Explainable AI

Christian Salvatore
Scuola Universitaria Superiore IUSS Pavia

christian.salvatore@iusspavia.it

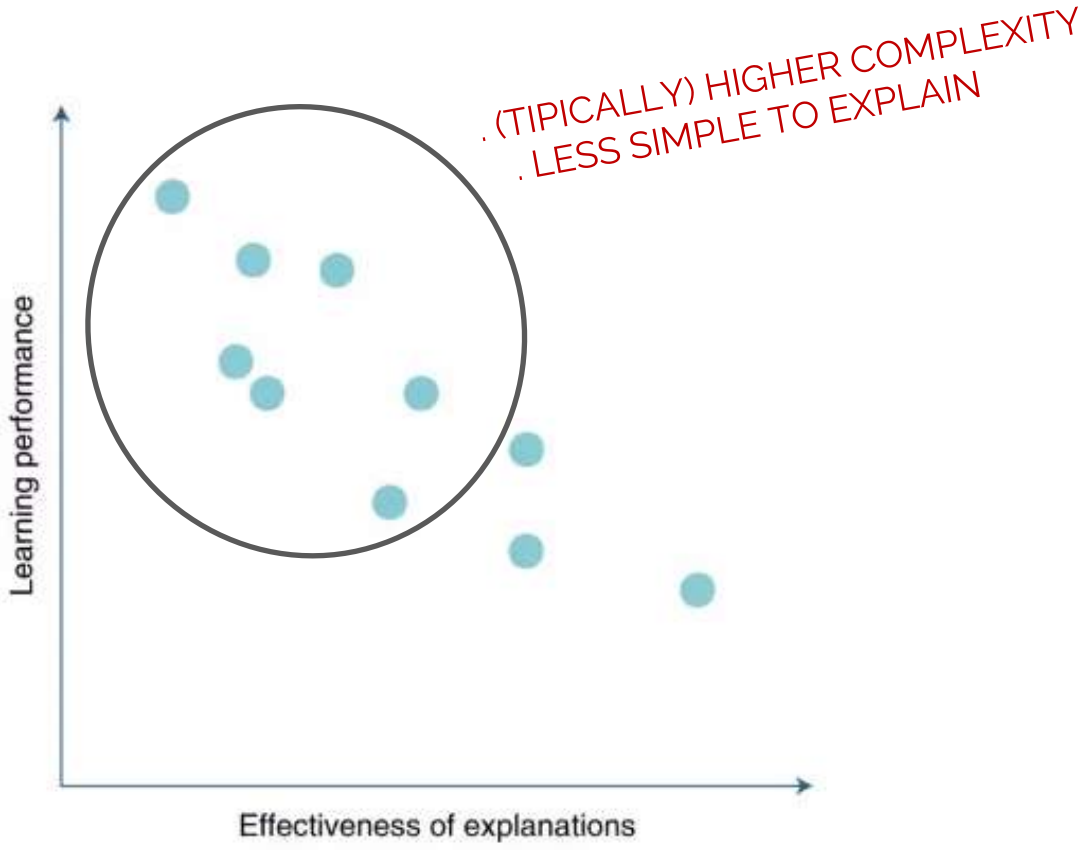
Improve model explainability

Interpretability

To observe the inner mechanics of the AI/ML method.
To understand the model's weights and features that are learned/used to determine the output of a classifier.

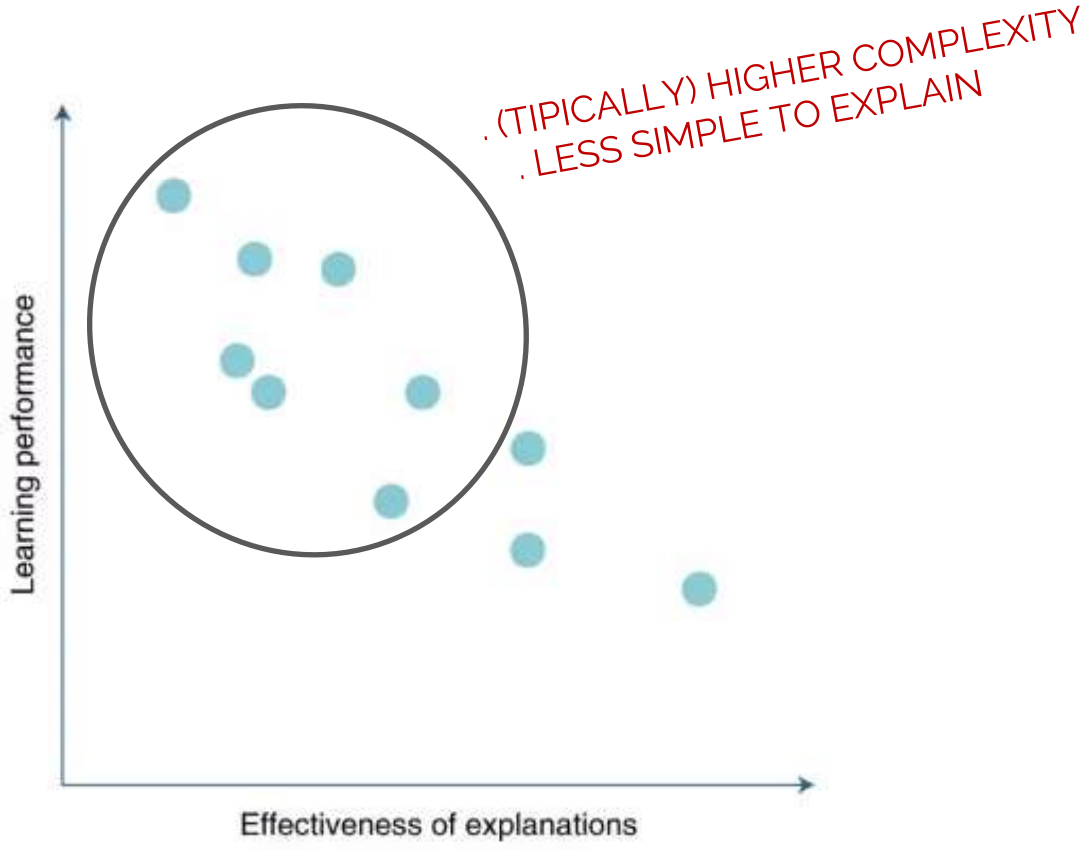
Improve model explainability

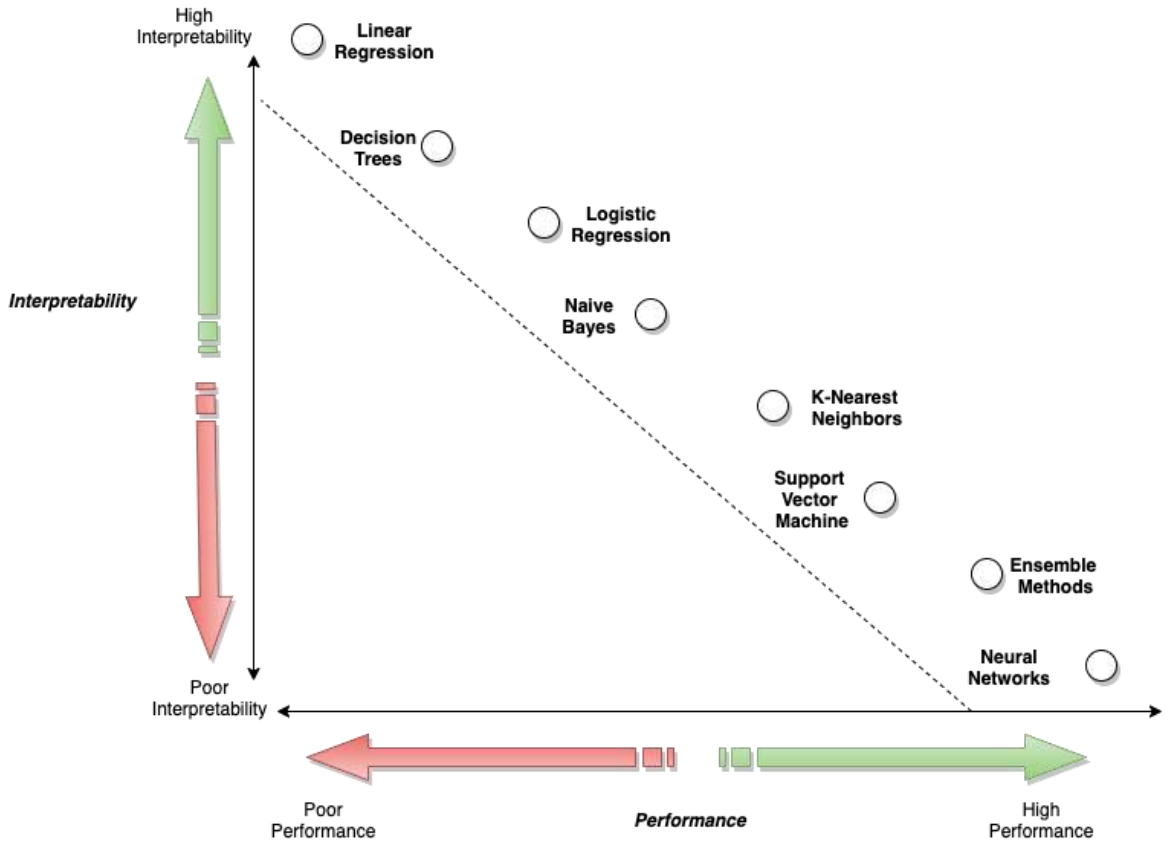
Performance-vs-interpretability tradeoff



Improve model explainability

Performance-vs-interpretability tradeoff





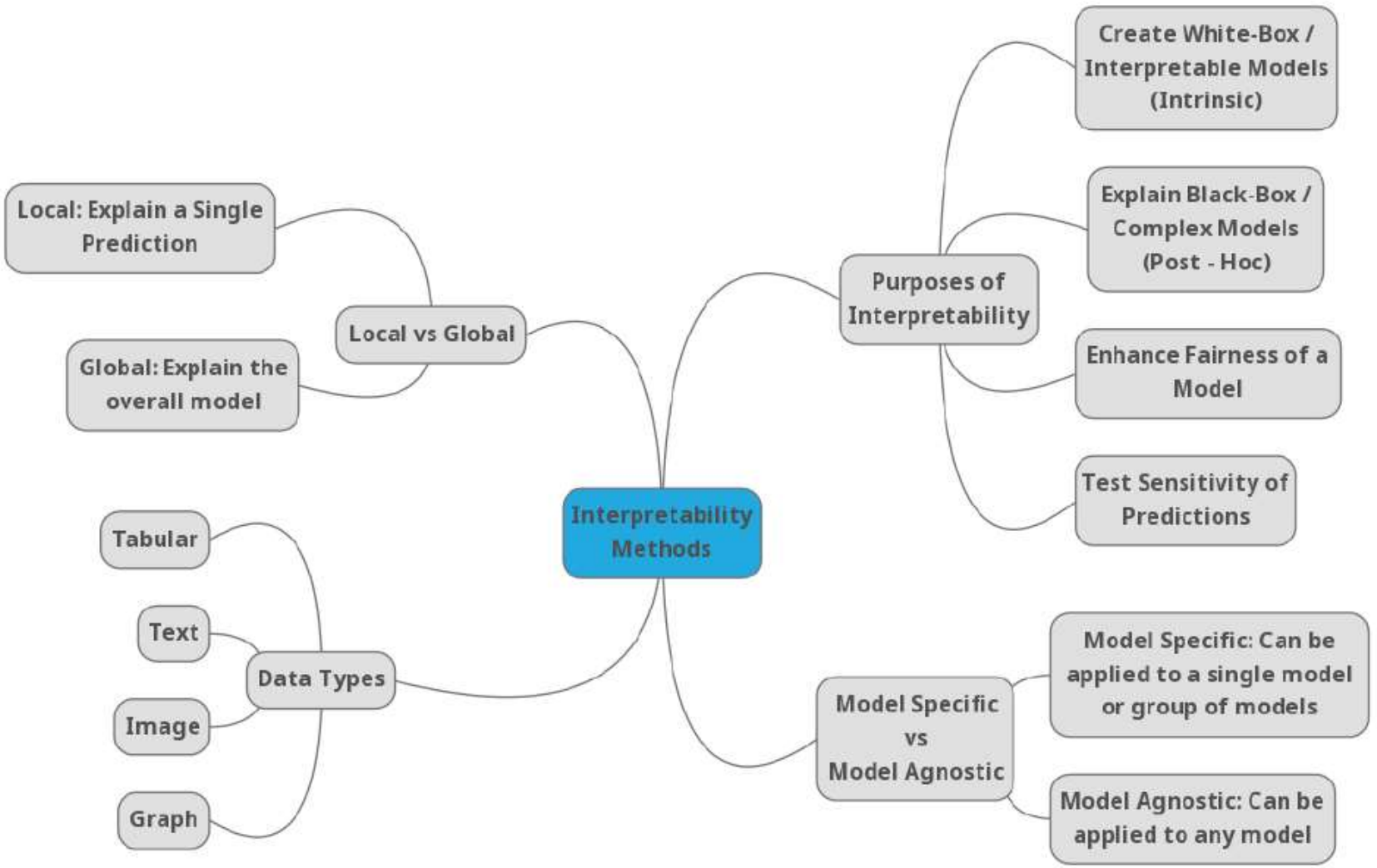
https://docs.aws.amazon.com/whitepapers/latest/model-explainability-aws-ai-ml/interpretability-versus-explainability.html

Improve model explainability

Explainability

To explain the behavior of a model at the decision level in human terms.

Improve model explainability



entropy

Review

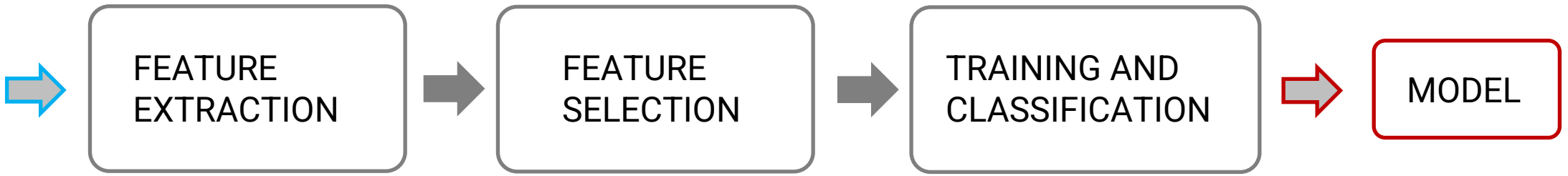
Explainable AI: A Review of Machine Learning Interpretability Methods

Pantelis Linardatos *, Vasilis Papastefanopoulos and Sotiris Kotsiantis

Figure 2. Taxonomy mind-map of Machine Learning Interpretability Techniques.

Improve model explainability

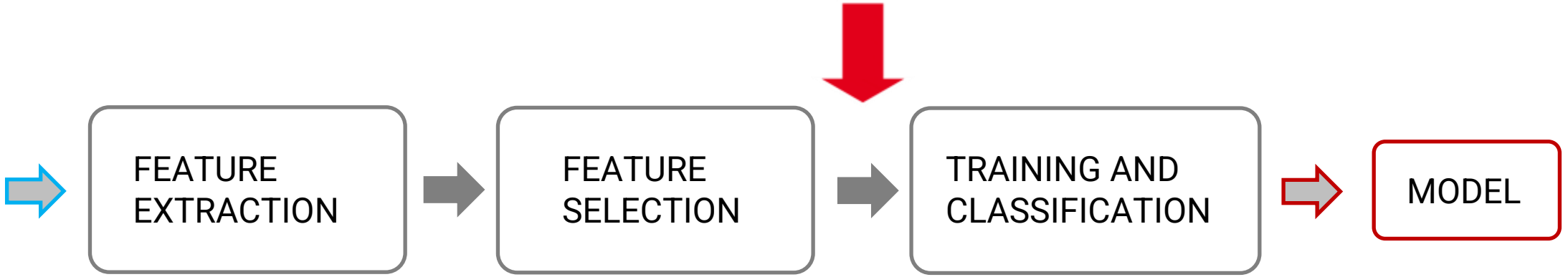
CONVENTIONAL MACHINE LEARNING



Improve model explainability

1. Feature-selection level

CONVENTIONAL MACHINE LEARNING

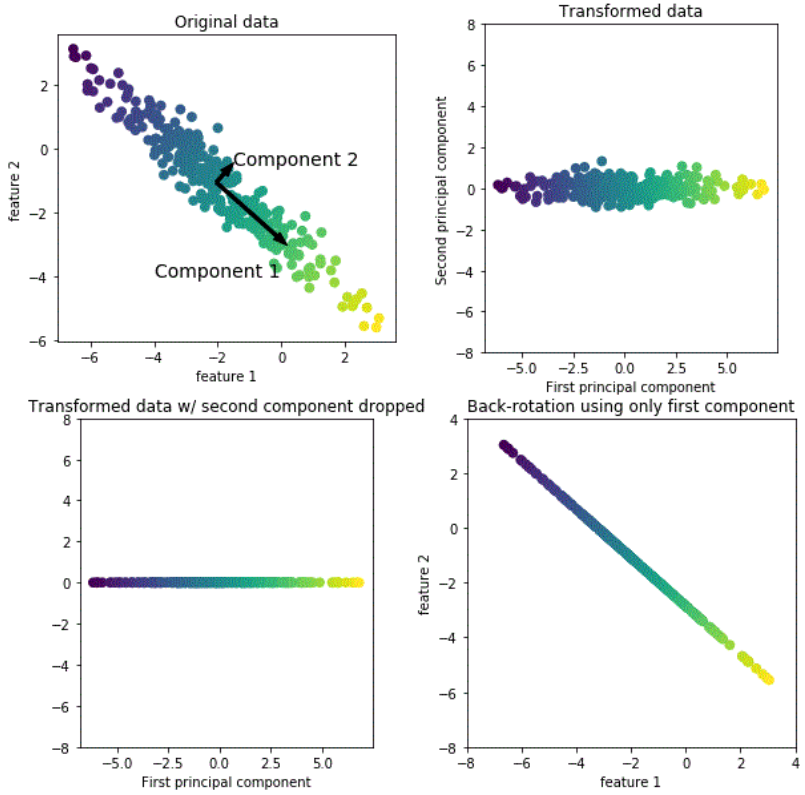


Improve model explainability

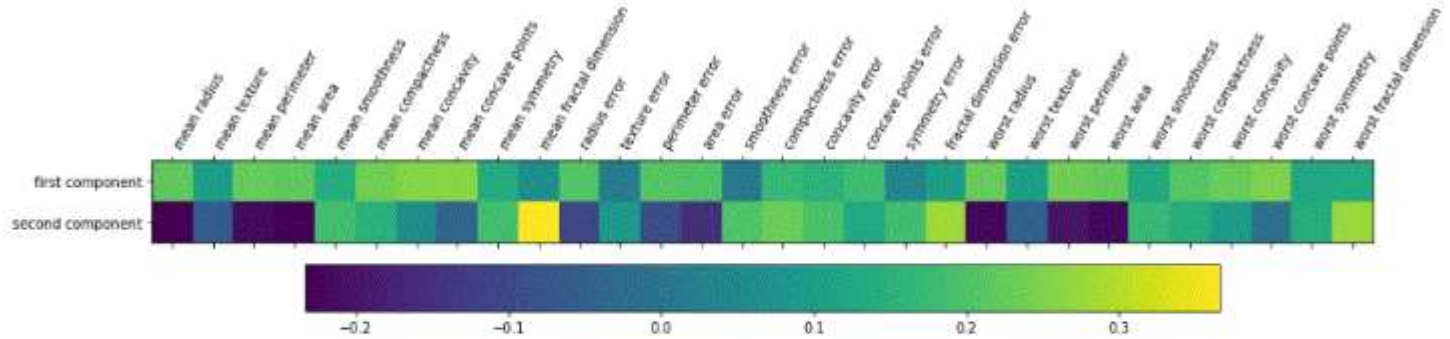
1. Feature-selection level

CONVENTIONAL MACHINE LEARNING

(CHARACTERISTICS OF) SELECTED FEATURES



Backprojecting PCA components

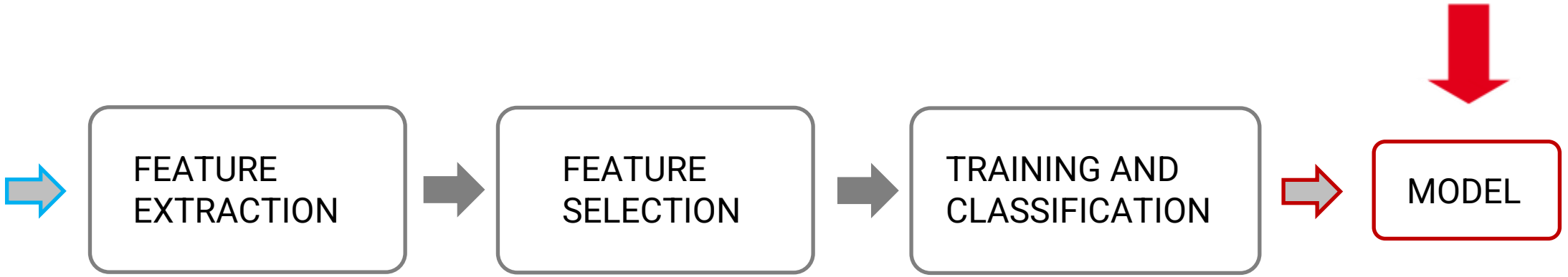


Above picture establishes (a) 1st Component has got all variables positively correlated meaning has got strong correlation (b) 2nd component has mixed sign meaning not so strong correlation (c) mixture of variables orients axes in such a way that 1st to n components have decresing order of relationship

Improve model explainability

2. Post-hoc wrt the output of the training process

CONVENTIONAL MACHINE LEARNING
DEEP LEARNING



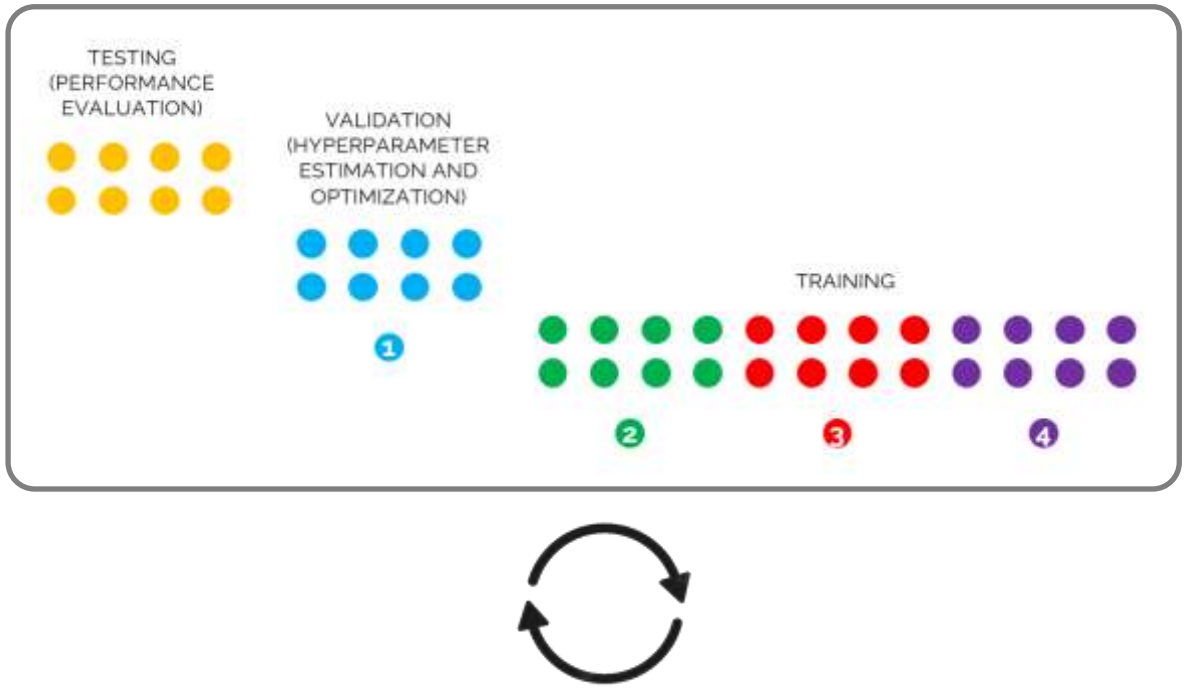
Improve model explainability

2. Post-hoc wrt the output of the training process

CONVENTIONAL MACHINE LEARNING

SELECTED FEATURES RANKED BY FREQUENCY IN (NESTED) CV

- For each loop i of the (nested) cross validation, perform feature selection
- Train the model i using the selected set of features
- Optimize the set of selected features by minimizing/maximizing a given parameter (e.g., model performance)
- Consider the set of selected features corresponding to the optimal models and compute the selection frequency for each feature
- The highest the selection frequency, the highest the importance of the feature



Improve model explainability

2. Post-hoc wrt the output of the training process

CONVENTIONAL MACHINE LEARNING
DEEP LEARNING

Table 2. Interpretability Methods to Explain any Black-Box Model.

Ref	Tool	Category	Local vs. Global	Model Specific vs. Model Agnostic	Data Type	Citations/ Year	Year
[45]	lime Eli5 InterpretML AIX360 Skater	PH	L	Agnostic	img txt tab	845.6	2016
[59]	PDPbox InterpretML Skater	PH	G	Agnostic	tab	589.2	
[48]	shap alibi AIX360 InterpretML	PH	L & G	Agnostic	img txt tab	504.5	
[50]	alibi Anchor	PH	L	Agnostic	img txt tab	158.3	
[53]	alibi	PH	L	Agnostic	tab img	124.5	

Ref	Tool	Category	Local vs. Global	Model Specific vs. Model Agnostic	Data Type	Citations/ Year	Year
[60]	PyCEbox	PH	L & G	Agnostic	tab	53.3	2015
[58]	L2X	PH	L	Agnostic	img txt tab	50.3	2018
[57]	Eli5	PH	G	Agnostic	tab	41.5	2010
[51]	alibi AIX360	PH	L	Agnostic	tab img	34.3	2018
[61]	Alibi	PH	G	Agnostic	tab	23.2	2016
[54]	alibi	PH	L	Agnostic	tab img	17	2019
[62]	pyBreakDown	PH	L	Agnostic	tab	8.3	2018
[62]	pyBreakDown	PH	G	Agnostic	tab	8.3	2018
[47]	DLIME	PH	L	Agnostic	img txt tab	7.5	2019
[56]	AIX360	PH	L	Agnostic	tab	7	2019
[52]	AIX360	PH	L	Agnostic	tab img	3	2019

Improve model explainability

2. Post-hoc wrt the output of the training process

CONVENTIONAL MACHINE LEARNING
DEEP LEARNING

LIME: Local Interpretable Model-agnostic Explanations

- For any given instance and its corresponding prediction, generate a set of simulated randomly-sampled data around the neighbourhood of input instance (“perturbed” instances)
- Classify these instances (using the model to “explain”)
- Weight these classifications by their proximity to the “real” input instance
- Train a simple, interpretable model using simulated instances and corresponding classification labels (e.g., a decision tree)
- Interpret this newly trained (local) model: this will result in an approximated interpretation of the original black-box model

Improve model explainability

2. Post-hoc wrt the output of the training process

CONVENTIONAL MACHINE LEARNING
DEEP LEARNING

LIME: Local Interpretable Model-agnostic Explanations

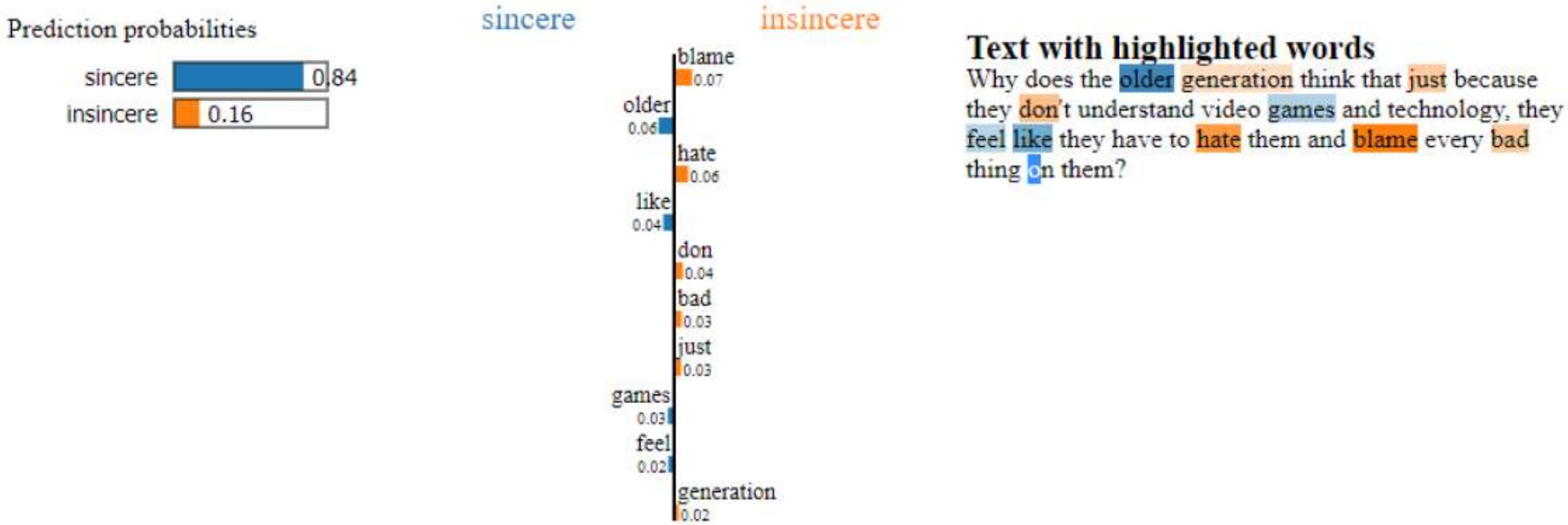


Figure 4. Local interpretable model-agnostic explanations (LIME) is used to explain the rationale behind the classification of an instance of the Quora Insincere Questions Dataset.

Improve model explainability

2. Post-hoc wrt the output of the training process

CONVENTIONAL MACHINE LEARNING
DEEP LEARNING

SHAP: Shapley Additive Explanations

- Classic result in game theory on distributing the total gain from a cooperative game
- Introduced by Lloyd Shapley in 1953 (Nobel Prize in Economics in 2012)

How it works:

Cooperative Game

- Players {1, ..., M} collaborating to generate some **gain**
  - Think: Employees in a company creating some profit
  - Described by a **set function v(S)** specifying the gain for any subset $S \subseteq \{1, ..., M\}$

- **Shapley values** are a fair way to attribute the total gain to the players
  - Think: Bonus allocation to the employees
  - Shapley values are commensurate with the player's contribution

On courtesy of Dr. Ankur Taly

Improve model explainability

2. Post-hoc wrt the output of the training process

CONVENTIONAL MACHINE LEARNING
DEEP LEARNING

SHAP: Shapley Additive Explanations

Shapley Value Algorithm [Conceptual]

$$\phi_i(v) = \mathop{\mathbb{E}}_{\boldsymbol{O}\sim\pi(M)} [v(\text{pre}_i(\boldsymbol{O}) \cup \{i\}) - v(\text{pre}_i(\boldsymbol{O}))]$$

- Consider all possible permutations $\pi(M)$ of players (**M! possibilities**)
- In each permutation $\boldsymbol{O} \sim \pi(M)$
  - Add players to the coalition in that order
  - Note the marginal contribution of each player i to set of players before it in the permutation, i.e., $v(pre_i(\boldsymbol{O}) \cup \{i\}) - v(pre_i(\boldsymbol{O}))$
- The average marginal contribution across all permutations is the Shapley Value

On courtesy of Dr. Ankur Taly

Improve model explainability

2. Post-hoc wrt the output of the training process

CONVENTIONAL MACHINE LEARNING
DEEP LEARNING

SHAP: Shapley Additive Explanations

Example

A company with two employees **Alice** and **Bob**

- No employees, no profit [v({}) = 0]
- Alice alone makes 20 units of profit [v({Alice}) = 20]
- Bob alone makes 10 units of profit [v({Bob}) = 10]
- Alice and Bob make 50 units of profit [v({Alice, Bob}) = 50]

What should the bonuses be?

On courtesy of Dr. Ankur Taly

Improve model explainability

2. Post-hoc wrt the output of the training process

CONVENTIONAL MACHINE LEARNING
DEEP LEARNING

SHAP: Shapley Additive Explanations

Example

A company with two employees **Alice** and **Bob**

- No employees, no profit [v({}) = 0]
- Alice alone makes 20 units of profit [v({Alice}) = 20]
- Bob alone makes 10 units of profit [v({Bob}) = 10]
- Alice and Bob make 50 units of profit [v({Alice, Bob}) = 50]

What should the bonuses be?

Permutation	Marginal for Alice	Marginal for Bob
Alice, Bob	20	30
Bob, Alice	40	10
Shapley Value	**30**	**20**

On courtesy of Dr. Ankur Taly

Improve model explainability

2. Post-hoc wrt the output of the training process

CONVENTIONAL MACHINE LEARNING
DEEP LEARNING

SHAP: Shapley Additive Explanations

Additivity
“SHAP values are additive, which means that the contribution of each feature to the final prediction can be computed independently and then summed up. This property allows for efficient computation of SHAP values, even for high-dimensional datasets.”

Local accuracy
“SHAP values add up to the difference between the expected model output and the actual output for a given input. This means that SHAP values provide an accurate and local interpretation of the model's prediction for a given input.”

Missingness
“SHAP values are zero for missing or irrelevant features for a prediction. This makes SHAP values robust to missing data and ensures that irrelevant features do not distort the interpretation.”

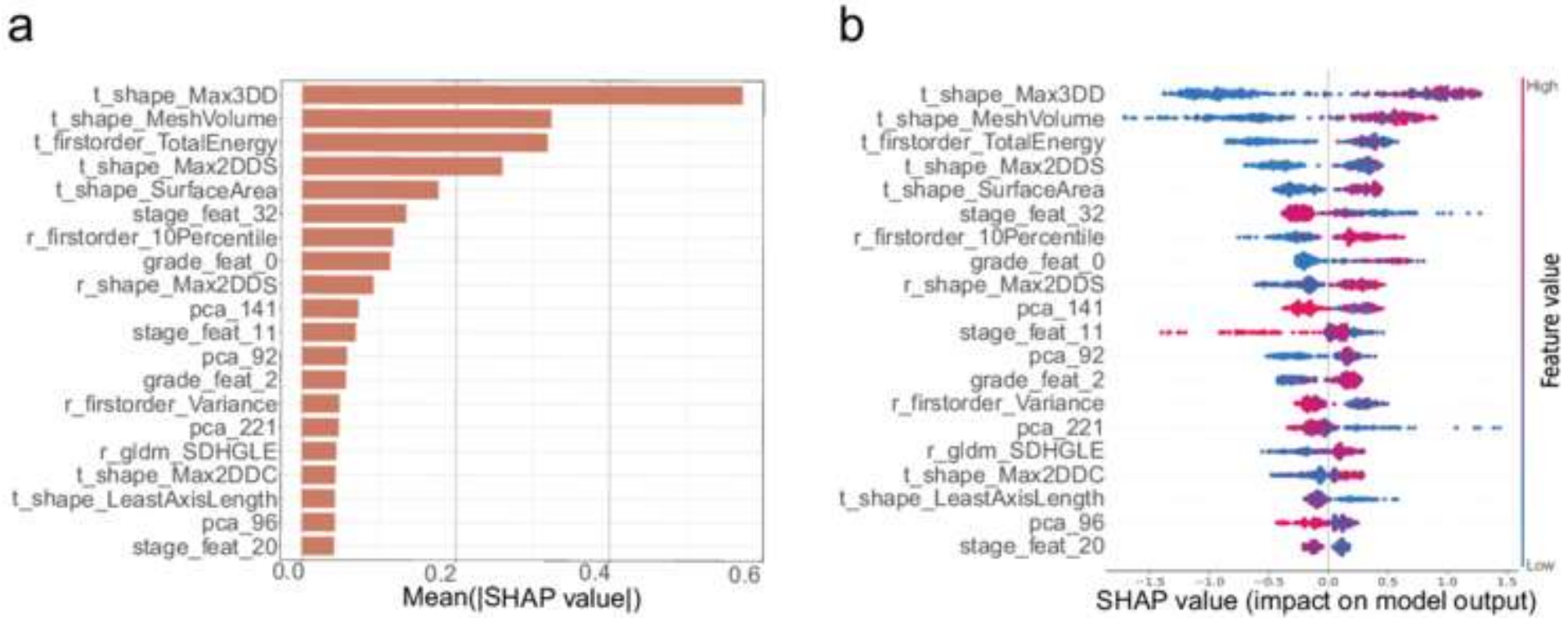
Consistency
“SHAP values do not change when the model changes unless the contribution of a feature changes. This means that SHAP values provide a consistent interpretation of the model's behavior, even when the model architecture or parameters change.”

Improve model explainability

2. Post-hoc wrt the output of the training process

CONVENTIONAL MACHINE LEARNING
DEEP LEARNING

SHAP: Shapley Additive Explanations



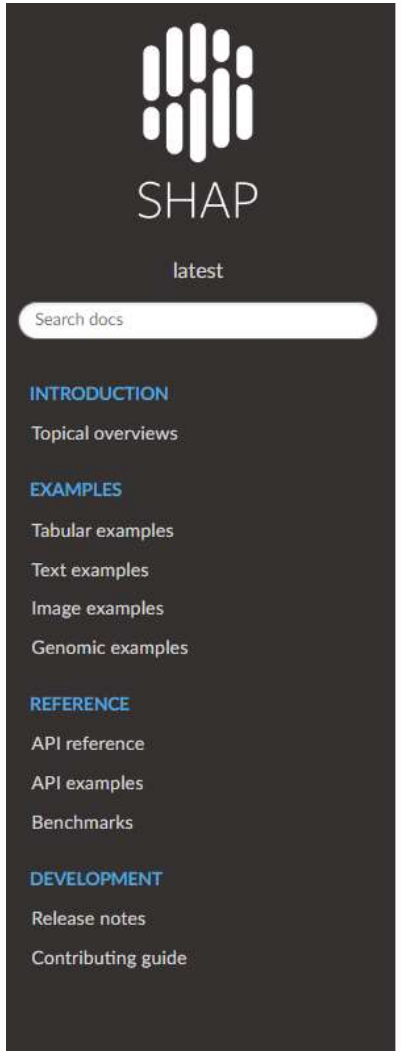
Improve model explainability

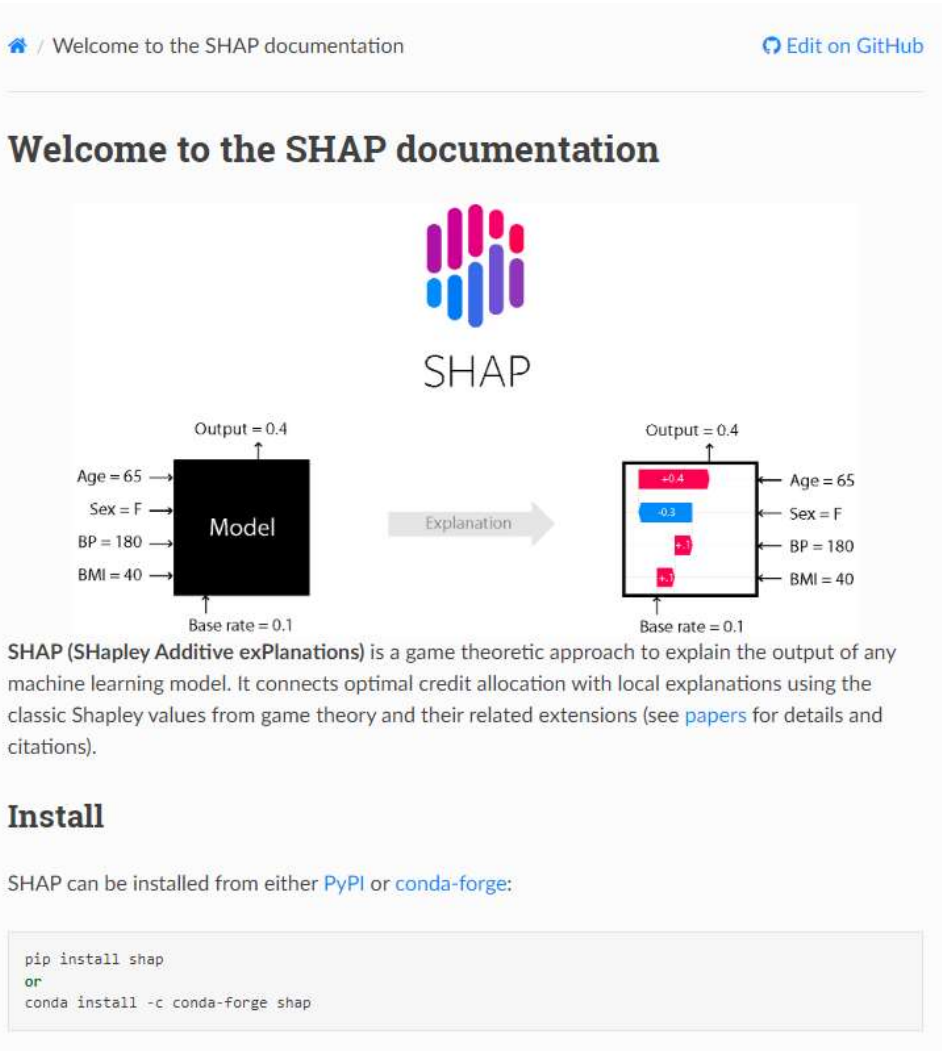
2. Post-hoc wrt the output of the training process

CONVENTIONAL MACHINE LEARNING
DEEP LEARNING

SHAP: Shapley Additive Explanations

https://shap.readthedocs.io/en/latest/

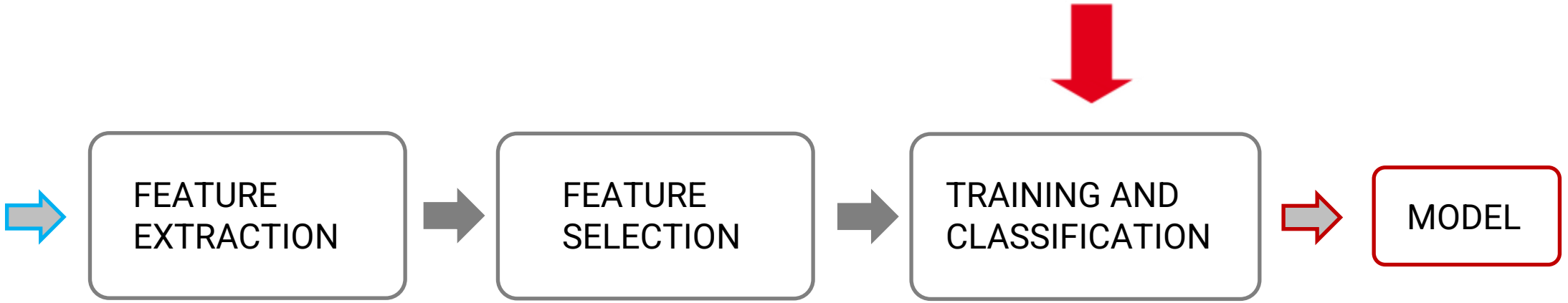




Improve model explainability

3. Embedded into the classifier

CONVENTIONAL MACHINE LEARNING



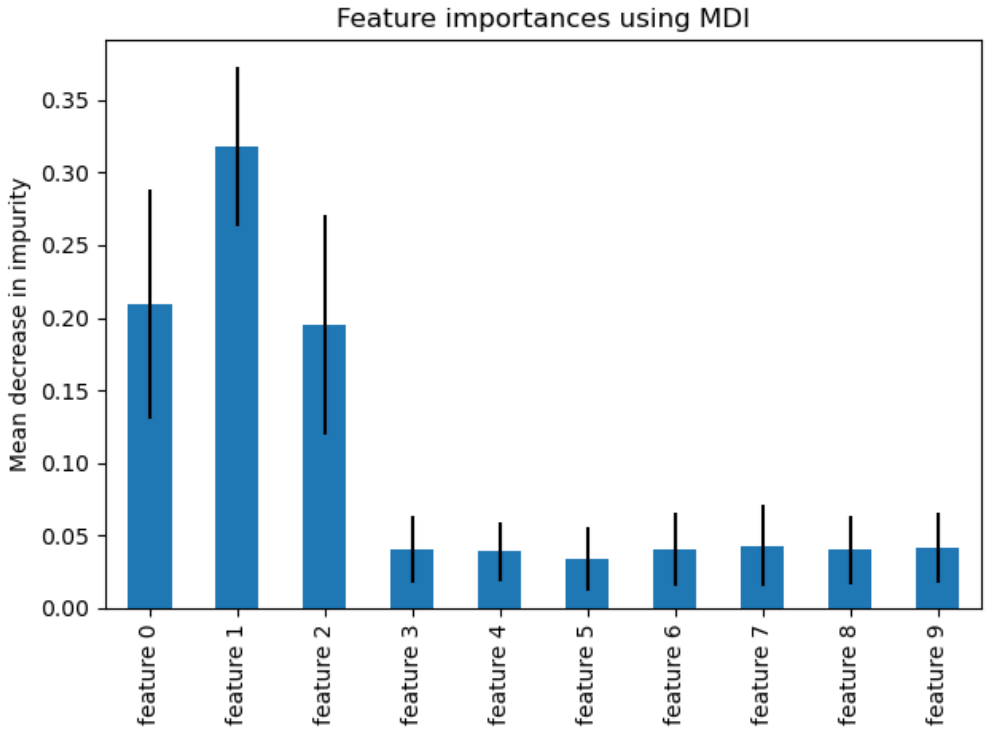
Improve model explainability

3. Embedded into the classifier

CONVENTIONAL MACHINE LEARNING

RANDOM-FOREST FEATURE IMPORTANCE

- Compute the decrease in Gini-impurity given by a feature at a given node
- Compute the mean-decrease of each feature for a given tree
- Compute the mean-decrease of each feature across all trained trees in the random forest to get MDI feature importance



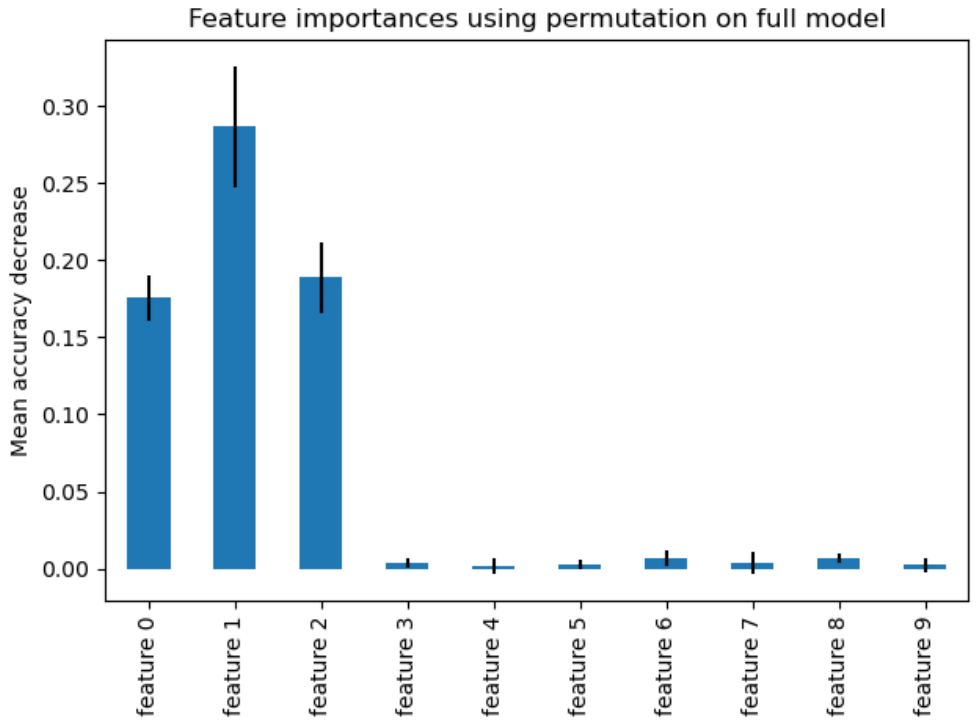
Improve model explainability

3. Embedded into the classifier

CONVENTIONAL MACHINE LEARNING

RANDOM-FOREST FEATURE
IMPORTANCE BASED ON PERMUTATIONS

- Compute the feature importance on permuted out-of-bag (OOB) samples based on mean decrease in the accuracy (or other metrics)
- The highest the performance decrease, the highest the importance of a feature

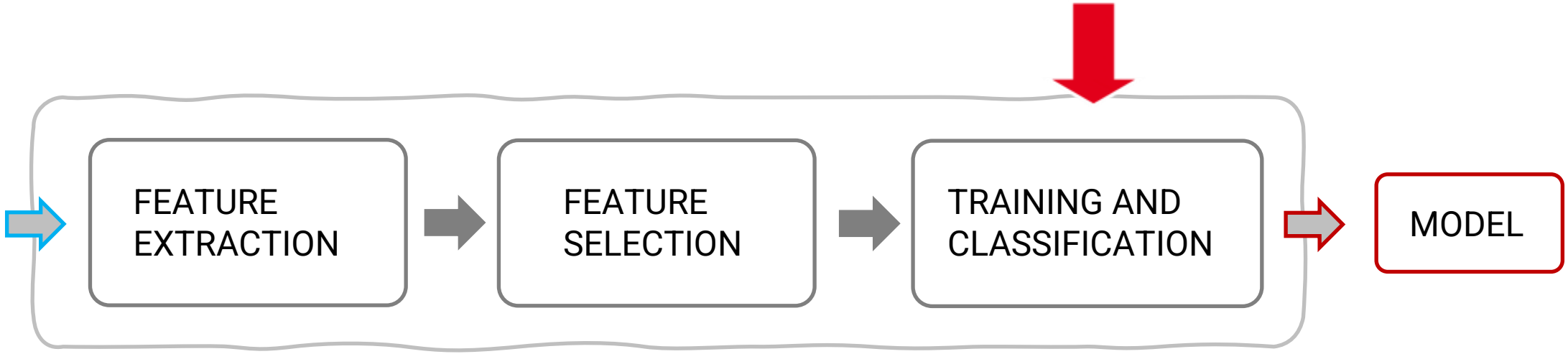


Improve model explainability

3. Embedded into the classifier

DEEP LEARNING

BASED ON DEEPNETS LAYER INFORMATION



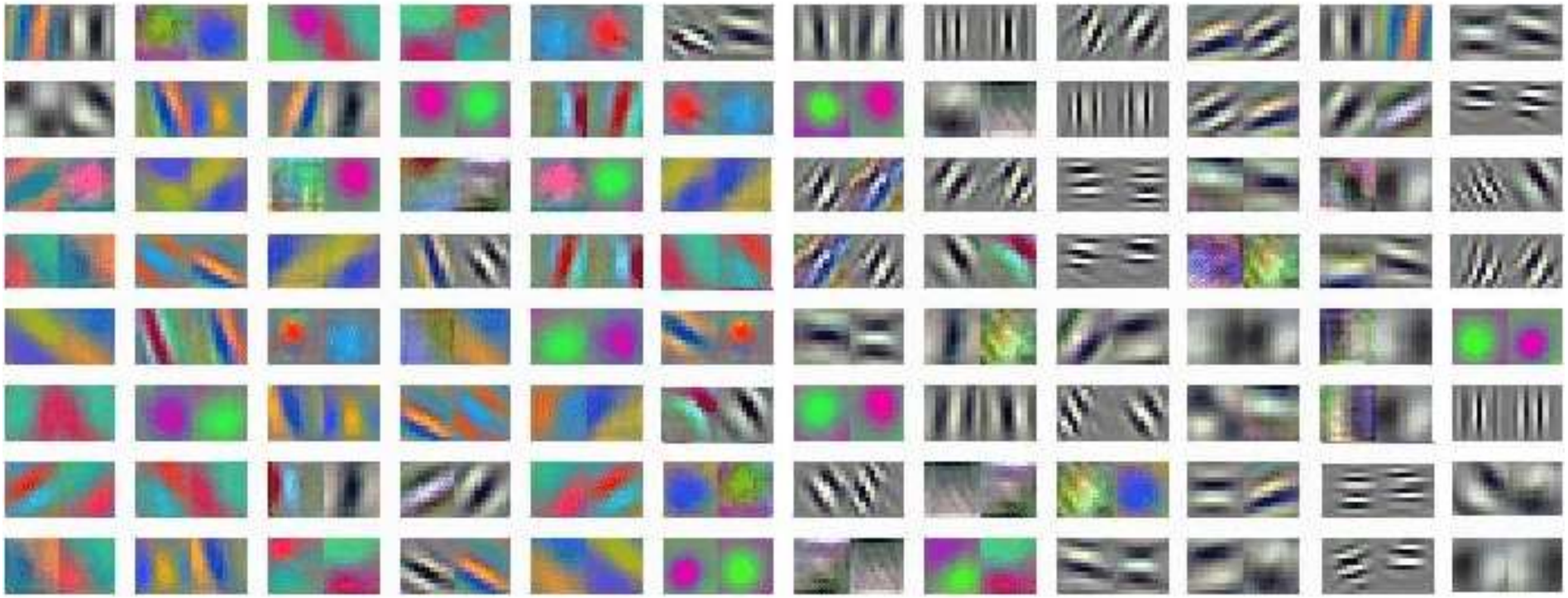
Improve model explainability

DEEP LEARNING

3. Embedded into the classifier

BASED ON DEEPNETS LAYER
INFORMATION -> WEIGHT FILTERS

ALEXNET CONV1 LEARNED FILTERS

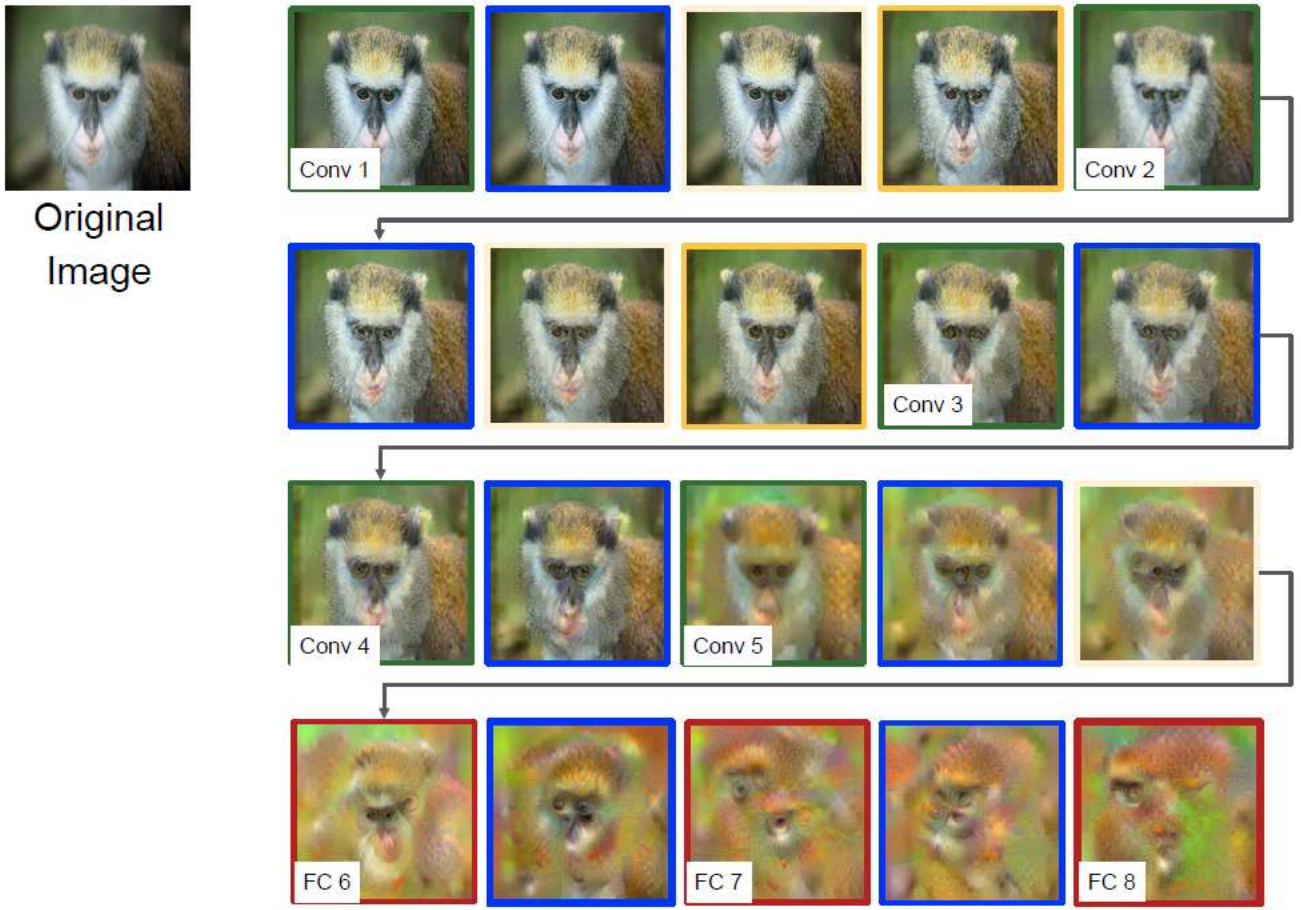


Improve model explainability

3. Embedded into the classifier

DEEP LEARNING

BASED ON DEEPNETS LAYER
INFORMATION -> TRANSFORMED INPUT



Improve model explainability

3. Embedded into the classifier

DEEP LEARNING

Table 1. Interpretability Methods to Explain Deep Learning Models.

Ref	Tool	Category	Local vs. Global	Model Specific vs. Model Agnostic	Data Type	Citations/ Year	Year
[32]	DeepExplain iNNvestigate tf-explain	PH	L	Specific	img	1548.3	2014
[35]	Grad-CAM tf-explain	PH	L	Specific	img	797.8	2017
[34]	CAM	PH	L	Specific	img	607.8	2016
[31]	iNNvestigate	PH	L	Specific	img	365.3	2014
[23]	DeepExplain iNNvestigate tf-explain	PH	L	Specific	img	278.3	2013
[27]	DeepExplain iNNvestigate Integrated Gradients tf-explain alibi Skater	PH	L	Specific	img txt tab	247	2017
[40]	Deep Visualization Toolbox	PH	L	Specific	img	221.7	2(
[37]	DeepExplain iNNvestigate The LRP Toolbox Skater	PH	L	Specific	img txt	217.8	2(
[29]	DeepExplain DeepLift iNNvestigate tf-explain Skater	PH	L	Specific	img	211.5	2017
[41]	iNNvestigate	PH	L	Specific	img	131.5	2017
[38]	iNNvestigate tf-explain	PH	L	Specific	img	113.3	2017
[42]	tcav	PH	L	Specific	img	95	2018
[43]	rationale	PH	L	Specific	txt	81.4	2016
[36]	Grad-CAM++	PH	L	Specific	img	81	2018
[39]	RISE	PH	L	Specific	img	43.3	2018
[44]	iNNvestigate	PH	L	Specific	img	41.8	2017

3. Embedded into the classifier

DEEP LEARNING

GradCAM

"Used to indicate the discriminative regions of an image used by a CNN to identify the category of the image"

Grad-CAM uses the gradient information flowing into the last convolutional layer of the model to obtain localization map and understand the importance of each pixel of the input image for a specific class. Let's assume, $L^c_{Grad-CAM} \in \mathbb{R}^{u \times v}$ represents the localization map with width u and height v for class c. To calculate $L^c_{Grad-CAM}$, the gradient of the score for class c (before softmax), with respect to feature map k, A^k, of the last convolutional layer is calculated and global average pooled to obtain neuron importance weight, α^c_k:

$$\alpha^c_k = \frac{1}{N} \sum_i \sum_j \frac{\partial y^c}{\partial A^k_{ij}}$$

Furthermore, a weighted combination of forward activation maps followed by ReLU is obtained:

$$M = \text{ReLU}\left(\sum_k \alpha^c_k A^k\right).$$

This results in a coarse heatmap of the same size as the convolutional feature maps. Using ReLU allows us to capture features that have positive influence on the class of interest, i.e. pixels whose intensity should be increased in order to increase y^c. Negative pixels are likely to belong to other categories in the image. Without ReLU, localization maps sometimes highlight more than just the desired class and achieve lower localization performance.

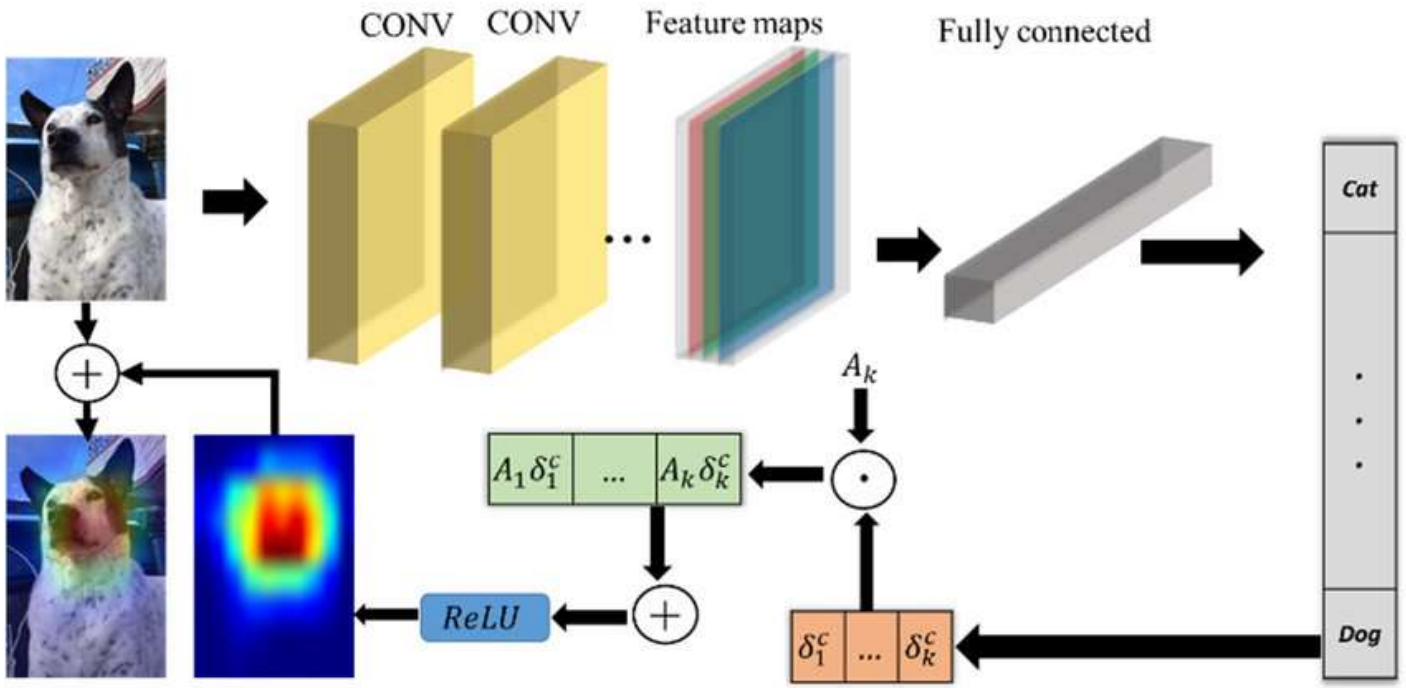
https://github.com/nejlag/Grad-CAM

DEEP LEARNING

3. Embedded into the classifier

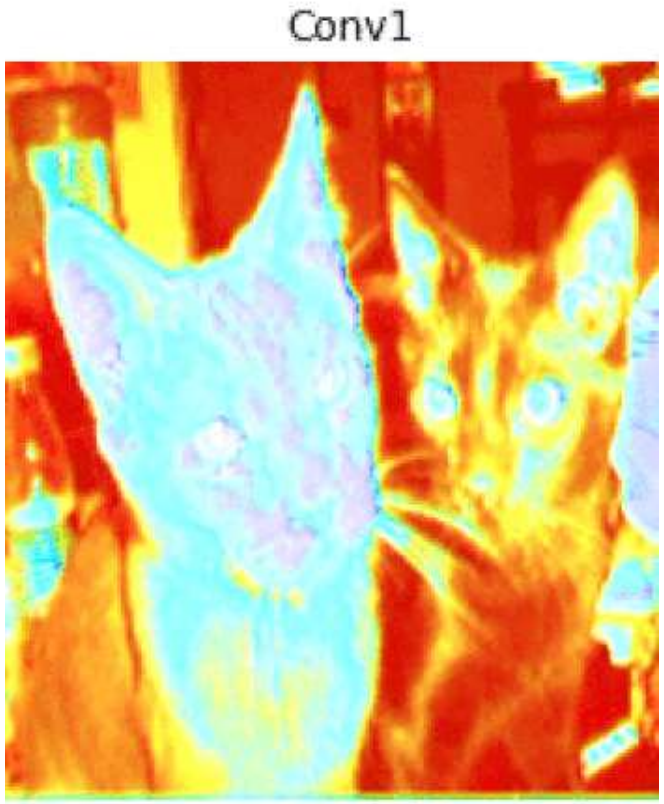
GradCAM

"Used to indicate the discriminative regions of an image used by a CNN to identify the category of the image"



Improve model explainability

DEEP LEARNING

3. Embedded into the classifier

GradCAM "Used to indicate the discriminative regions of an image used by a CNN to identify the category of the image"