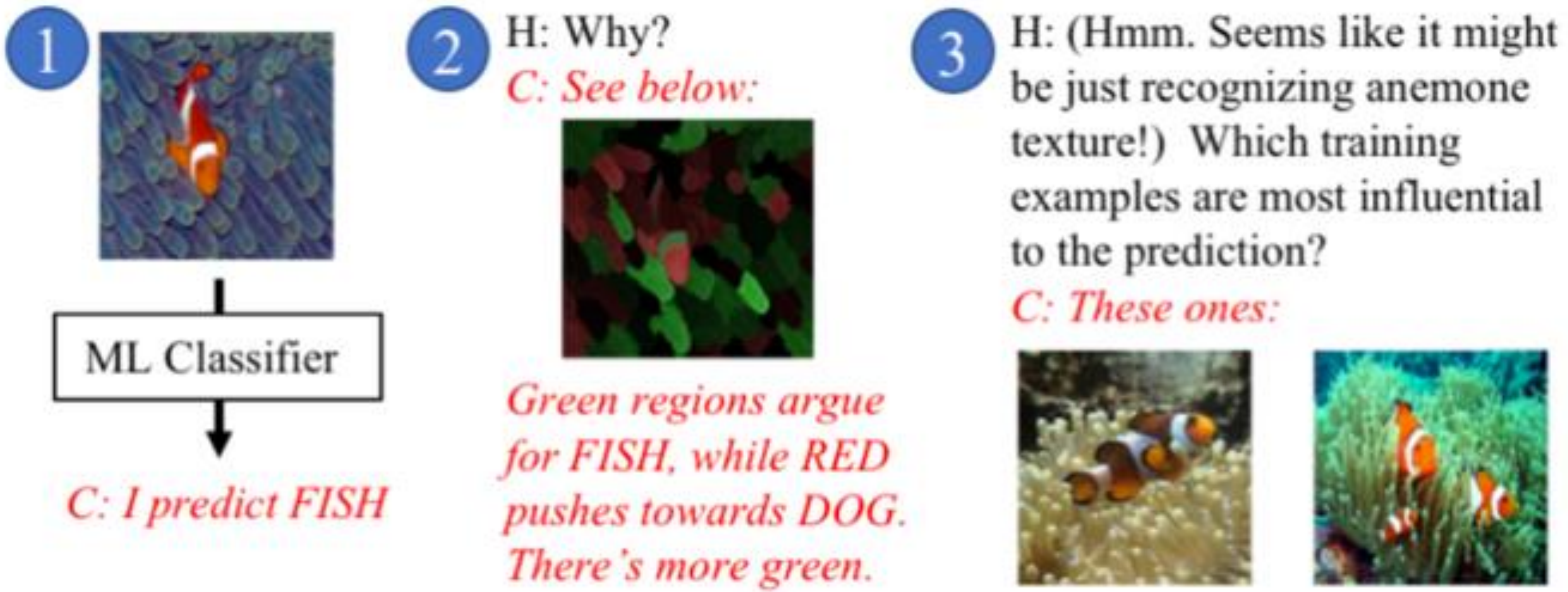
Explanation as *Machine-Human Conversation*

[Weld and Bansal 2018]



- Humans may have follow-up questions
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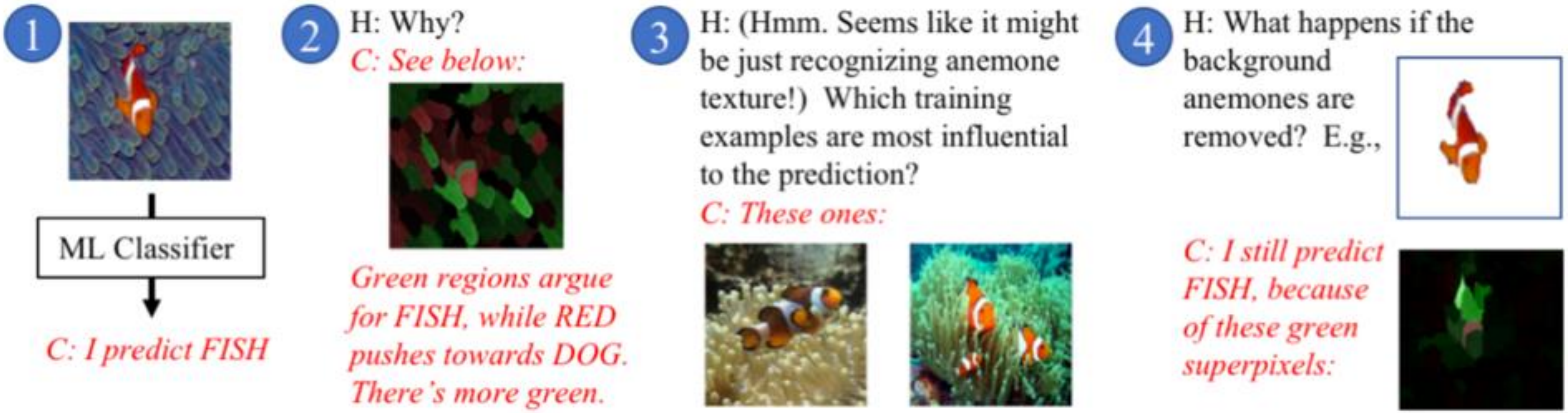
Explanation as *Machine-Human Conversation*

[Weld and Bansal 2018]



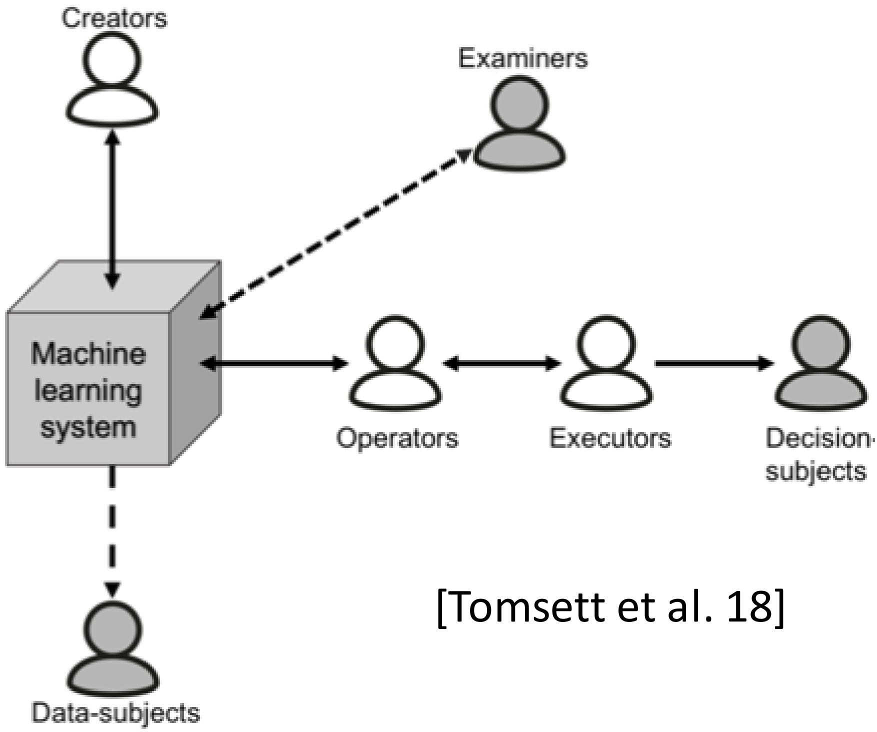
- Humans may have follow-up questions
- Explanations cannot answer all users' concerns

Role-based Interpretability

"~~Is the explanation interpretable~~?" → "*To whom* is the explanation interpretable?"

No Universally Interpretable Explanations!

- **End users** "Am I being treated fairly?"
  "Can I contest the decision?"
  "What could I do differently to get a positive outcome?"
- **Engineers, data scientists**: "Is my system working as designed?"
- **Regulators** " Is it compliant?"



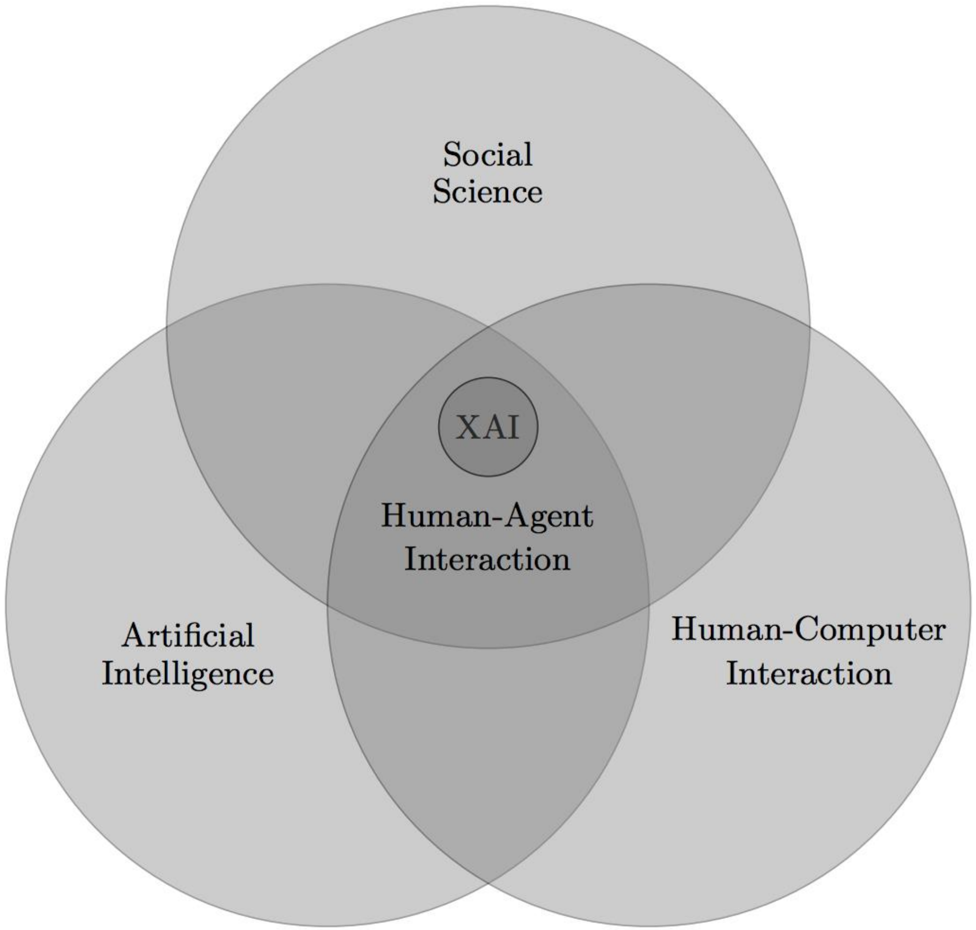
[Tomsett et al. 18]

An ideal explainer should model the *user background.*

[Tomsett et al. 2018, Weld and Bansal 2018, Poursabzi-Sangdeh 2018, Mittelstadt et al. 2019]

XAI is Interdisciplinary

- For millennia, philosophers have asked the questions about what constitutes an explanation, what is the function of explanations, and what are their structure
- **[Tim Miller 2018]**

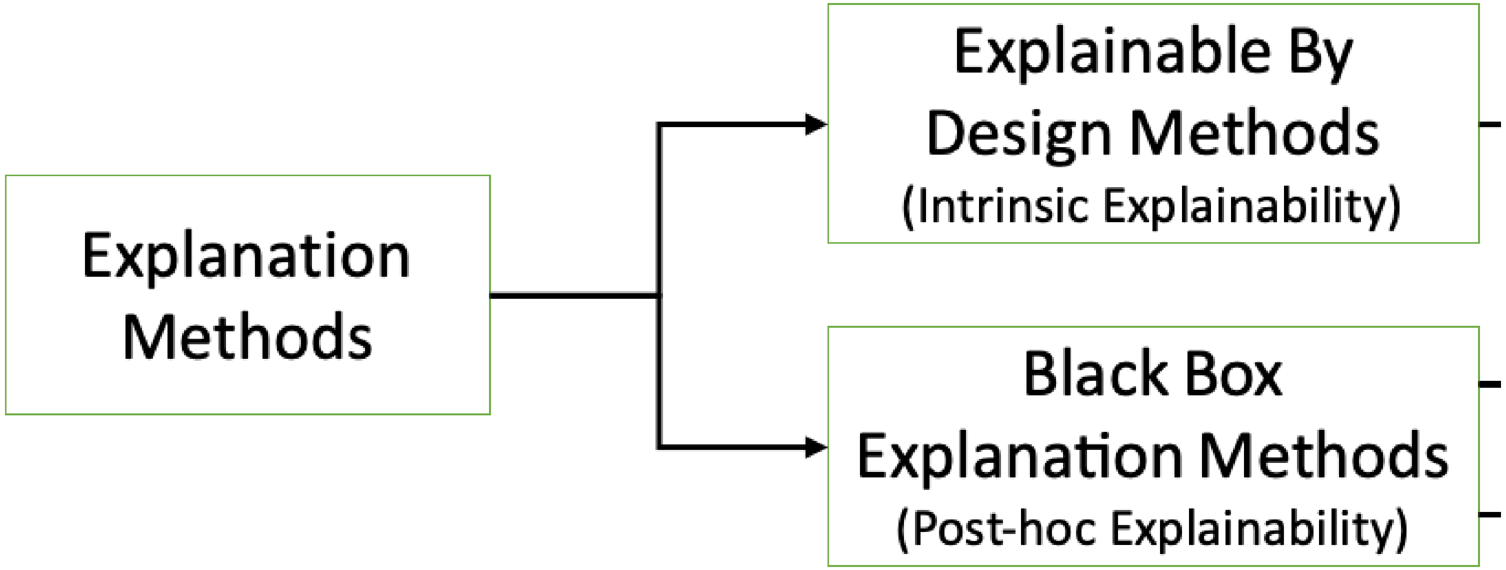


How to Open the Black Box

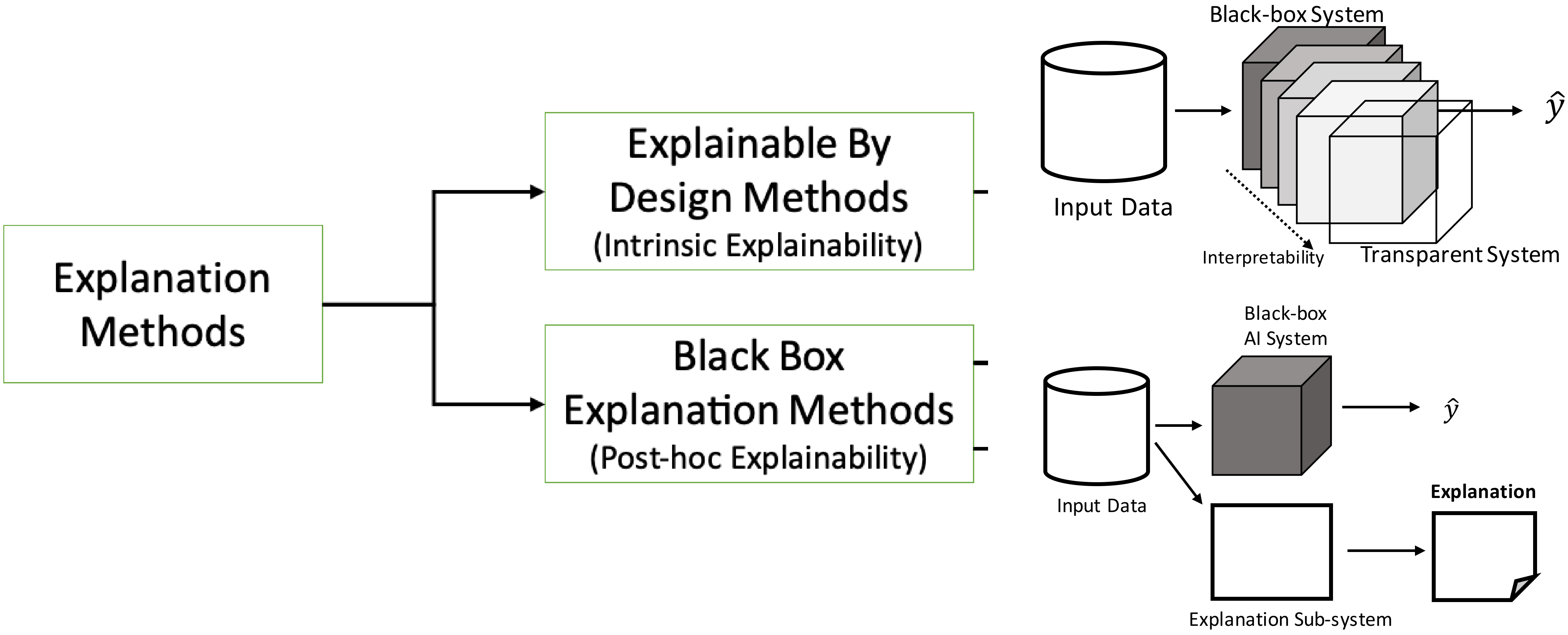
XAI Taxonomy of Explanation Methods

Explanation Methods

XAI Taxonomy of Explanation Methods



XAI Taxonomy of Explanation Methods



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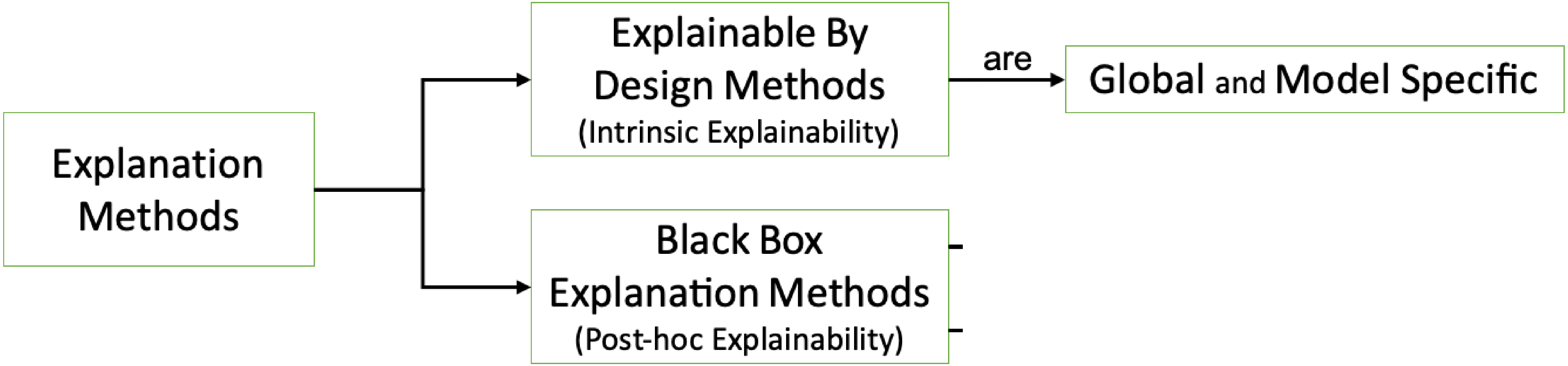
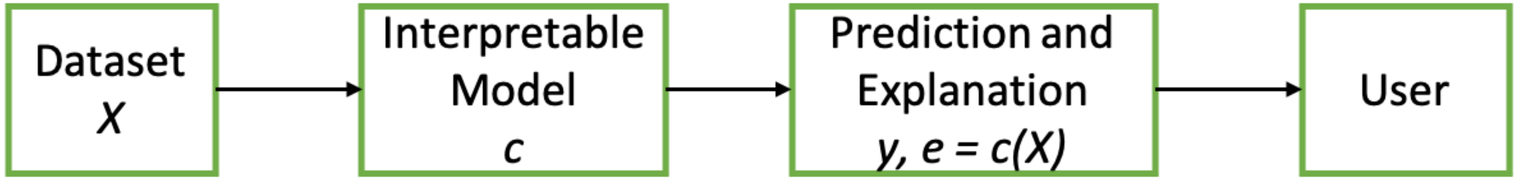
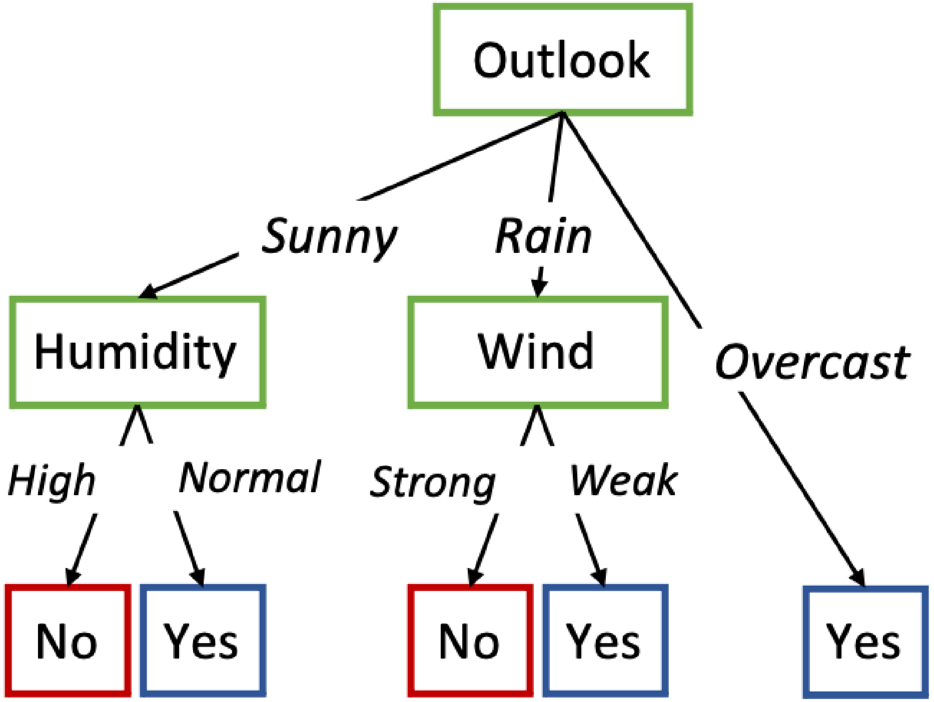
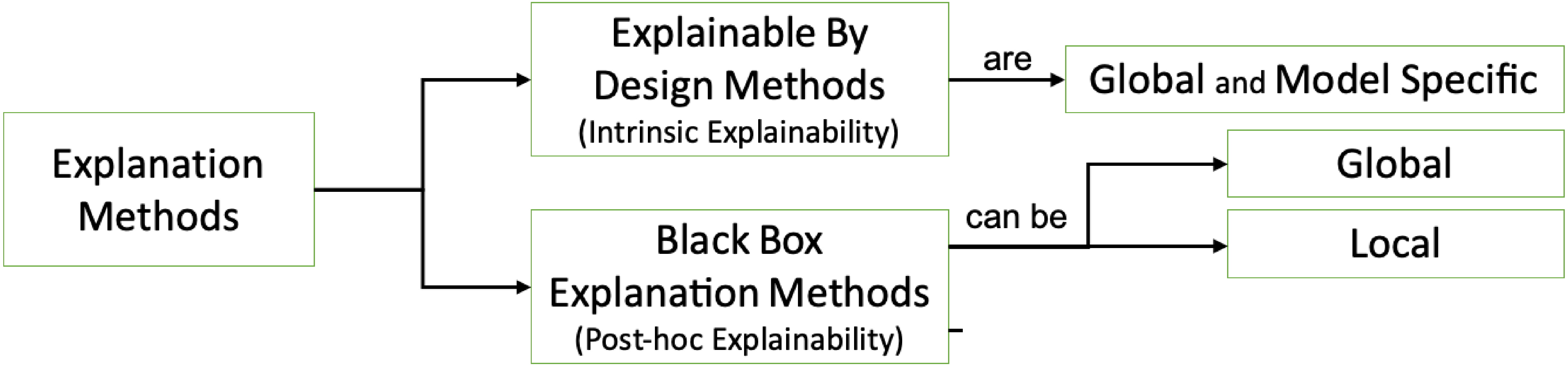


Explainable by Design Method

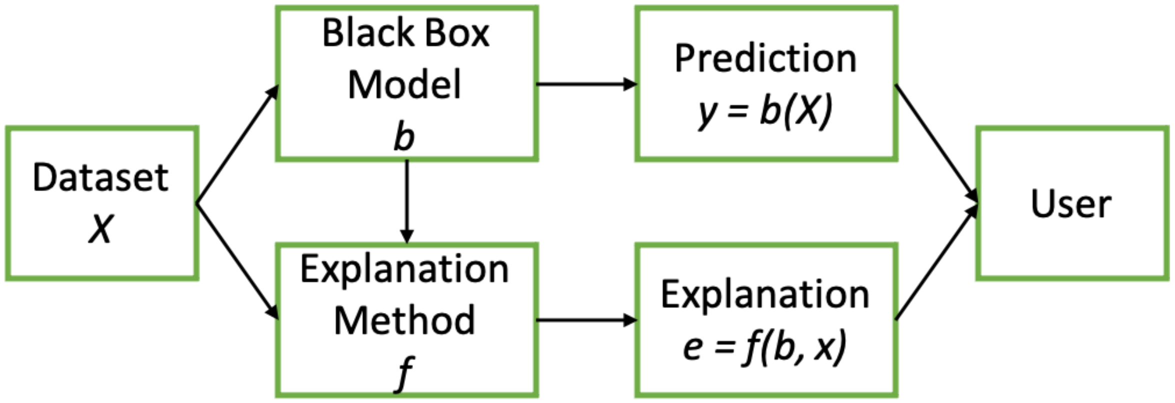


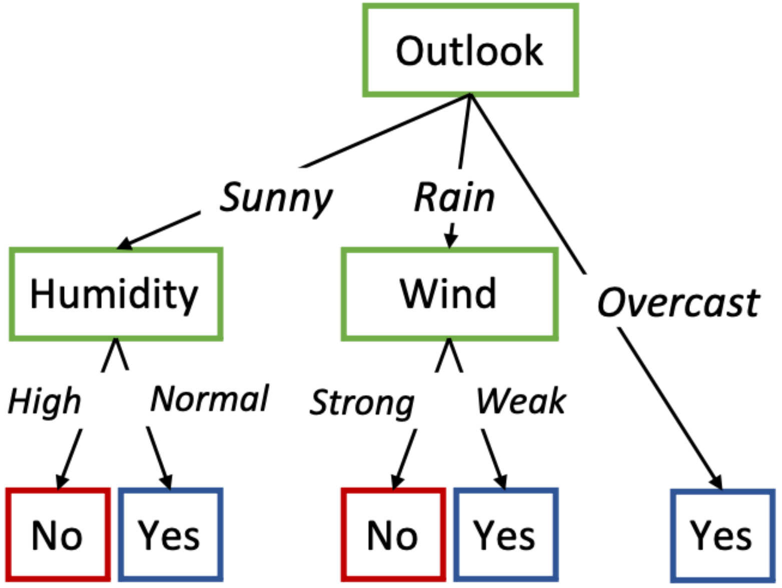


XAI Taxonomy of Explanation Methods



Black Box Explanations: Global vs Local





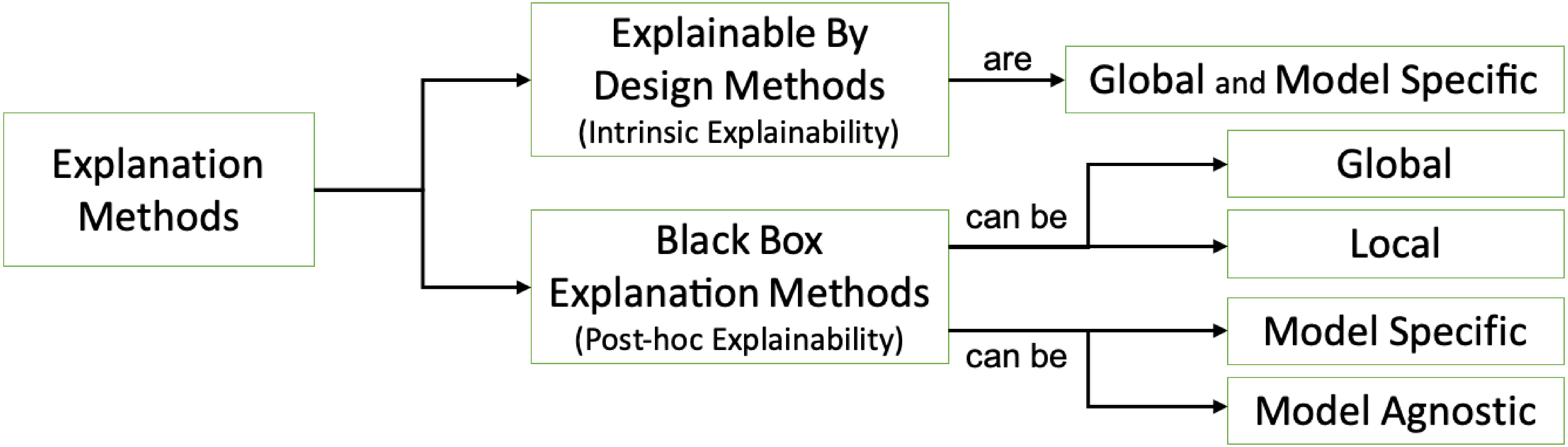
If Outlook = *Sunny* and Humidity = *Normal*
then Play Tennis = ***Yes***

- Outlook: *0.7*
- Humidity: *-0.4*
- Wind: *0.0*

Global Explanation

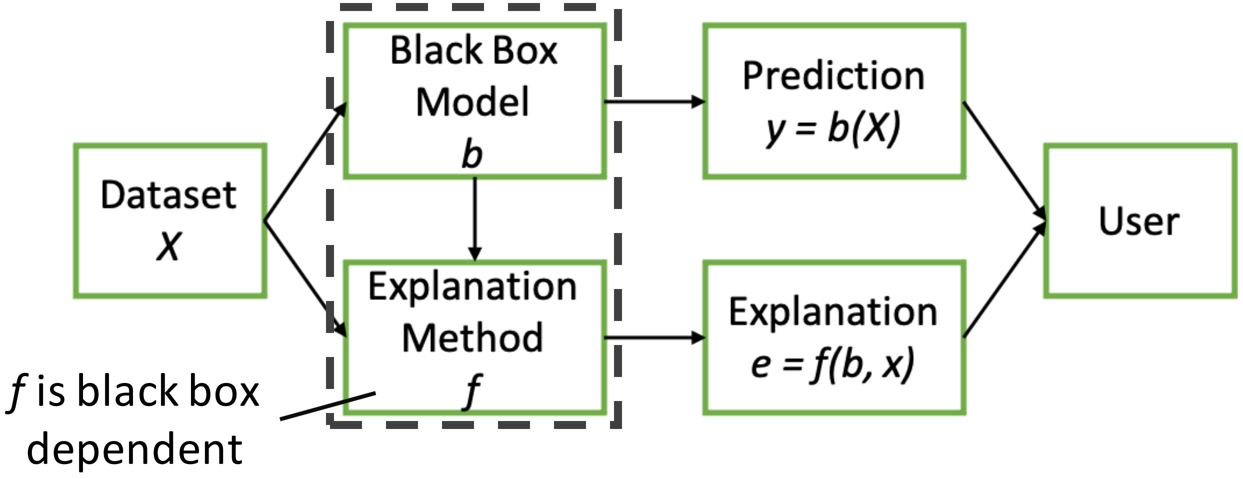
Local Explanations

XAI Taxonomy of Explanation Methods

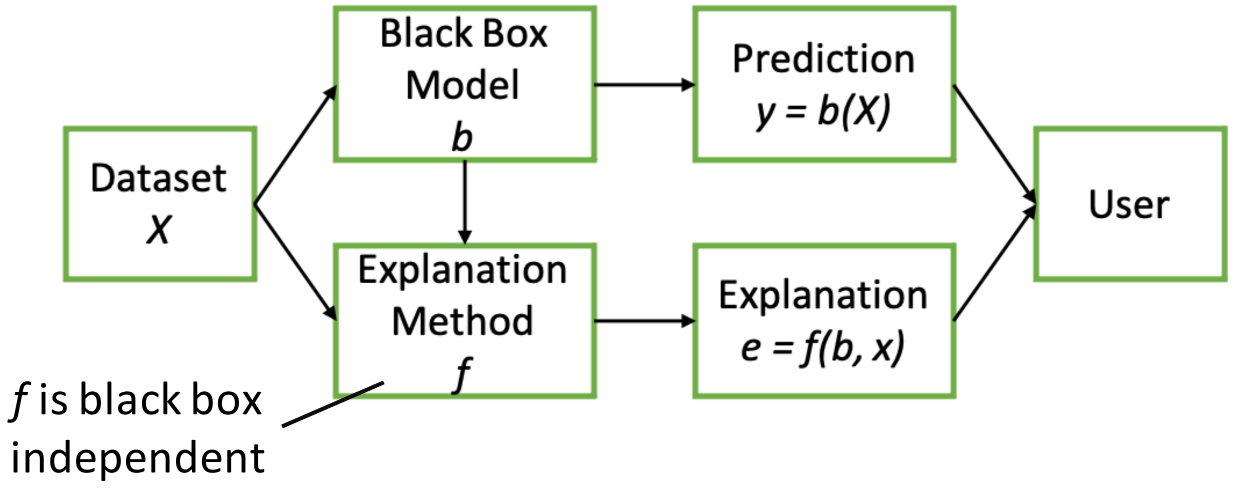


Black Box Explanations: Specific vs Agnostic

Model Specific



Model Agnostic



Types of Data

Table of baby-name data
(baby-2010.csv)

name	rank	gender	year
Jacob	1	boy	2010
Isabella	1	girl	2010
Ethan	2	boy	2010
Sophia	2	girl	2010
Michael	3	boy	2010

Field names

One row (4 fields)

2000 rows all told

Tabular

(TAB)

Images

(IMG)

Text

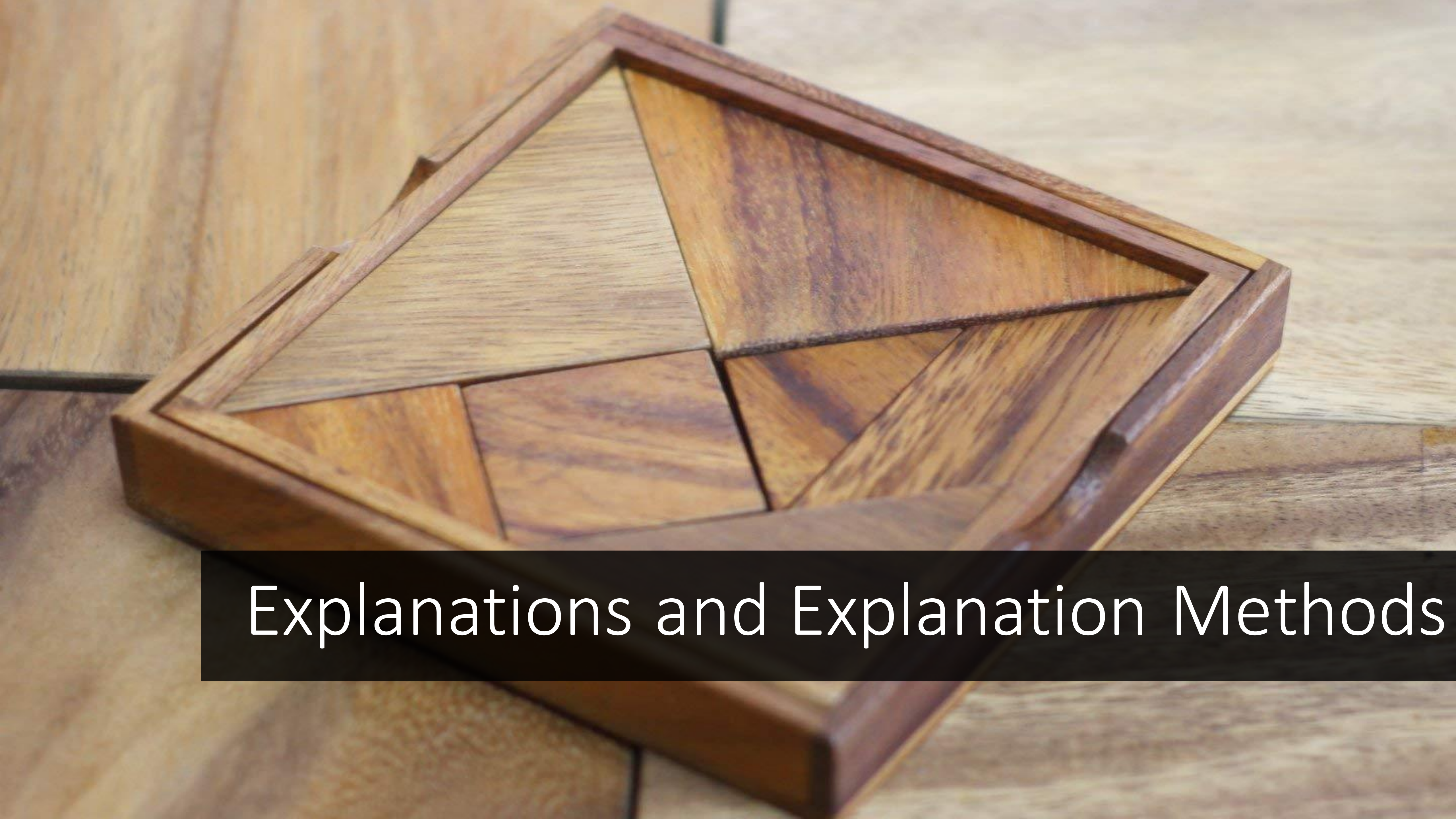
(TXT)

Types of Explanations

- Tabular Data
  - Rule-based
  - Decision Tree
  - Features Importance
  - Prototypes
  - Counter-exemplars
- Images
  - Saliency Maps
  - Concept Attributions
  - Prototypes
  - Counter-exemplars
- Text
  - Sentence Highlighting
  - Attention-based
  - Prototypes
  - Counter-exemplars

If Outlook = *Sunny* and Humidity = *Normal*
then Play Tennis = ***Yes***

- Outlook: *0.7*
- Humidity: *-0.4*
- Wind: *0.0*

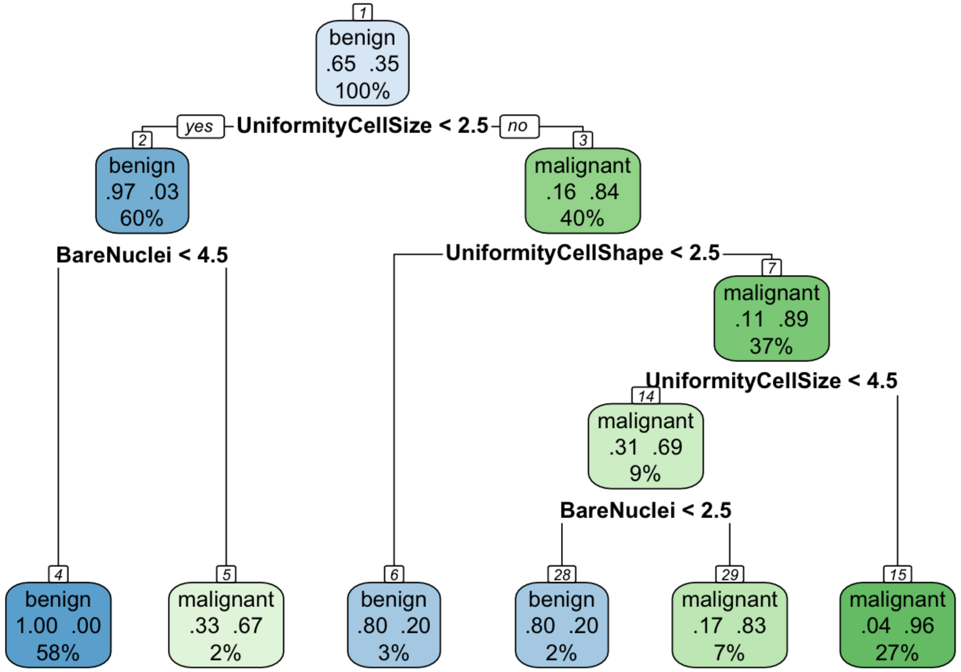


Explanations and Explanation Methods

TREPAN

Trepan

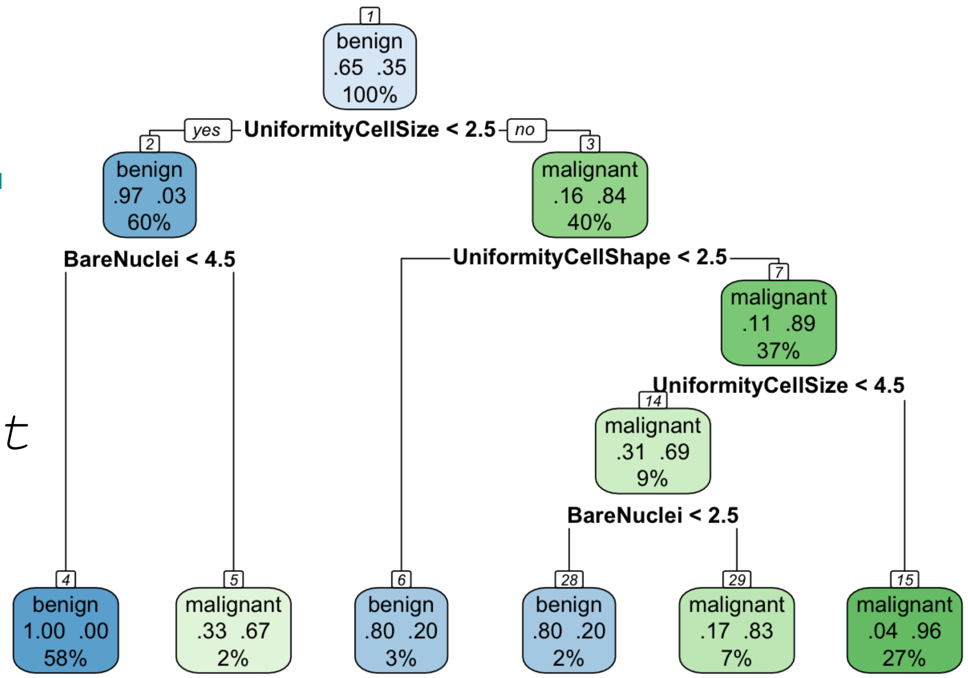
- Global explainer designed to explain NN but usable for any type of black box.
- It aims at approximating a NN with a DT classifier using best-m-of-n rules.
- At each node split the feature to split is selected on the original data extended with random samples respecting the current path.
- It learns to predict the label returned by the black box, not the original one.



Trepan

```
T = root_of_the_tree()
Q = <T, X, {}>
while Q not empty & size(T) < limit
    N, X_N, C_N = pop(Q)
    Z_N = random(X_N, C_N)
    y_Z = b(Z), y = b(X_N)
    if same_class(y U y_Z)
        continue
    S = best_split(X_N U Z_N, y U y_Z)
    S' = best_m-of-n_split(S)
    N = update_with_split(N, S')
    for each condition c in S'
        C = new_child_of(N)
        C_C = C_N U {c}
        X_C = select_with_constraints(X_N, C_N)
        put(Q, <C, X_C, C_C>)
```

black box auditing

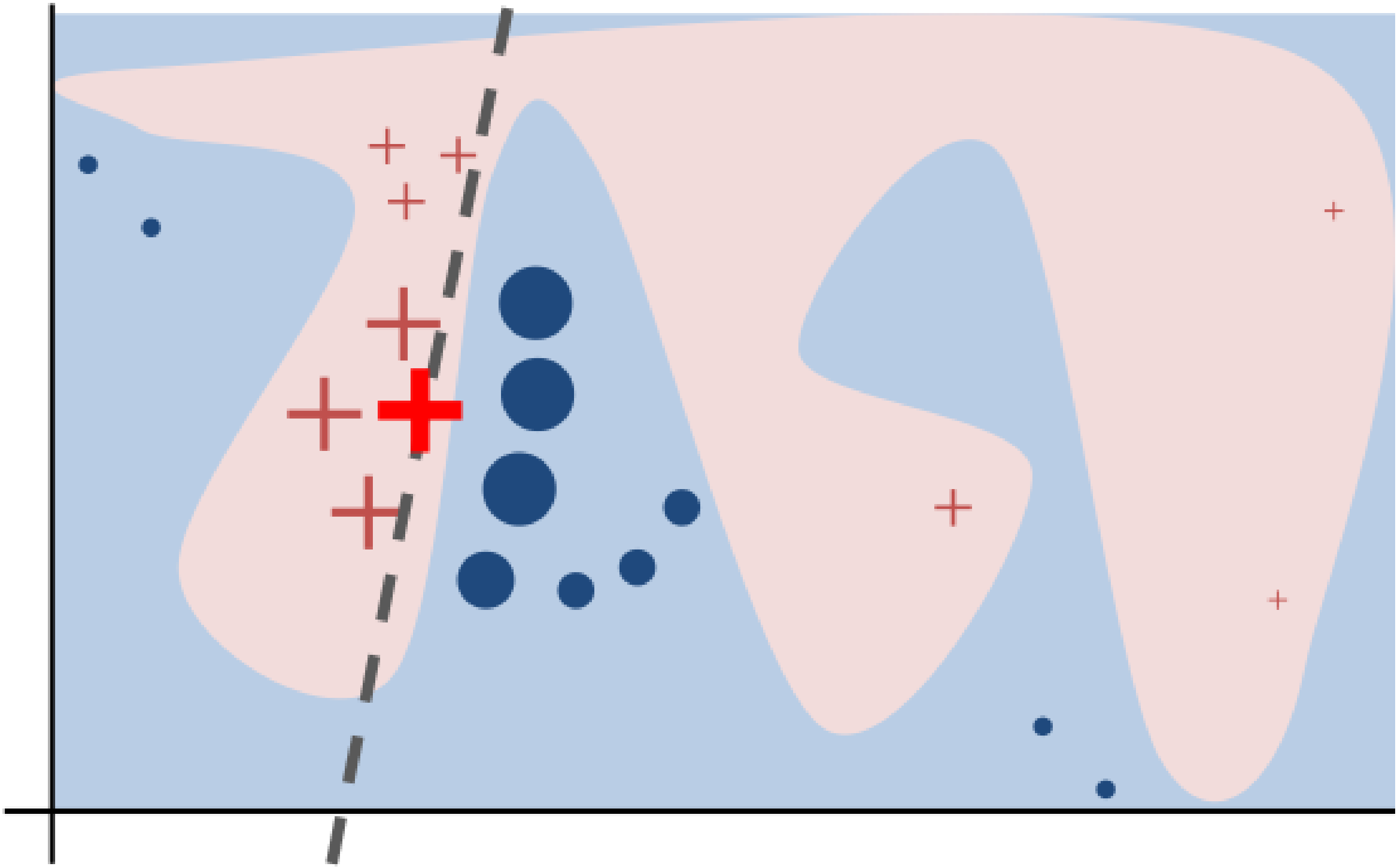


- Mark Craven and JudeW. Shavlik. 1996. ***Extracting tree-structured representations of trained networks***. NIPS.

LIME

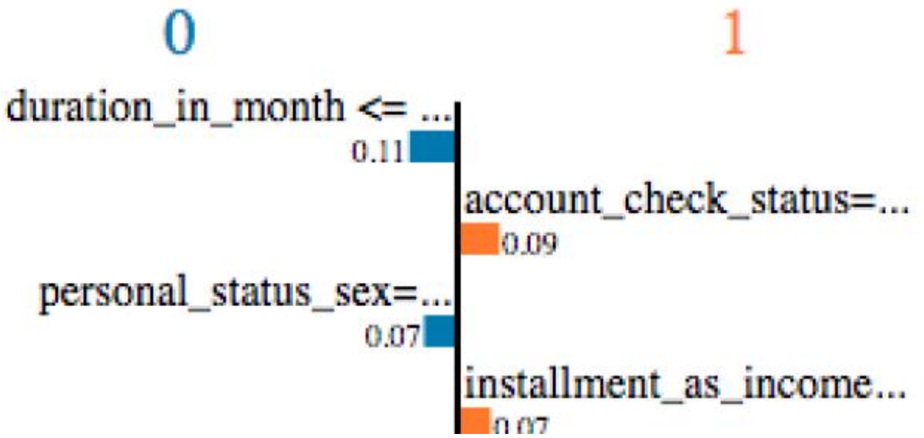
Local Explanation

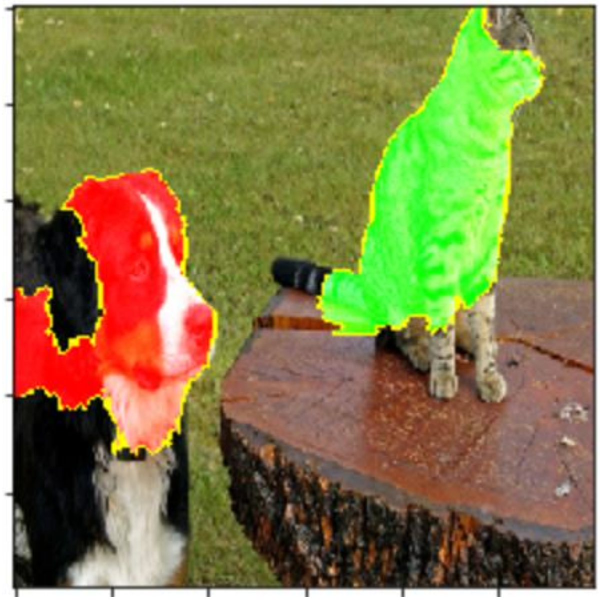
- The overall decision boundary is complex
- In the neighborhood of a single decision, the boundary is simple
- A single decision can be explained by auditing the black box around the given instance and learning a *local* decision.



Local Interpretable Model-agnostic Explanations

- Local model-agnostic explainer that reveals the black box decisions through features importance/saliency maps.
- It locally approximates the behavior of a black box with a local surrogate expressed as a logistic regressor (with Lasso or Ridge penalization).
- Synthetic neighbors are weighted w.r.t. the distance with the instance to explain.





LIME

Sepal length	Sepal width	Petal length	Petal width	b(setosa)	b(versic)	b(virgi)
3	4	3	6	0.1	0.7	0.2

LIME

Sepal length	Sepal width	Petal length	Petal width	b(setosa)	b(versic)	b(virgi)
3	4	3	6	0.1	0.7	0.2
3	4	5	6	0.4	0.4	0.6

LIME

Sepal length	Sepal width	Petal length	Petal width	b(setosa)	b(versic)	b(virgi)
3	4	3	6	0.1	0.7	0.2
3	4	5	6	0.4	0.4	0.6
3	2	3	8	0.3	0.6	0.1

LIME

Sepal length	Sepal width	Petal length	Petal width	b(setosa)	b(versic)	b(virgi)
3	4	3	6	0.1	0.7	0.2
3	4	5	6	0.4	0.4	0.6
3	2	3	8	0.3	0.6	0.1
5	2	3	6	0.0	0.3	0.7
2	4	4	7	0.0	0.8	0.2

LIME

Sepal length	Sepal width	Petal length	Petal width	b(setosa)	b(versic)	b(virgi)
3	4	3	6	0.1	0.7	0.2
3	4	5	6	0.4	0.4	0.6
3	2	3	8	0.3	0.6	0.1
5	2	3	6	0.0	0.3	0.7
2	4	4	7	0.0	0.8	0.2

Train a Linear Regressor

LIME

Sepal length	Sepal width	Petal length	Petal width	b(setosa)	b(versic)	b(virgi)
3	4	3	6	0.1	0.7	0.2
3	4	5	6	0.4	0.4	0.6
3	2	3	8	0.3	0.6	0.1
5	2	3	6	0.0	0.3	0.7
2	4	4	7	0.0	0.8	0.2

Train a Linear Regressor

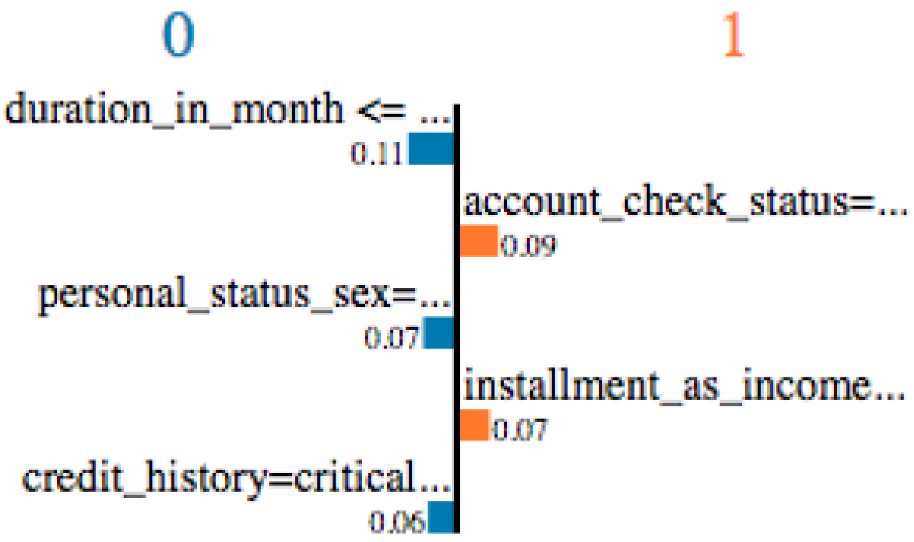
Returns the coefficients as Explanation

LIME

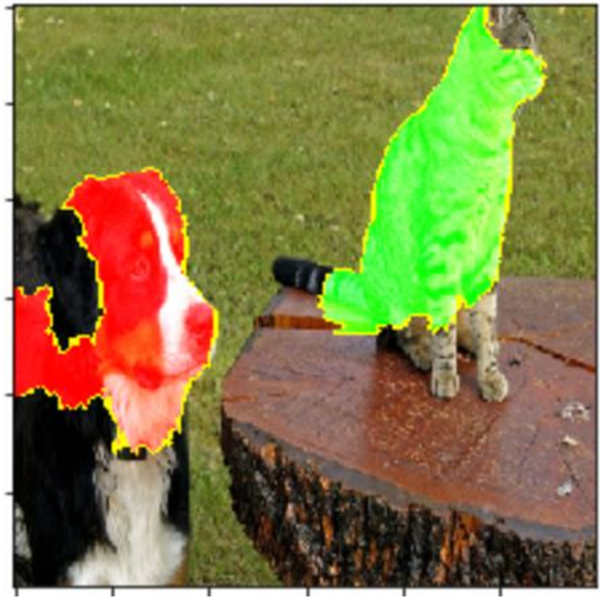
```
Z = {}
x instance to explain
x' = real2interpretable(x)
for i in {1, 2, …, N}
        z_i= sample_around(x')
        z = interpretabel2real(z')
        Z = Z U {<z_i, b(z_i), d(x, z)>}
w = solve_Lasso(Z, k)
return w
```

black box auditing

Features Importance



Saliency Map

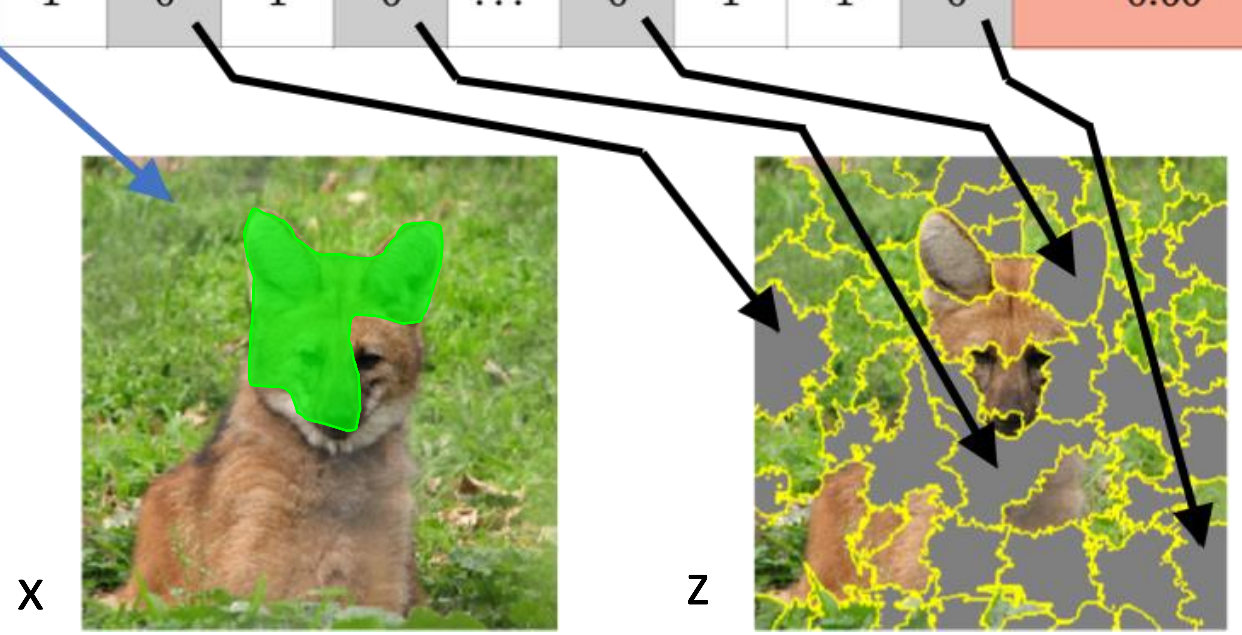


- Marco Tulio Ribeiro, Sameer Singh, and Carlos Guestrin. 2016. Why should i trust you?: Explaining the predictions of any classifier. KDD.

LIME

- LIME ***turns*** an image x to a vector x’ of interpretable superpixels expressing presence/absence.
- It ***generates*** a synthetic neighborhood Z by randomly perturbing x’ and labels them with the black box.
- It ***trains*** a linear regression model (interpretable and locally faithful) and assigns a weight to each superpixel.

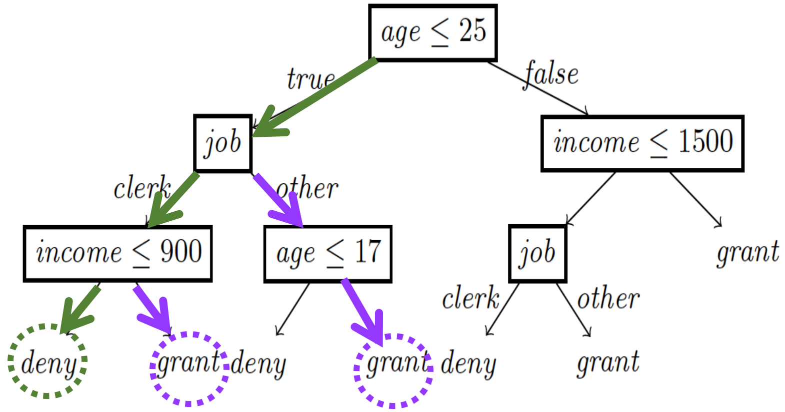
x'	1	1	1	1	...	1	1	1	1	0.94
	1	1	0	0	...	1	1	1	1	0.58
	1	1	1	0	...	0	0	1	1	0.15
z'	1	0	1	0	...	0	1	1	0	0.66



LORE

*LO*cal *R*ule-based *E*xplainer

- LORE extends LIME adopting as local surrogate a decision tree classifier and by generating synthetic instances through a genetic procedure that accounts for both instances with the same labels and different ones.
- It can be generalized to work on images and text using the same data representation adopted by LIME.



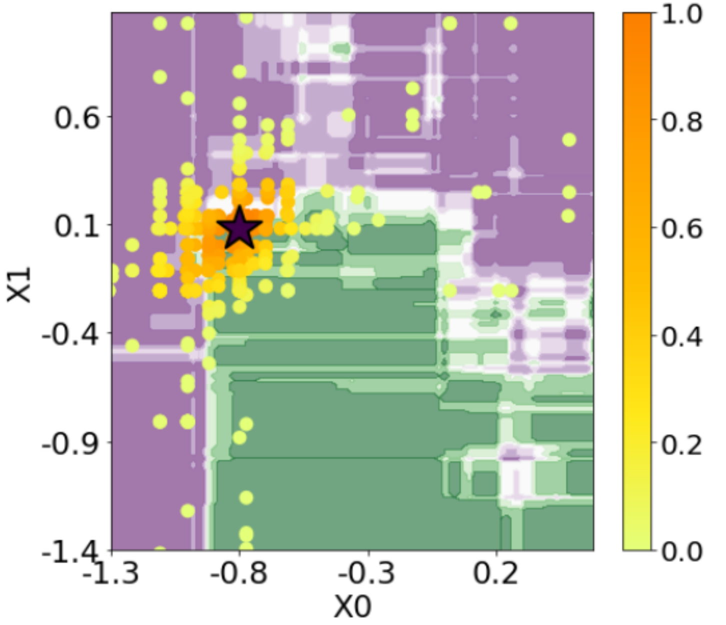
LORE

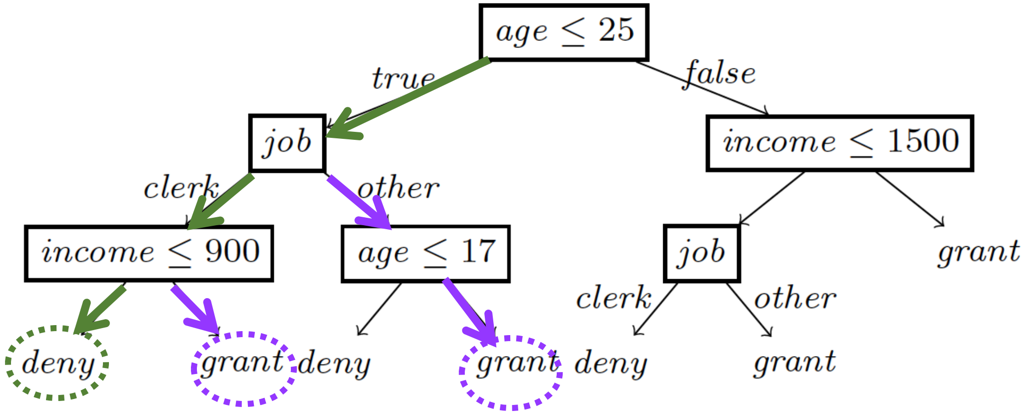
parent 1	25	clerk	10k	yes
parent 2	30	other	5k	no
children 1	25	other	5k	yes
children 2	30	clerk	10k	no

```
x instance to explain
Z_= = geneticNeighborhood(x, fitness_=, N/2)
Z_≠ = geneticNeighborhood(x, fitness_≠, N/2)
Z = Z_= ∪ Z_≠
c = buildTree(Z, b(Z))
r = (p -> y) = extractRule(c, x)
ϕ = extractCounterfactual(c, r, x)
return e = <r, ϕ>
```

black box auditing

parent	25	clerk	10k	yes
children	27	clerk	7k	yes





r = {age ≤ 25, job = clerk, income ≤ 900} -> deny

Φ = {({income > 900} -> grant),
({17 ≤ age < 25, job = other} -> grant)}

LORE

$$x_1 = \{ \textit{Education} = \textit{Bachelors}, \textit{Occupation} = \textit{Prof-specialty}, \textit{Sex} = \textit{Male}, \textit{NativeCountry} = \textit{Vietnam}, \textit{Age} = 35, \textit{Workclass} = 3, \textit{HoursWeek} = 40, \textit{Race} = \textit{Asian-Pac-Islander}, \textit{MaritialStatus} = \textit{Married-civ}, \textit{Relationship} = \textit{Husband}, \textit{CapitalGain} = 0, \textit{CapitalLoss} = 0\}, > 50k$$

$$r_{lore} = \{ \textit{Education} > \textit{5-6th}, \textit{Race} > 0.86, \textit{WorkClass} \leq 3.41, \textit{CapitalGain} \leq 20000, \textit{CapitalLoss} \leq 1306 \} \rightarrow > 50k$$

$$c_{lore} = \{\textit{CapitalLoss} \geq 436 \} \rightarrow \leq 50k$$

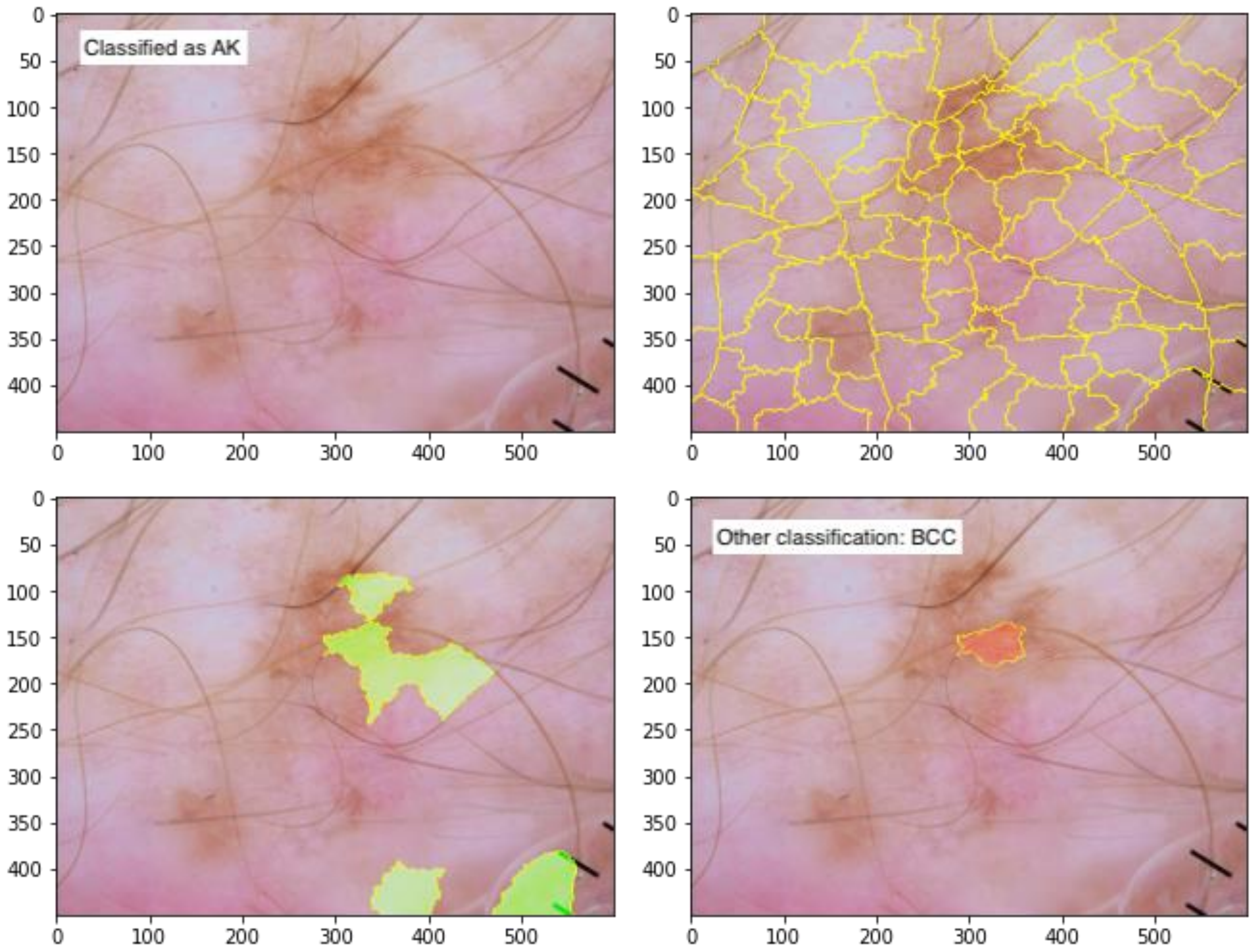
$$x_2 = \{ \textit{Education} = \textit{College}, \textit{Occupation} = \textit{Sales}, \textit{Sex} = \textit{Male}, \textit{NativeCountry} = \textit{US}, \textit{Age} = 19, \textit{Workclass} = 2, \textit{HoursWeek} = 15, \textit{Race} = \textit{White}, \textit{MaritialStatus} = \textit{Married-civ}, \textit{Relationship} = \textit{Husband}, \textit{CapitalGain} = 2880, \textit{CapitalLoss} = 0 \}, \leq 50k$$

$$r_{lore} = \{\textit{Education} \leq \textit{Masters}, \textit{Occupation} > -0.34, \textit{HoursWeek} \leq 40, \textit{WorkClass} \leq 3.50, \textit{CapitalGain} \leq 10000, \textit{Age} \leq 34\} \rightarrow \leq 50k$$

$$c_{lore} = \begin{array}{l} \{\textit{Education} > \textit{Masters} \} \rightarrow > 50k \\ \{\textit{CapitalGain} > 20000 \} \rightarrow > 50k \\ \{\textit{Occupation} \leq -0.34 \} \rightarrow > 50k \end{array}$$

LORE on Medical Images

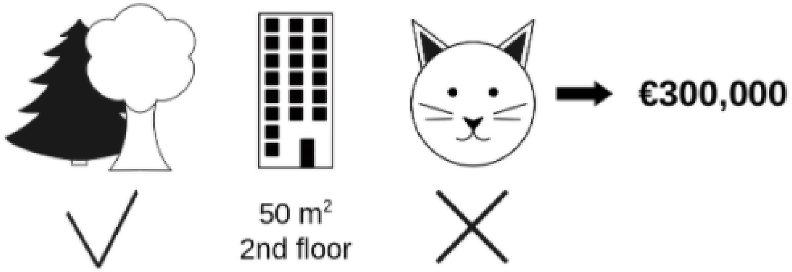
- The goal is to classify dermoscopic images among categories such as: Melanoma (MEL), Melanocytic Nevus (NV); Basal Cell Carcinoma (BCC), Actinic Keratosis (AK), etc.
- The original is classified as AK
- The counterfactual as BCC.



SHAP

Shapely Values

- A prediction can be explained by assuming that each feature value of the instance is a "player" in a game where the prediction is the payout. Shapley values -- a method from coalitional game theory -- tells us how to fairly distribute the "payout" among the features.
- Example: A black box predicts apartment prices. For a certain apartment it predicts €300,000 and you need to explain this prediction. The apartment has an area of 50 m^2, is located on the 2nd floor, has a park nearby and cats are banned.

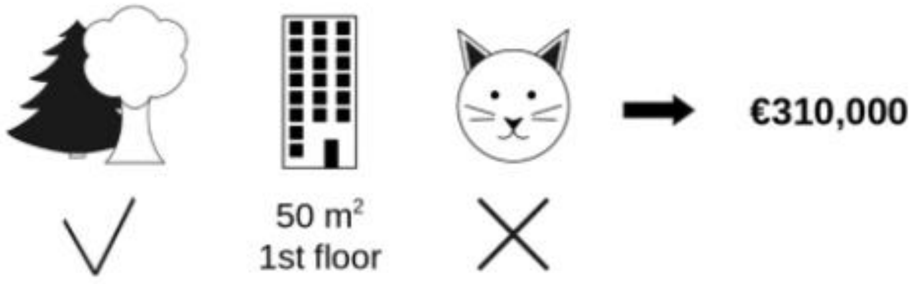


Shapely Values and Game Theory

- The average prediction is €310,000. How much has each feature value contributed to the prediction compared to the average prediction?
- The "game" is the prediction task for a single instance of the dataset.
- The "gain" is the actual prediction for this instance minus the average prediction for all instances.
- The "players" are the feature values of the instance that collaborate to receive the gain (= predict a certain value).
- The explanation could be: The park-nearby contributed €30,000; area-50 contributed €10,000; floor-2nd contributed €0; cat-banned contributed -€50,000. The contributions add up to -€10,000, the final prediction minus the average predicted apartment price.

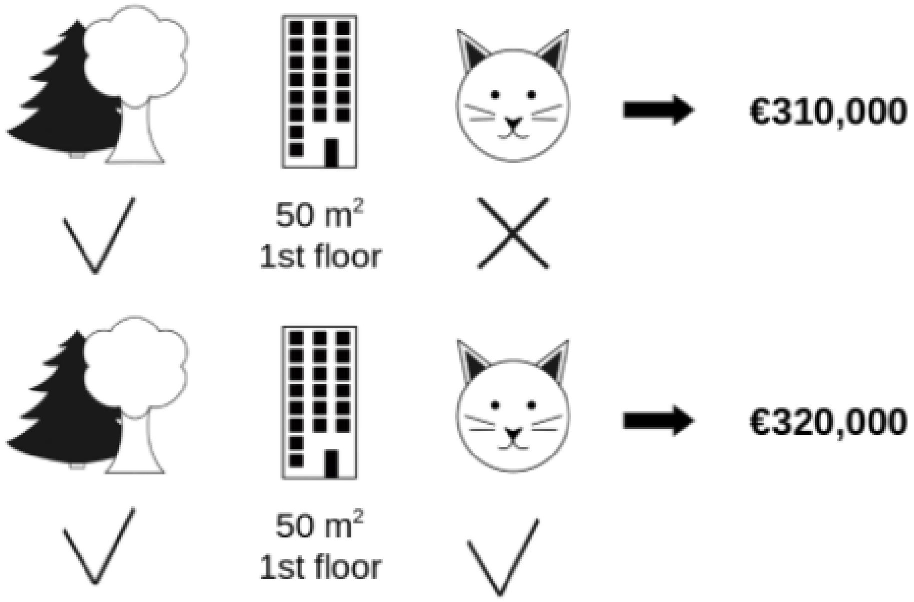
Shapely Values Example

- The Shapley value is the average marginal contribution of a feature value across all possible *coalitions* (combination of fixed feature values).
- We evaluate the contribution of *cat-banned when it is added to a coalition of park-nearby and area-50*.
- We simulate that only park-nearby, cat-banned and area-50 are in a coalition by randomly drawing another apartment from the data and using its value for the floor feature.
- The floor-2nd is replaced by the randomly drawn floor-1st.
- Then we predict the price of the apartment with this combination (€310,000).



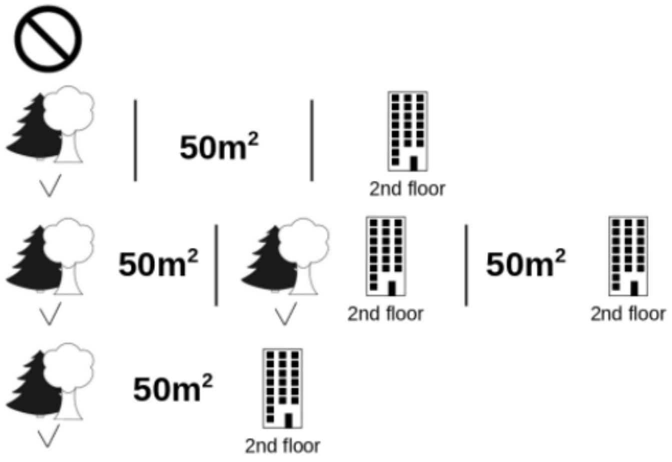
Shapely Values Example

- In a second step, we remove cat-banned from the coalition by replacing it with a random value of the cat allowed/banned from the randomly drawn apartment. In the example it was cat-allowed, but it could have been cat-banned again.
- We predict the apartment price for the coalition of park-nearby and area-50 (€320,000).
- The contribution of cat-banned was €310,000 - €320,000 = -€10,000. This estimate depends on the values of the randomly drawn apartment that served as a "donor" for the cat and floor feature values.
- We get better estimates if we repeat this sampling step and average the contributions.

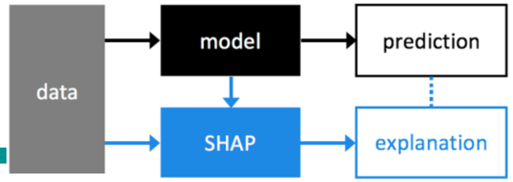


Shapely Values Example

- We repeat this computation for all possible coalitions.
- The Shapley value is the average of all the marginal contributions to all possible coalitions.
- The computation time increases exponentially with the number of features.
- For each of these coalitions we compute the predicted apartment price with and without the feature value cat-banned and take the difference to get the marginal contribution.
- We replace the feature values of features that are not in a coalition with random feature values from the apartment dataset to get a prediction from the black box.
- If we estimate the Shapley values for all feature values, we get the complete distribution of the prediction (minus the average) among the feature values.



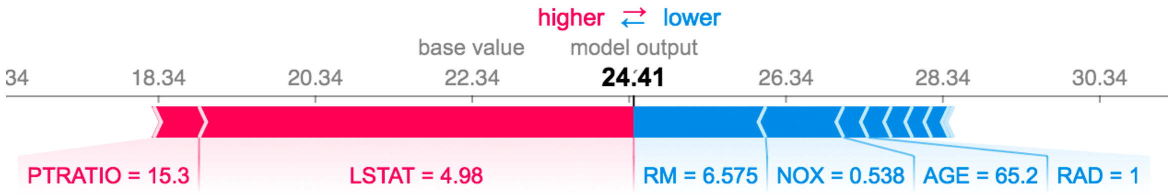
SHAP

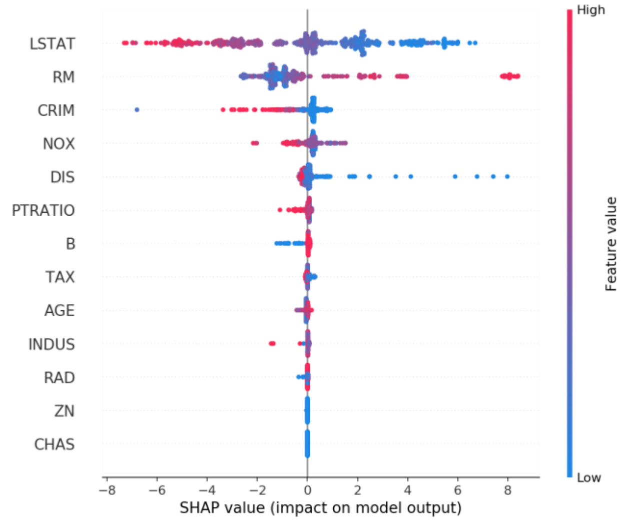


- SHAP (SHapley Additive exPlanations) assigns each feature an importance value for a particular prediction by means of an additive feature attribution method.
- It assigns an importance value to each feature that represents the effect on the model prediction of including that feature

$$g(z') = \phi_0 + \sum_{i=1}^{M} \phi_i z'_i,$$

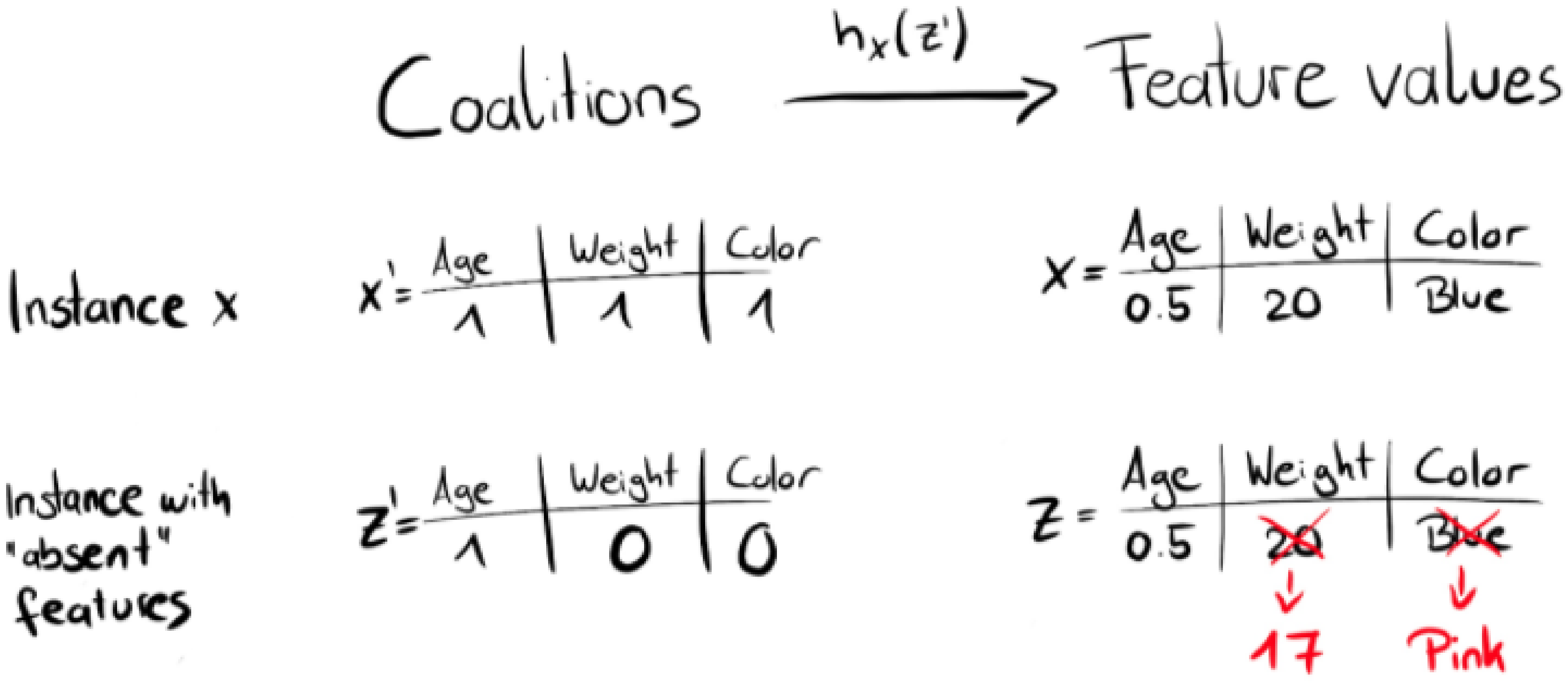
$$\phi_i = \sum_{S \subseteq F \setminus \{i\}} \frac{|S|!(|F| - |S| - 1)!}{|F|!} \left[f_{S \cup \{i\}}(x_{S \cup \{i\}}) - f_S(x_S) \right]$$



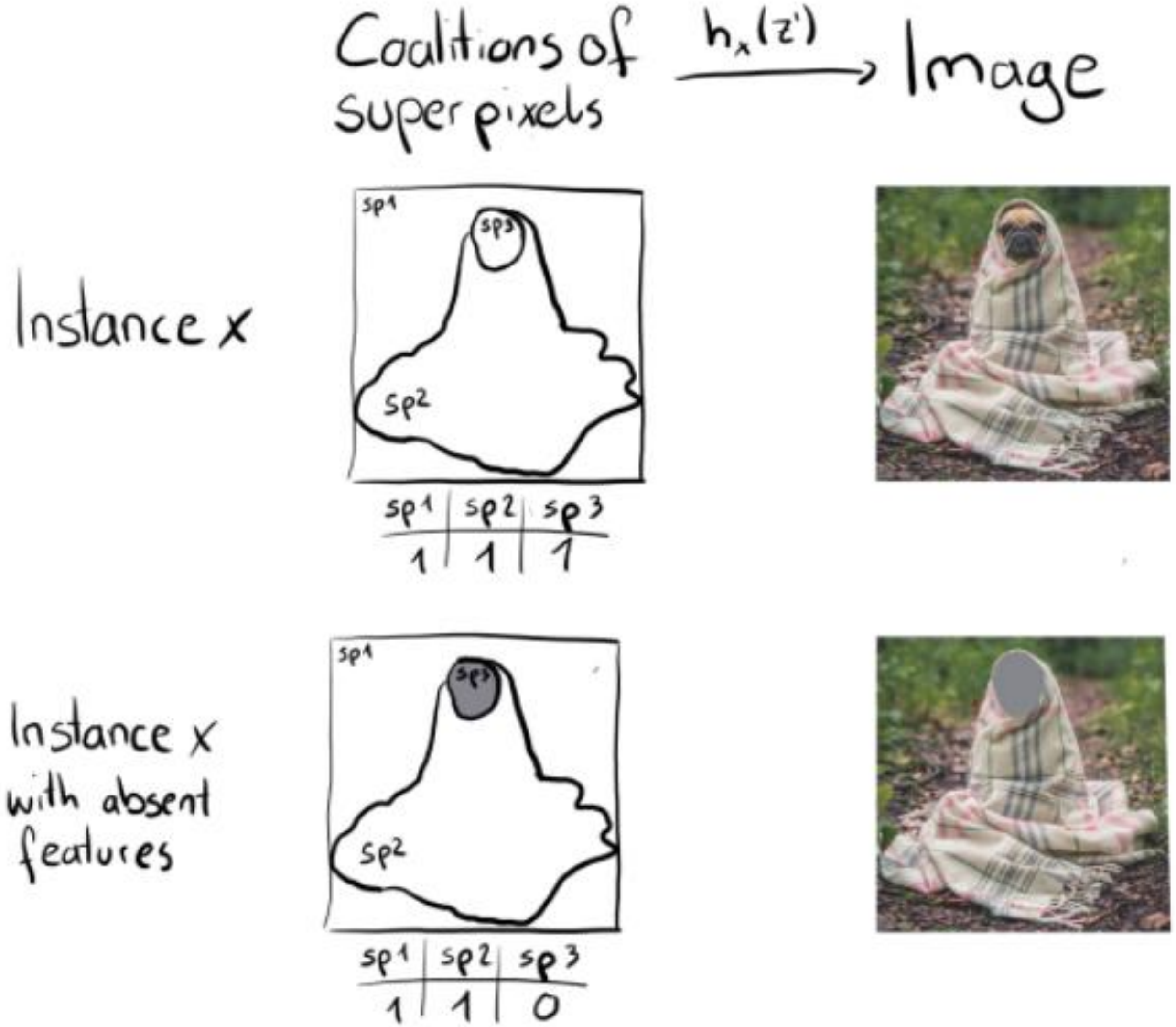


- Lundberg, Scott M., and Su-In Lee. ***A unified approach to interpreting model predictions***. *Advances in Neural Information Processing Systems*. 2017.

SHAP on Tabular Data



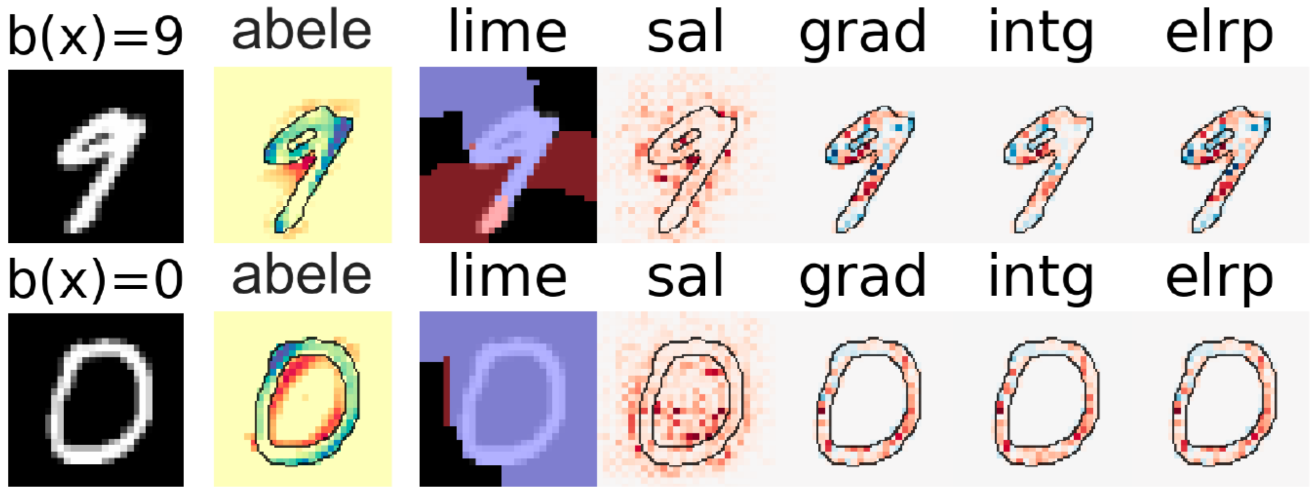
SHAP on Images



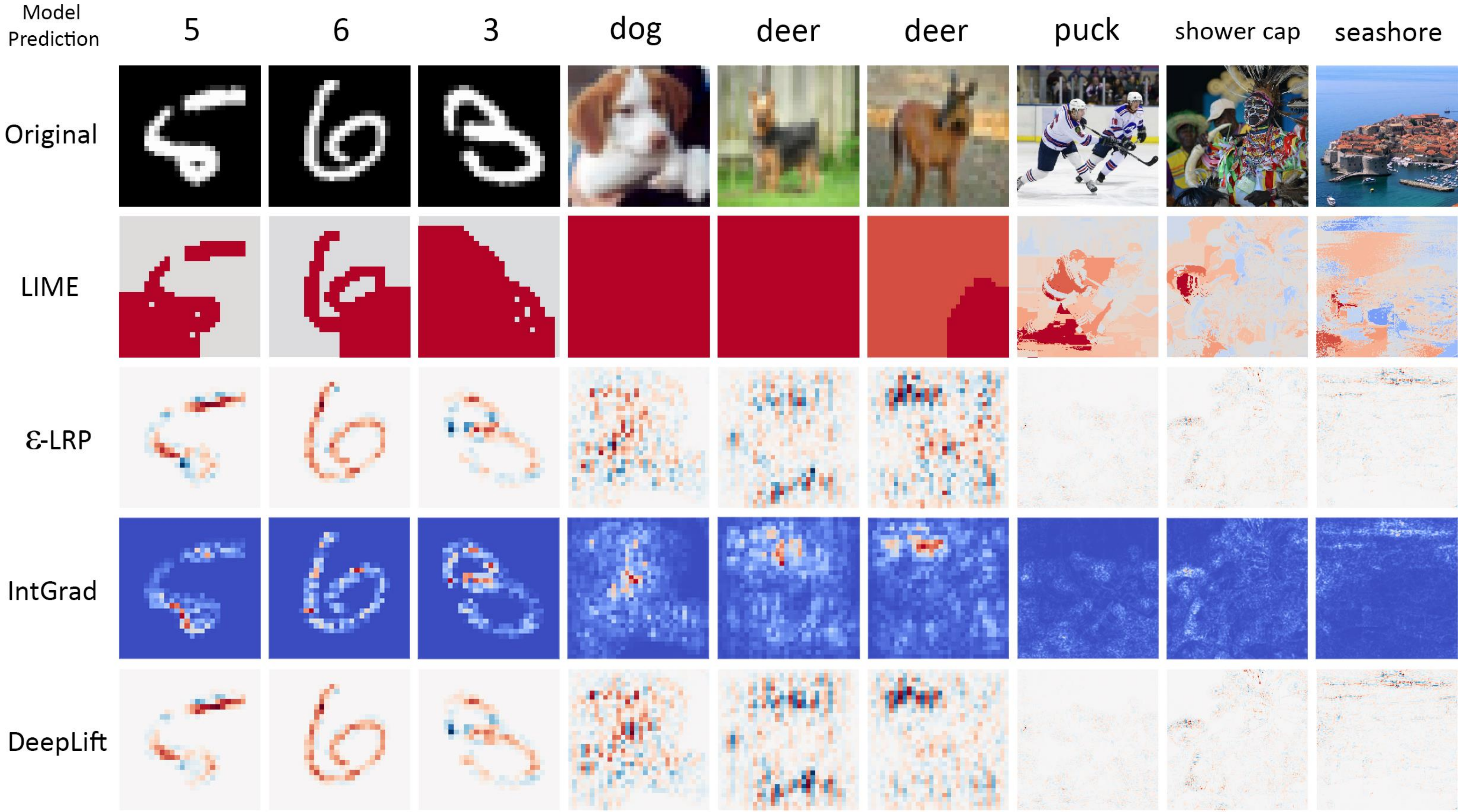
Saliency Maps

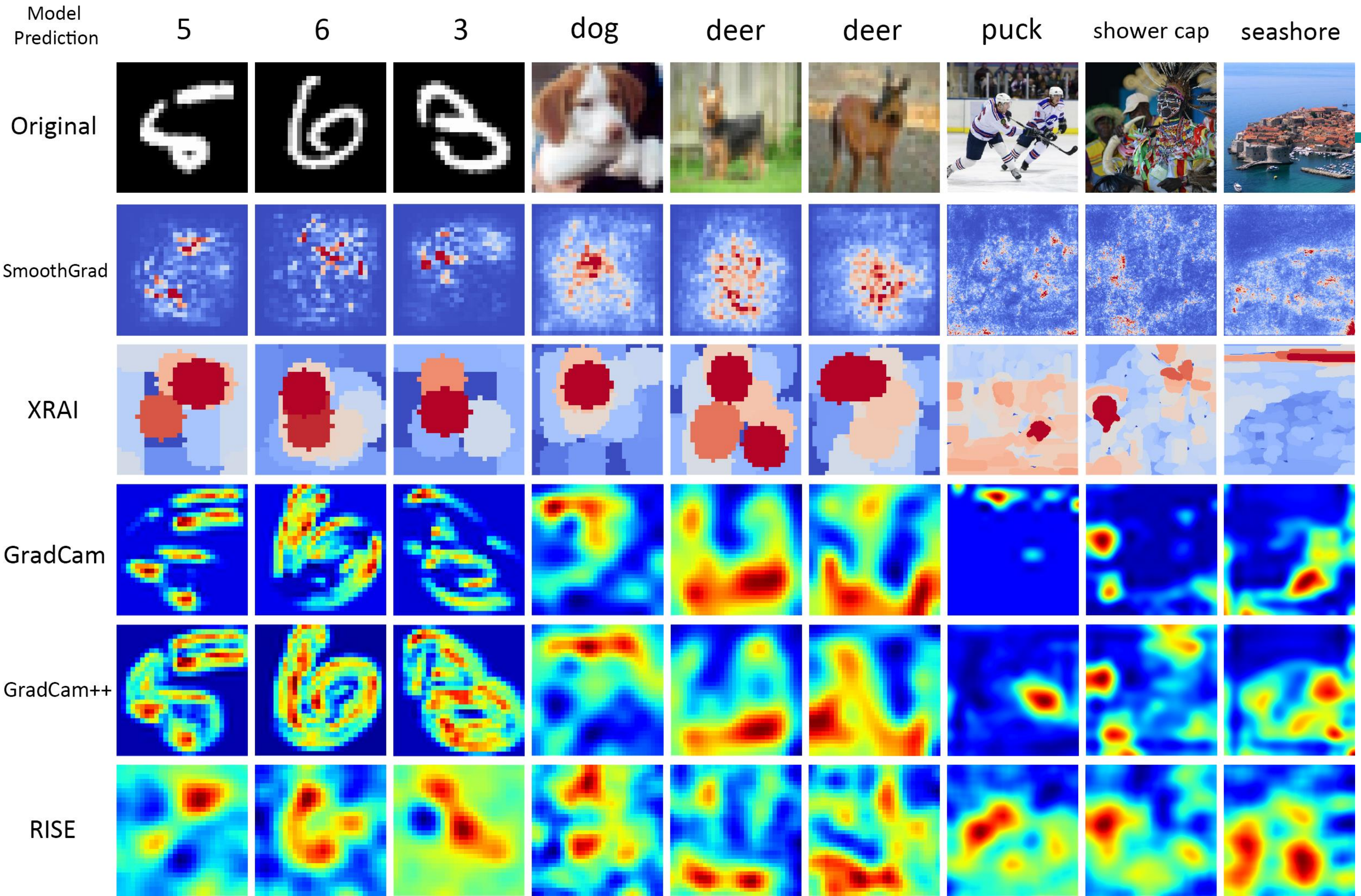
Saliency Maps

- A saliency map is an image in which a pixel's brightness represents how salient the pixel is. A positive value (red) means that the pixel has contributed positively to the classification, while a negative one (blue) means that has contributed negatively.
- There are two methods for creating SMs.
  1. Assign to ***every pixel*** a saliency value.
  2. Segment the image into different ***pixel groups (superpixels or segments)*** and then assign a saliency value for each group.



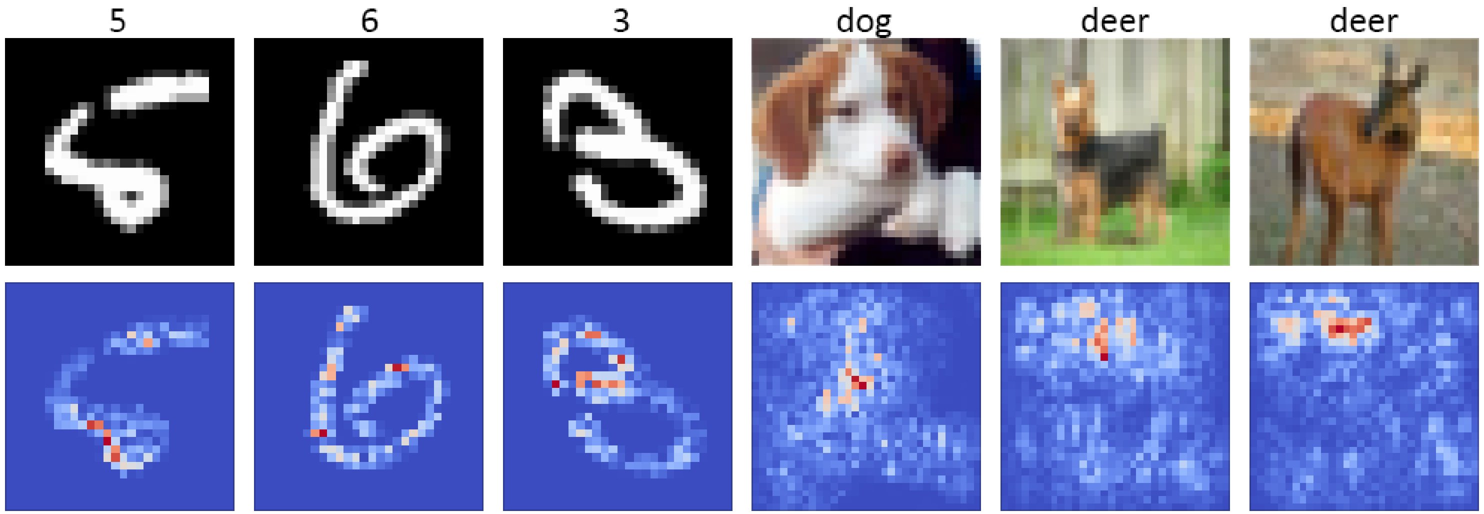
Saliency Maps




Model Prediction
5
6
3
dog
deer
deer
puck
shower cap
seashore
Original
SmoothGrad
XRAI
GradCam
GradCam++
RISE

Integrated Gradient

- INTGRAD can only be applied to differentiable models.
- INTGRAD constructs a path from the baseline image x' to the input x and computes the gradients of points along the path.
- The points are taken by overlapping x with x', and gradually modifying the opacity of x. Saliency maps are obtained by cumulating the gradients of these points.



- Mukund Sundararajan, Ankur Taly, Qiqi Yan. ***Axiomatic Attribution for Deep Networks***. arXiv preprint arXiv:1703.01365. 2017

MASK

01 x instance to explain

02 ***varying*** x into x′ maximizing $b(x) \sim b(x')$ ← ***black box auditing***

03 the variation runs replacing a region R of x with:

constant value, noise, blurred image

04 reformulation: find ***smallest*** R such that $b(x_R) \ll b(x)$

- Ruth Fong and Andrea Vedaldi. 2017. ***Interpretable explanations of black boxes by meaningful perturbation***. arXiv:1704.03296 (2017).

Sentence Highlighting

Instance-based Explanations

Instance-based Explanations

- Instance-based explanation methods select particular instances of the dataset or generate synthetic instances to explain black box behaviors.
- Instance-based explainers are mainly local explainers.
- Instance-based explanations only make sense if we can represent an instance of the data in a humanly understandable way.
- This works well for:
  - images
  - tabular data with not many features
  - short texts

Instance-based Explanations

- We mainly recognize the following example-based explanations:
  - ***Prototypes***: a selection of representative instances having the same class of the instance under analysis. Among prototypes we also recognize:
    - ***Criticisms:*** instances that are not well represented by prototypes.
    - ***Influential Instances:*** training points that were the most influential for the training of the black-box or for the prediction itself.
  - **Counterfactuals:** a selection of representative instances having a different class w.r.t. the instance under analysis.

Counterfactual Explanations

- A counterfactual explanation describes a causal situation in the form: "If X had not occurred, Y would not have occurred".
- Thinking in counterfactual terms requires imagining a hypothetical reality that contradicts the observed facts.
- Even if the relationship between the inputs and the outcome to be predicted might not be causal, we can see the inputs of a model as the cause of the prediction.
- ***A counterfactual explanation of a prediction describes the smallest change to the feature values that changes the prediction to a predefined output.***

Counterfactual Explan

- Counterfactuals answer why a decision has been made by highlighting what changes in the input would lead to a different outcome.
- CF are not generalizations!!!

income: 1200$
car owner: no
other debts: yes

Denied!

income: 1200$
car owner: yes
other debts: yes

income: 1500$
car owner: no
other debts: yes

Accepted!

Generating Counterfactual Explanations

- A simple and naive approach to generating counterfactual explanations is ***searching by trial and error:*** randomly changing feature values of the instance of interest and stopping when the desired output is predicted.
- As an alternative we can define *a loss function* that consider the instance of interest, a counterfactual and the desired (counterfactual) outcome. Then, we can find the ***counterfactual explanation that minimizes this loss using an optimization algorithm***.
- Many methods proceed in this way but differ in their definition of the loss function and optimization method.

Counterfactuals with a Brute Force Procedure

age	income	other debts	car owner
25	1200$	yes	no

age	income	other debts	car owner
25	500$	yes	no

age	income	other debts	car owner
25	10000$	yes	no

age	income	other debts	car owner
25	1200$	no	no

age	income	other debts	car owner
25	1200$	yes	yes

age	income	other debts	car owner
25	500$	no	no

age	income	other debts	car owner
25	500$	yes	yes

Counterfactuals by Optimization Problems

- Most of the counterfactual explainers return counterfactuals by solving an optimization problem.
- The problem is typically designed through the *definition of a loss function* aimed at guaranteeing a set of desired properties.
- The objective is to find a counterfactual instance that minimizes this loss using an optimization (OPT) algorithm.

Optimized CF Search

Wachter et al. suggest minimizing the following loss:

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

$$d(x, x') = \sum_{j=1}^{p} \frac{|x_j - x'_j|}{MAD_j}$$

balance the prediction

$$MAD_j = \text{median}_{i \in \{1,\dots,n\}}(|x_{i,j} - \text{median}_{l \in \{1,\dots,n\}}(x_{l,j})|)$$

1. Sample a random CF x'
2. Optimize the loss L
3. If not $|\hat{f}(x') - y'| \leq \epsilon$
4. Increase Lambda. Go to 2.
5. Return the CF x' that minimizes the loss.

- Wachter, Sandra and Mittelstadt, Brent and Russell, Chris. ***Counterfactual explanations without opening the black box: Automated decisions and the GDPR.*** 2017. Harv. JL & Tech

Optimized CF Search

- The loss function minimized by Wachter et al. is

$$\lambda(b(x') - y')^2 + d(x, x')$$

- where the first term is the quadratic distance between the desired outcome ***y'*** and the classifier prediction on ***x'***, and the second term is the distance between ***x*** and ***x'***.
- Lambda balances the contribution of the first term against the second term.

Wachter S, Mittelstadt BD, Russell C (2017) Counterfactual explanations without opening the black box: Automated decisions and the GDPR. HarvJL & Tech 31:841

Distance Functions

- Manhattan distance weighed with the inverse median absolute deviation MAD (used by Wachter)

$$d(x, x') = \sum_{j=1}^{p} \frac{|x_j - x'_j|}{MAD_j} \quad MAD_j = \text{median}_{i \in \{1,...,n\}}(|x_{i,j} - \text{median}_{l \in \{1,...,n\}}(x_{l,j})|)$$

- Mixed Distance (used by Mothilal)

$$d(a, b) = \frac{m_{con}}{n_{con}} \sum_{i \in con} \frac{|a_i - b_i|}{MAD_i} + \frac{m_{cat}}{n_{cat}} \sum_{i \in cat} \mathbb{1}_{a_i \neq b_i}$$

DICE - Diverse Counterfactual Explanations

- DICE solves an optimization problem with penalization terms to ensure plausibility by similarity and diversity.
- It returns a set of ***k*** plausible and different counterfactuals for ***x***.

$$C(\boldsymbol{x}) = \underset{\boldsymbol{c}_1,\ldots,\boldsymbol{c}_k}{\arg\min} \frac{1}{k}\sum_{i=1}^{k} \mathrm{yloss}(f(\boldsymbol{c}_i), y) + \frac{\lambda_1}{k}\sum_{i=1}^{k} dist(\boldsymbol{c}_i, \boldsymbol{x}) - \lambda_2\, \mathrm{dpp\_diversity}(\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k)$$

Mothilal RK, Sharma A, Tan C (2020) Explaining machine learning classifiers through diverse counterfactual explanations. In: FAT*, ACM, pp 607–617

Mothilal RK, Mahajan D, Tan C, Sharma A (2021) Towards unifying feature attribution and counterfactual explanations: Different means to the sameend. In: AIES, ACM, pp 652–663

Counterfactuals through Heuristic Strategies

- Heuristic strategies are typically much more efficient than optimization algorithms.
- Efficiency is paid with solutions that are not necessarily optimal.
- The search strategy is typically designed such that at each iteration, $\boldsymbol{x}'$ is updated with the objective of *minimizing a cost function*.
- The cost function is based on a local and heuristic choice aiming for a valid counterfactual similar to $\boldsymbol{x}$.

SEDC - Search for Explanations for Document Classification

- The search is guided by local improvements via best-first search with pruning.

- b("the quick brown fox jumps over the lazy dog") = y (0.8)

Prob. of y

Input

- b("~~the~~ quick brown fox jumps over the lazy dog") = y (0.8)
- b("the ~~quick~~ brown fox jumps over the lazy dog") ≠ y'(0.3)
- b("the quick ~~brown~~ fox jumps over the lazy dog") = y (0.7)

Iter 1

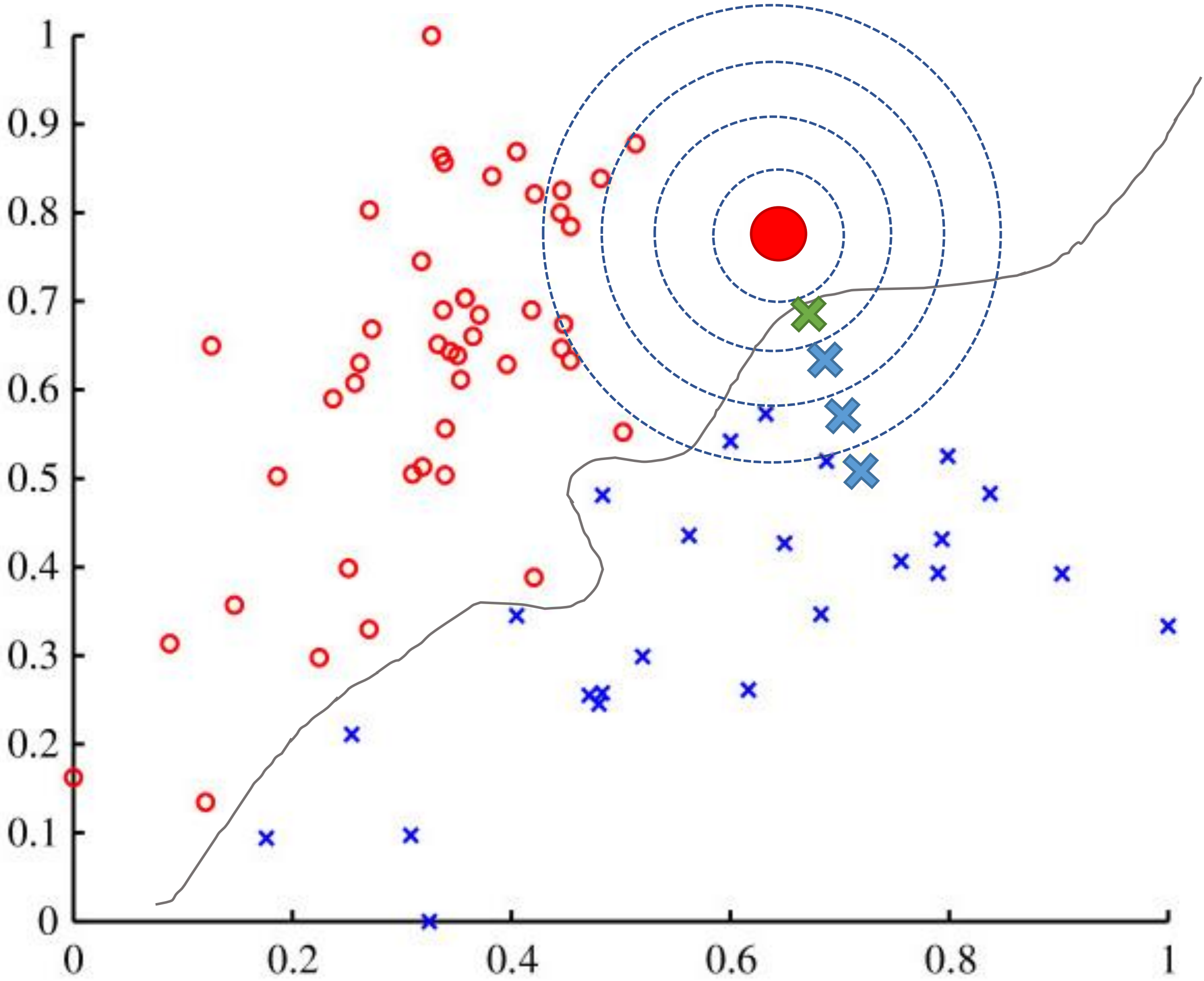
- …
- b("~~the~~ quick ~~brown~~ fox jumps over the lazy dog") = y (0.6)
- b("the quick ~~brown~~ ~~fox~~ jumps over the lazy dog") = y (0.6)
- b("the quick ~~brown~~ fox ~~jumps~~ over the lazy dog") ≠ y'(0.4)

Iter 2

Martens D, Provost FJ (2014) Explaining data-driven document classifications. MIS Q 38(1):73–99

GSG - Growing Spheres Generation

- GSG relies on a generative approach growing a *sphere* of synthetic instances around ***x*** to find the closest counterfactual ***x'***.
- GSG ignores in which direction the closest classification boundary might be.



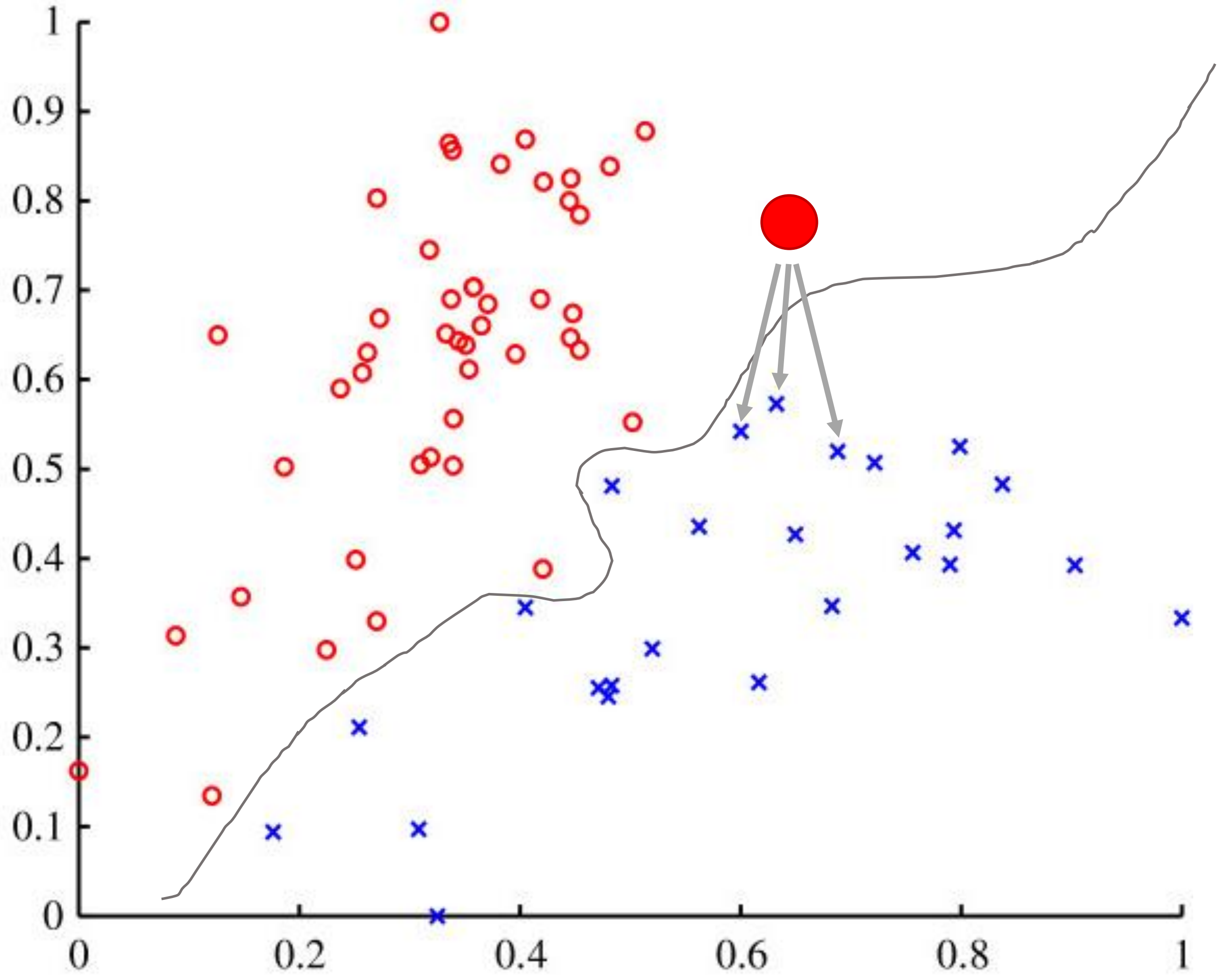
Laugel T, Lesot M, Marsala C, Renard X, Detyniecki M (2018) Comparison-based inverse classification for interpretability in machine learning. In:IPMU (1), Springer, Communications in Computer and Information Sci-ence, vol 853, pp 100–111

Counterfactuals with Instance-Based Strategies

- The very simple but effective idea of instance-based (or case-based) approaches for counterfactual explanation is to search into a reference population instances to be used as counterfactuals.

NNCE - Nearest-Neighbor Counterfactual Explainer

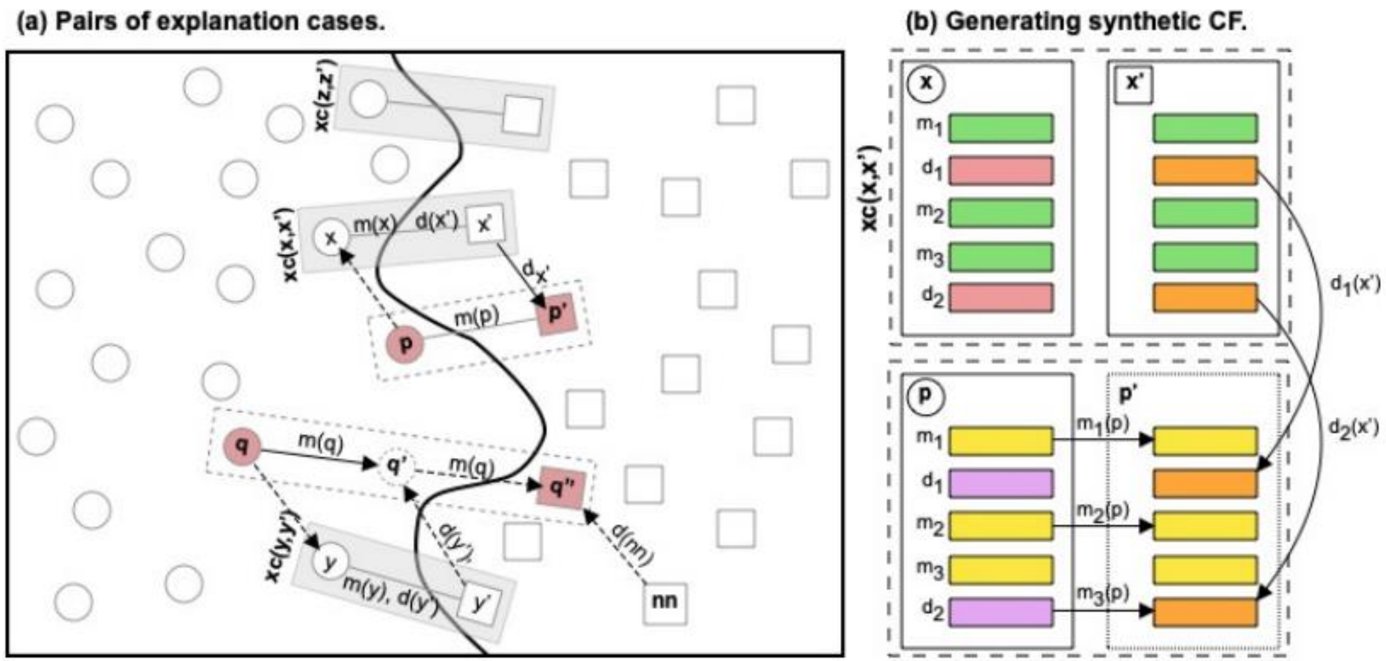
- NNCE is an endogenous counterfactual explainer inspired by kNN classifiers that select as counterfactual(s) the instances in ***x'∈X*** most similar to ***x*** and with a different label, i.e., ***b(x') ≠ b(x)***.
- Candidate counterfactuals are sorted with respect to the distance between ***x,*** and the ***k*** most similar ones are selected.



Shakhnarovich G, Darrell T, Indyk P (2008) Nearest-neighbor methods inlearn

CBCE - Case-Based Counterfactual Explainer

- CBCE refines NNCE.
- It adopts the notion of *explanation case (**xc**).*
- *G*iven ***X***, an ***xc*** is a couple of instances ***(x,x')*** such that ***(x,x')*** are the two most similar instances in ***X*** and ***b(x') ≠ b(x)***.



Keane MT, Smyth B (2020) Good counterfactuals and where to find them: A case-based technique for generating counterfactuals for explainable AI(XAI). In: ICCBR, Springer, Lecture Notes in Computer Science, vol 12311,pp 163–178

Take Home Message

Open The Black Box!

- ***To empower*** individual against undesired effects of automated decision making
- ***To reveal*** and protect new vulnerabilities
- ***To implement*** the “right of explanation”
- ***To improve*** industrial standards for developing AI-powered products, increasing the trust of companies and consumers
- ***To help*** people make better decisions
- ***To align*** algorithms with human values
- ***To preserve*** (and expand) human autonomy

Open Research Questions

- There is ***no agreement*** on ***what an explanation is***
- There is ***not a formalism*** for ***explanations***
- How to evaluate the ***goodness of explanations***?
- There is ***no work*** that seriously addresses the problem of ***quantifying*** the grade of ***comprehensibility*** of an explanation for humans
- What if there is a ***cost*** for querying a black box?

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Explanation Toolboxes and Repositories

- https://github.com/jphall663/awesome-machine-learning-interpretability
- https://github.com/pbiecek/xai_resources
- https://github.com/ModelOriented/DrWhy
- https://fat-forensics.org/
- https://github.com/Trusted-AI/AIX360
- https://captum.ai/
- https://github.com/interpretml/interpret
- https://github.com/SeldonIO/alibi
- https://github.com/pair-code/what-if-tool