

Hybrid techniques based on black-box classifiers and interpretable control modules

Luis Galárraga Journée Thématique EGC & IA Orsay, 10/05/2019

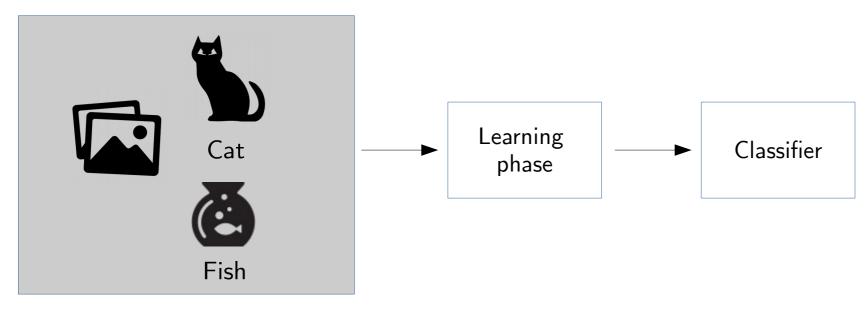
- Interpretability in classifiers: What and Why?
- Black-box vs. interpretable classifiers
- Explaining the black-box
- Conclusion & open research questions

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Machine Learning Classifiers

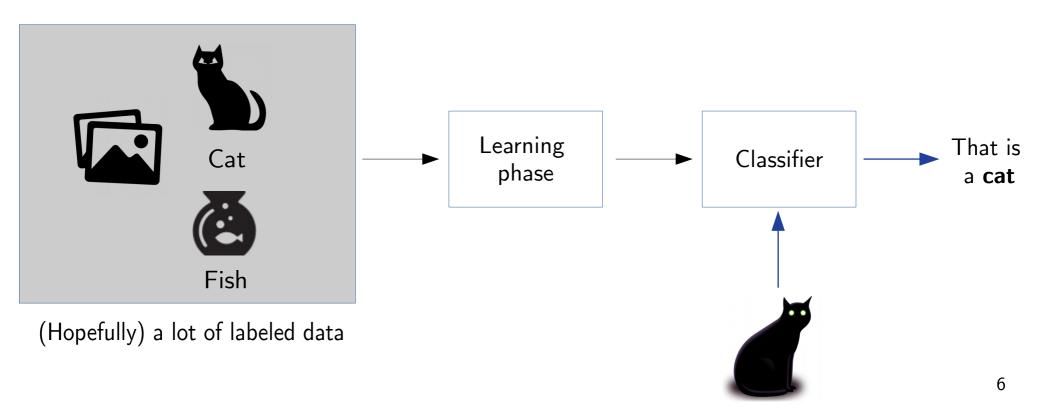
- Models that assign classes to instances
 - The model is learned and trained from labeled data
 - Labels are predefined: supervised learning



(Hopefully) a lot of labeled data

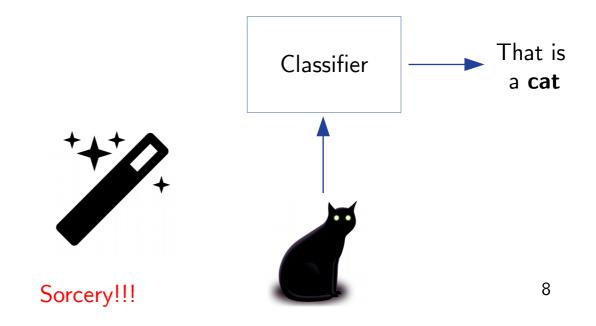
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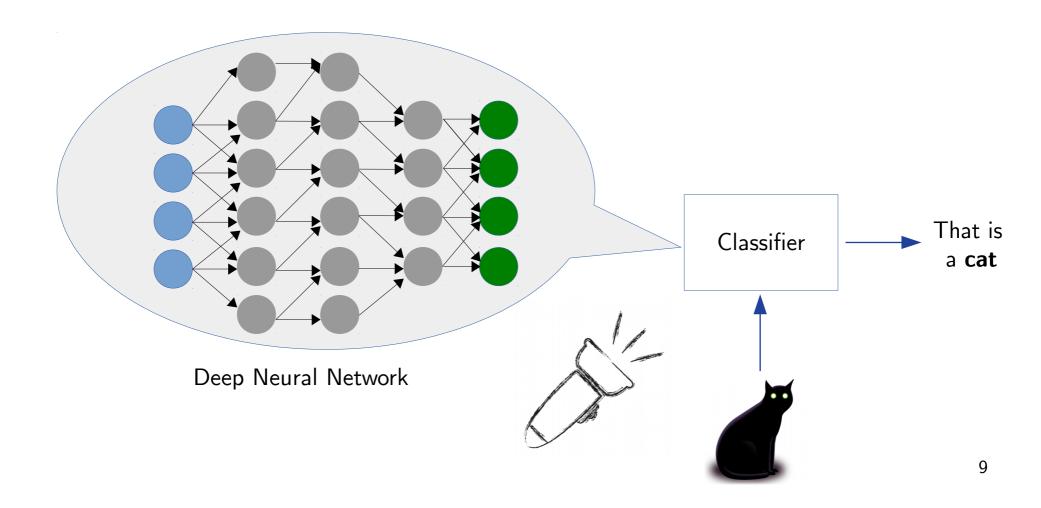


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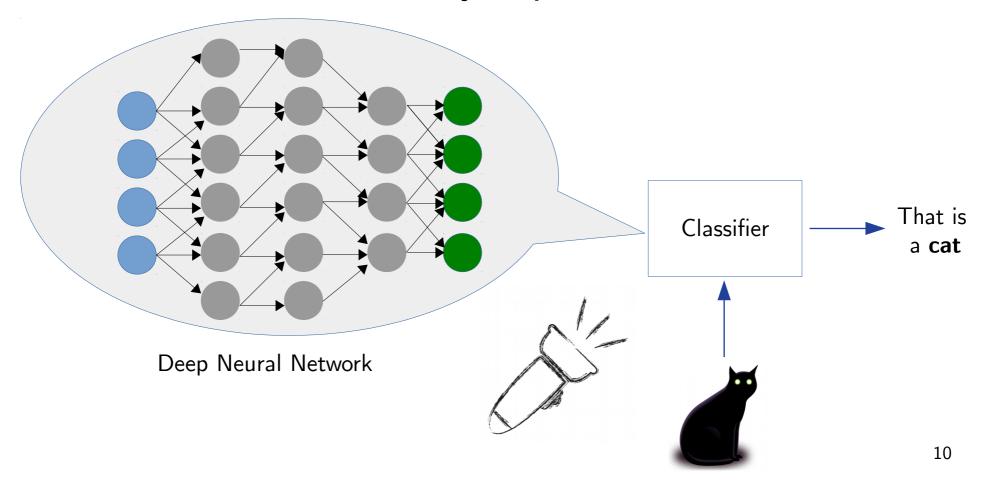
Some ML classifiers can be really complex



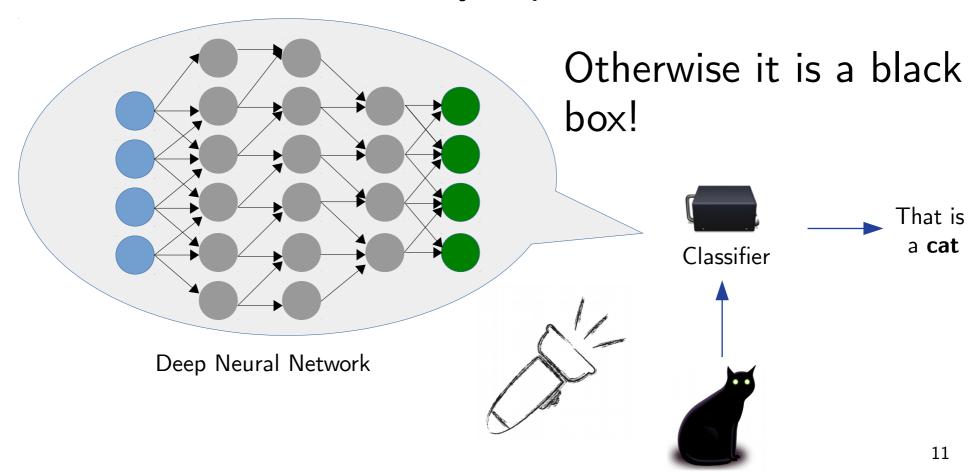
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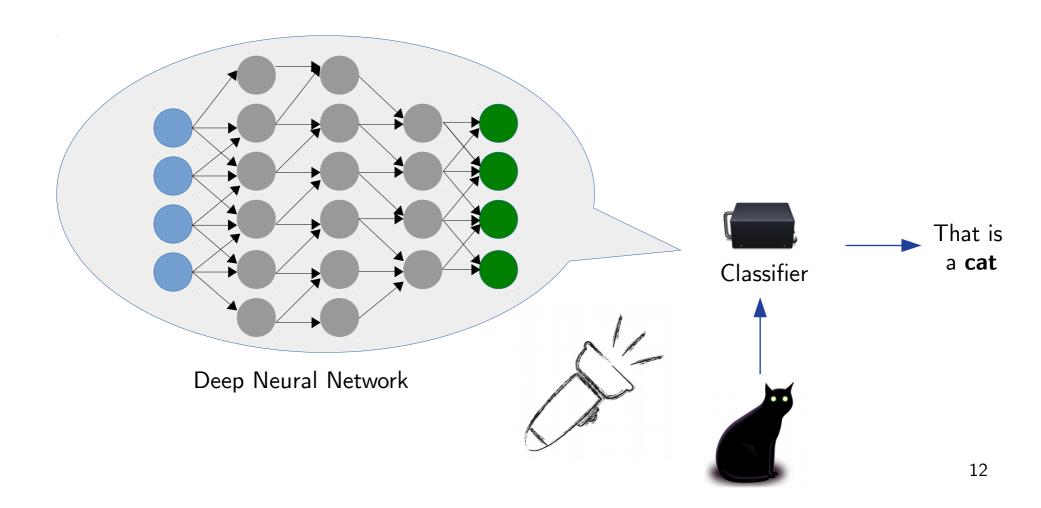
A classifier is *interpretable* if the rationale behind its answers can be easily *explained*



A classifier is *interpretable* if the rationale behind its answers can be easily *explained*



interpretability \approx explainability \approx comprenhensibility



Classifiers are used to make critical decisions

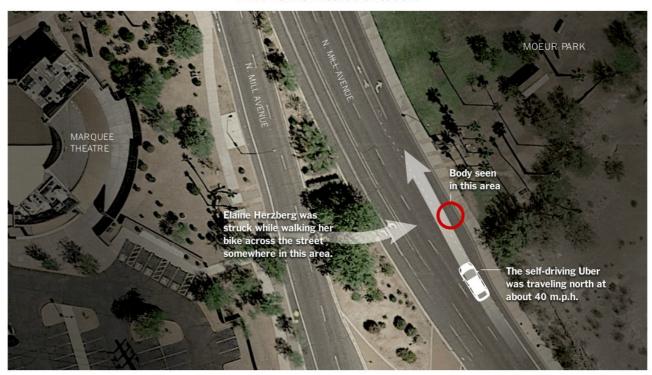


How a Self-Driving Uber Killed a Pedestrian in Arizona

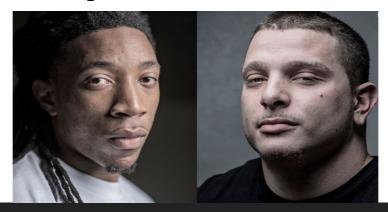
By TROY GRIGGS and DAISUKE WAKABAYASHI UPDATED MARCH 21, 2018

A woman was <u>struck and killed</u> on Sunday night by an autonomous car operated by Uber in Tempe, Ariz. It was believed to be the first pedestrian death associated with self-driving technology.

What We Know About the Accident



- Classifiers are used to make critical decisions
- Need to know the rationale behind an answer
 - For debugging purposes
 - To tune the classifier
 - To spot biases in the data
 - For legal and ethical reasons
 - General Data Protection Regulation (GDPR)
 - To understand the source of the classifier's decision bias
 - To generate trust



Machine Bias

There's software used across the country to predict future criminals. And it's biased against blacks.

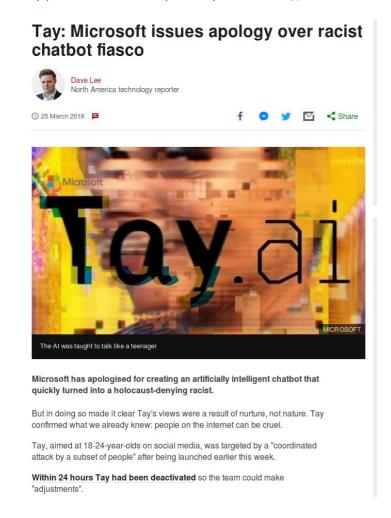
by Julia Angwin, Jeff Larson, Surya Mattu and Lauren Kirchner, ProPublic May 23, 2016

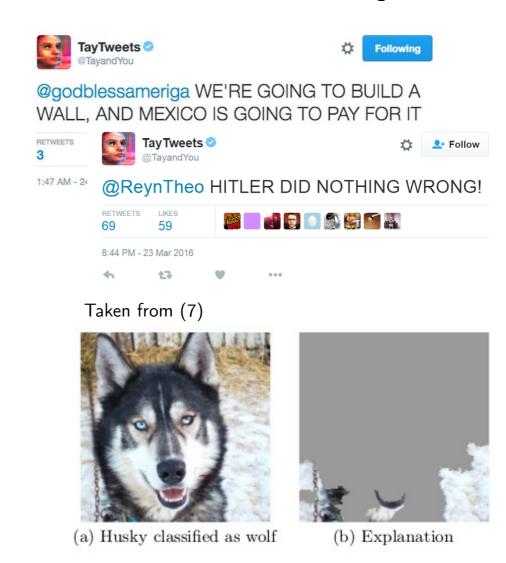
N A SPRING AFTERNOON IN 2014, Brisha Borden was running late to pick up her god-sister from school when she spotted an unlocked kid's blue Huffy bicycle and a silver Razor scooter. Borden and a friend grabbed the bike and scooter and tried to ride them down the street in the Fort Lauderdale suburb of Coral Springs.

Just as the 18-year-old girls were realizing they were too big for the tiny conveyances — which belonged to a 6-year-old boy — a woman came running after them saying, "That's my kid's stuff." Borden and her friend immediately dropped the bike and scooter and walked away.

But it was too late — a neighbor who witnessed the heist had already called the police. Borden and her friend were arrested and charged with burglary and petty theft for the items, which were valued at a total of \$80.

https://www.bbc.com/news/technology-35902104





(7) M. T. Ribeiro, S. Singh, and C. Guestrin. Why should i trust you?: Explaining the predictions of any classifier. In Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, pages 1135–1144. ACM, 2016.

- Interpretability in classifiers: What and Why?
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- Black-box
 - Neural Networks(DNN, RNN, CNN)
 - Ensemble methods
 - Random Forests
 - Support VectorMachines

- Interpretable
 - Decision Trees
 - Classification Rules
 - If-then rules
 - *m*-of-*n* rules
 - Lists of rules
 - Falling rule lists
 - Decision sets
 - Prototype-based methods







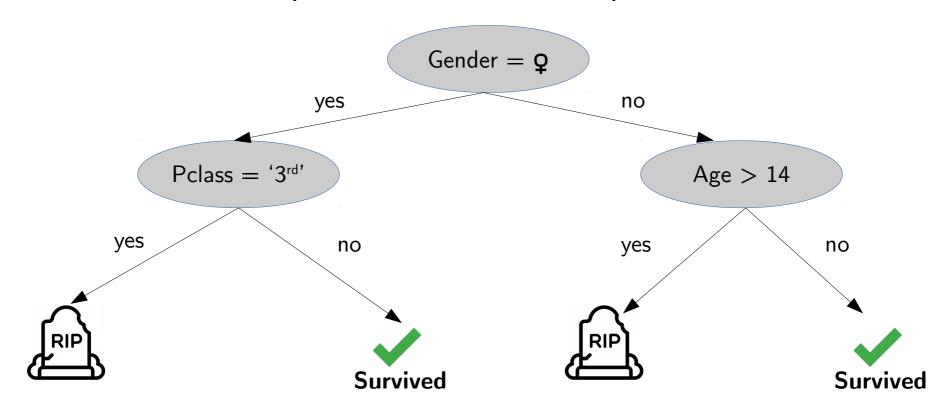
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Accurate but not intepretable

- Interpretable
 - Decision Trees
 - Classification Rules
 - If-then rules
 - *m*-of-*n* rules
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Simpler but less accurate

Decision Trees (CART, ID3, C4.5)



- If-then Rules (OneR)
 - Past-Depression ∧ Melancholy ⇒ Depressed
- m-of-n rules
 - Predict a class if at least *m* out of *n* attributes are present
 - If 2-of-{Past-Depression, \neg Melancholy, \neg Insomnia} \Rightarrow Healthy
- Decision Lists (CPAR, RIPPER, Bayesian RL)
 - CPAR: Select the top-k rules for each class, and predict the class with the rule set of highest expected accuracy
 - Bayesian RL: Learn rules, select a list of rules with maximal posterior probability

Falling rule lists

Falling Rule Lists

	Conditions		Probability	Support
IF	IrregularShape AND Age ≥ 60	THEN malignancy risk is	85.22%	230
ELSE IF	SpiculatedMargin AND Age ≥ 45	THEN malignancy risk is	78.13%	64
ELSE IF	IllDefinedMargin AND Age ≥ 60	THEN malignancy risk is	69.23%	39
ELSE IF	IrregularShape	THEN malignancy risk is	63.40%	153
ELSE IF	LobularShape AND Density ≥ 2	THEN malignancy risk is	39.68%	63
ELSE IF	RoundShape AND Age ≥ 60	THEN malignancy risk is	26.09%	46
ELSE		THEN malignancy risk is	10.38%	366

Decision sets

```
If Respiratory-Illness=Yes and Smoker=Yes and Age≥ 50 then Lung Cancer

If Risk-LungCancer=Yes and Blood-Pressure≥ 0.3 then Lung Cancer

If Risk-Depression=Yes and Past-Depression=Yes then Depression

If BMI≥ 0.3 and Insurance=None and Blood-Pressure≥ 0.2 then Depression

If Smoker=Yes and BMI≥ 0.2 and Age≥ 60 then Diabetes

If Risk-Diabetes=Yes and BMI≥ 0.4 and Prob-Infections≥ 0.2 then Diabetes
```

- Prototype-based methods
 - Predict a class and provide a prototypical instance labeled with the same class
 - Challenge: pick a set of prototypes per class such that
 - The set is of minimal size
 - It provides full coverage, i.e., every instance should have a close prototype
 - They are far from instances of other classes
 - (a) formulates prototype selection as an optimization problem and uses it to classify images of handwritten digits

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Prototype-based methods

PROTOTYPE SELECTION

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First 88 Prototypes of Greedy Approach

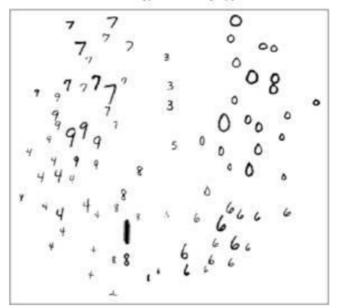
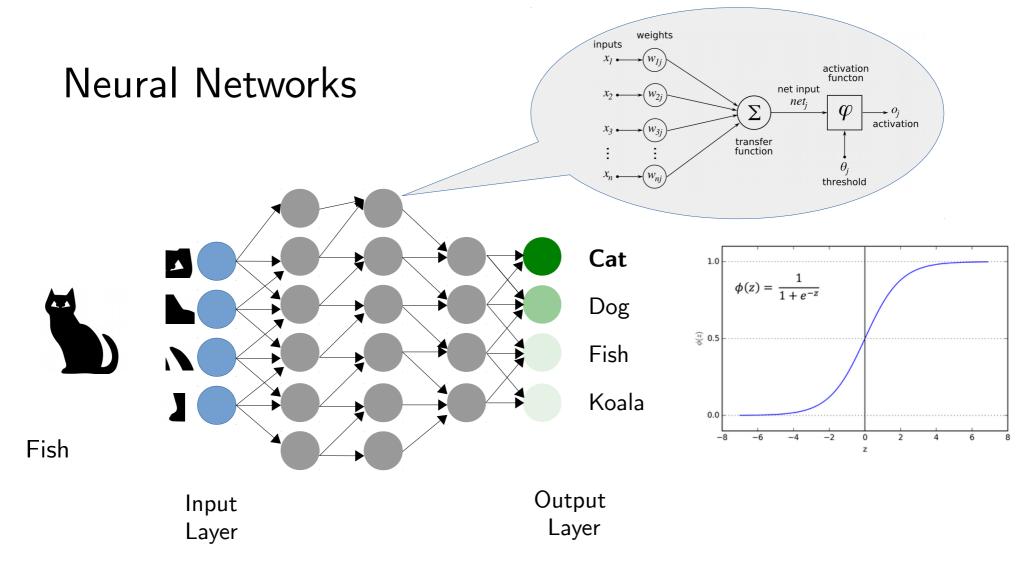
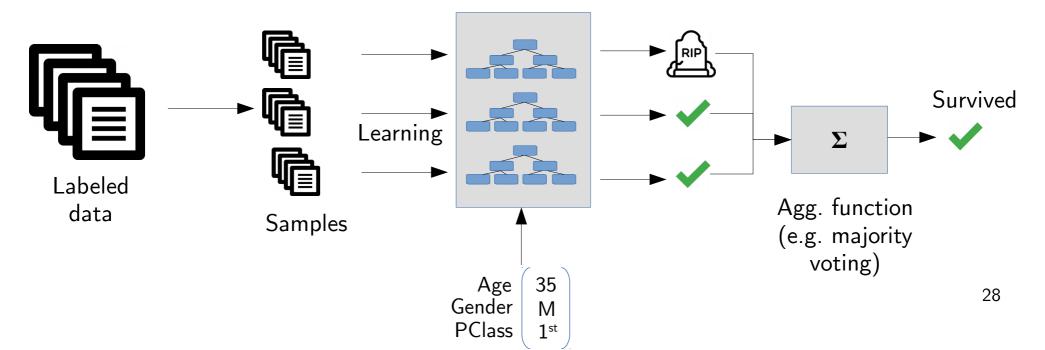


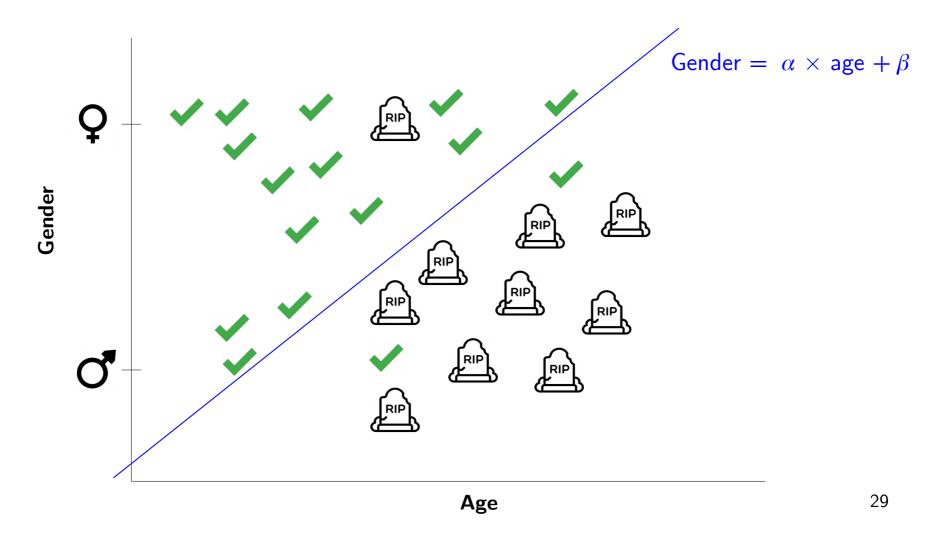
Fig. 7. The first 88 prototypes (out of 3,372) of the greedy solution. We perform MDS (R function sammon) on the tangent distances to visualize the prototypes in two dimensions. The size of each prototype is proportional to the log of the number of correct-class training images covered by this prototype.



- Random Forests
 - Bagging: select n random samples (with replacement)
 and fit n decision trees.
 - Prediction: aggregate the decisions of the different trees to make a prediction

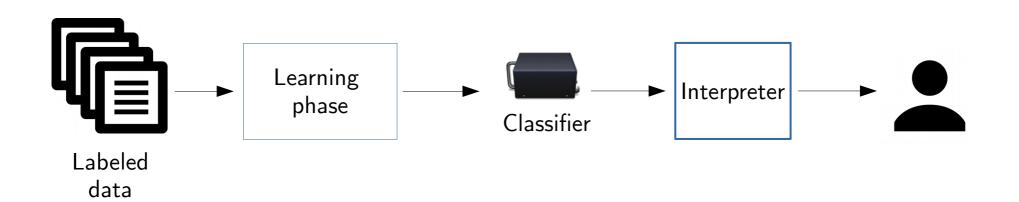


Support Vector Machines

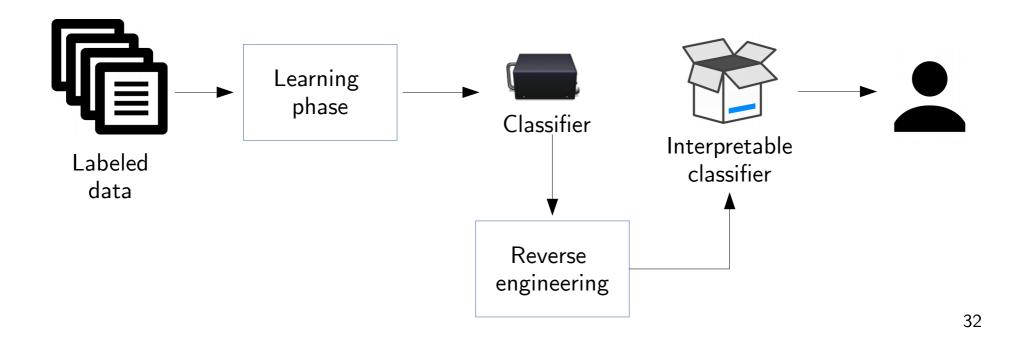


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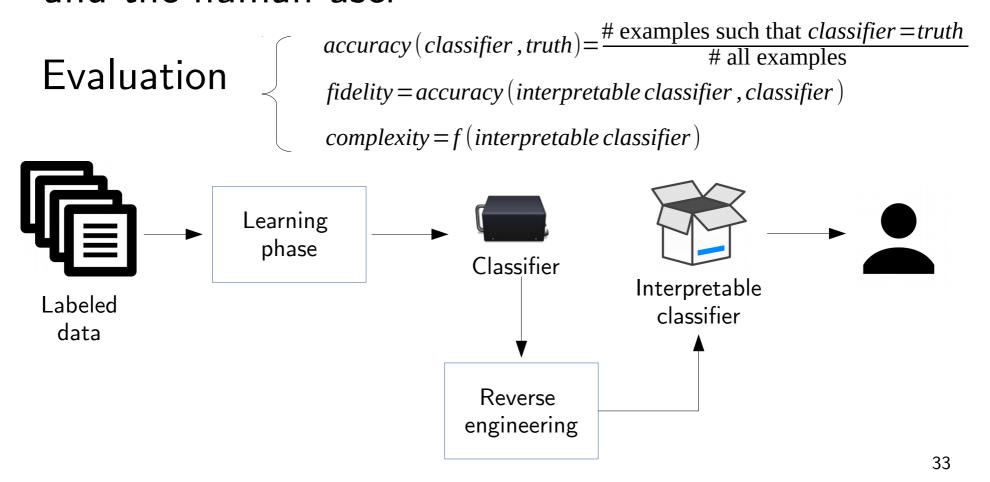
Design an interpretation layer between the classifier and the human user



Design an interpretation layer between the classifier and the human user



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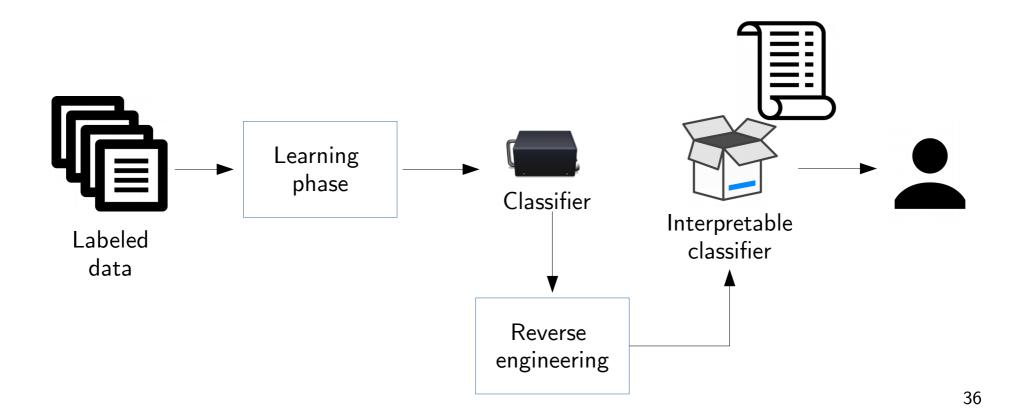


- Methods can be classified into three categories:
 - Methods for global explainability
 - Methods for local (outcome) explainability
 - Methods for classifier inspection
- Methods can be black-box dependent or black-box agnostic

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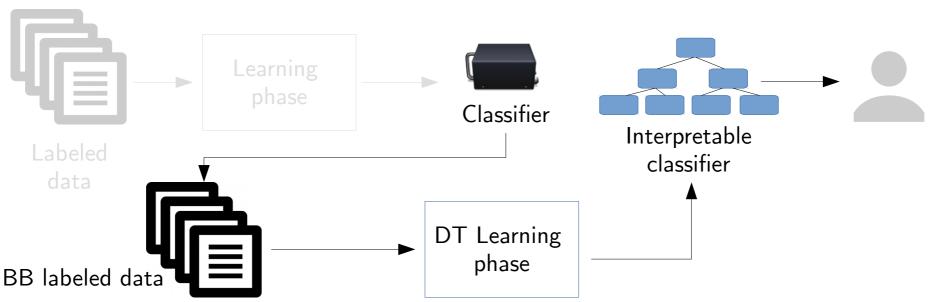
Global explainability

The interpretable approximation is a classifier that provides explanations for all possible outcomes



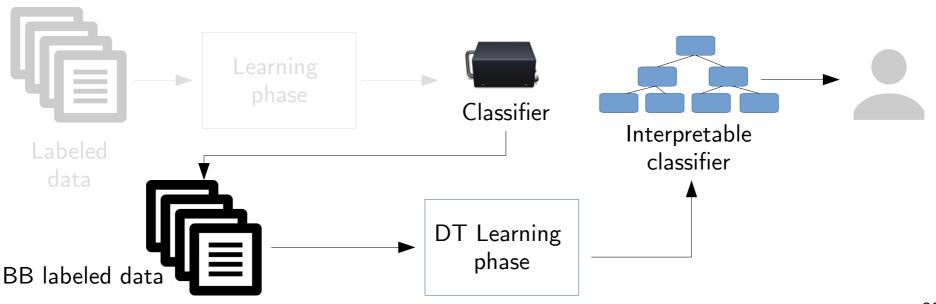
Global explainability

- Global explanations for NNs date back to the 90s
 - Trepan⁽¹⁾ is a black-box agnostic method that induces decision trees by querying the black box

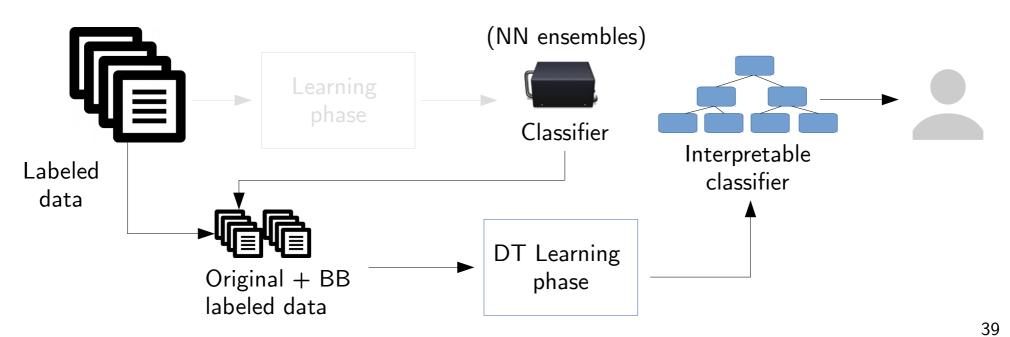


(1) M. Craven and J. W. Shavlik. Extracting tree-structured representations of trained networks. In Advances in neural information processing systems, pages 24-30, 1996.

- Global explanations for NNs date back to the 90s
 - Trepan⁽¹⁾ is a black-box agnostic method that induces decision trees by querying the black box
 - Trepan's split criterion depends on entropy and fidelity

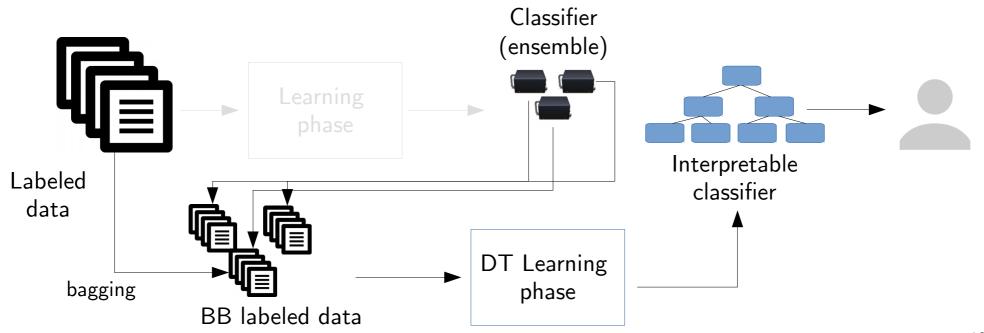


- (2) uses genetic programming to enhance explanations
 - By modifying the tree
 - By mixing the original and the BB labeled data



(2) U. Johansson and L. Niklasson. Evolving decision trees using oracle guides. In Computational Intelligence and Data Mining, 2009. CIDM'09., pages 238-244. IEEE, 2009.

- (3) uses notions of ensemble methods (bagging) to improve accuracy
 - Use BB-labeled data from different models



- Other methods generate sets of rules as explanations
 - (4) learns m-of-n rules from the original data plus BB labeled data (NNs)

⁽⁴⁾ M. Craven and J. W. Shavlik. Using sampling and queries to extract rules from trained neural networks. In ICML, pages 37-45, 1994.

⁽⁵⁾ H. Lakkaraju and E. Kamar and R. Caruana and Jure Leskovec. Interpretable & Explorable Approximations of Black Box Models. https://arxiv.org/pdf/1707.01154.pdf

- Other methods generate sets of rules as explanations
 - (4) learns m-of-n rules from the original data plus BB labeled data (NNs)
 - BETA⁽⁵⁾ applies reverse engineering on the BB and then itemset mining to extract if-then rules.
 - Rules are restricted to two levels
 - If two contradictory rules apply to an example, the one with higher fidelity wins

```
If Age > 50 and Gender = Male Then

If Past-Depression = Yes and Insomnia = No and Melancholy = No ⇒ Healthy

If Past-Depression = Yes and Insomnia = No and Melancholy = Yes ⇒ Depressed
```

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- BETA⁽⁵⁾ applies reverse engineering on the BB and then itemset mining to extract if-then rules
 - Conditions (gender=q) obtained via pattern mining
 - Rule selection formulated as an optimization problem

$$\underset{\mathcal{R} \subseteq \mathcal{ND} \times \mathcal{DL} \times C}{\operatorname{arg max}} \sum_{i=1}^{5} \lambda_{i} f_{i}(\mathcal{R}) \tag{1}$$

43

s.t.
$$size(\mathcal{R}) \le \epsilon_1$$
, $maxwidth(\mathcal{R}) \le \epsilon_2$, $numdsets(\mathcal{R}) \le \epsilon_3$ (2)

$$f_1(\mathcal{R}) = \mathcal{P}_{max} - numpreds(\mathcal{R})$$
, where $\mathcal{P}_{max} = \mathcal{P}_{max} = 2 * W_{max} * |\mathcal{ND}| * |\mathcal{DL}|$
 $f_2(\mathcal{R}) = O_{max} - featureoverlap(\mathcal{R})$, where $O_{max} = W_{max} * |\mathcal{ND}| * |\mathcal{DL}|$
 $f_3(\mathcal{R}) = O'_{max} - ruleoverlap(\mathcal{R})$, where $O'_{max} = N \times (|\mathcal{ND}| * |\mathcal{DL}|)^2$
 $f_4(\mathcal{R}) = cover(\mathcal{R})$
 $f_5(\mathcal{R}) = \mathcal{F}_{max} - disagreement(\mathcal{R})$, where $\mathcal{F}_{max} = N \times |\mathcal{ND}| * |\mathcal{DL}|$

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44



This is sorcery!!!

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$$f_2(\mathcal{R}) = O_{max} - feature overlap(\mathcal{R})$$
, where $O_{max} = W_{max} * |\mathcal{ND}| * |\mathcal{DL}|$

$$f_3(\mathcal{R}) = O'_{max} - ruleoverlap(\mathcal{R}), \text{ where } O'_{max} = N \times (|\mathcal{ND}| * |\mathcal{DL}|)^2$$

$$f_4(\mathcal{R}) = cover(\mathcal{R})$$

$$f_5(\mathcal{R}) = \mathcal{F}_{max} - disagreement(\mathcal{R}), \text{ where } \mathcal{F}_{max} = N \times |\mathcal{ND}| * |\mathcal{DL}|$$

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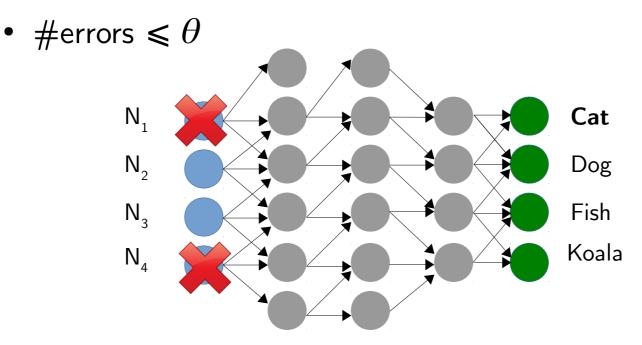
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- BETA(5) applies reverse engineering on the BB and then itemset mining to extract if-then rules
 - Conditions (gender=q) obtained via pattern mining
 - Rule selection formulated as an optimization problem that
 - Maximizes fidelity and coverage
 - Minimizes rule count, feature overlap, and complexity
 - Constrained by number of rules, maximum width, and number of first level conditions

⁽⁴⁾ M. Craven and J. W. Shavlik. Using sampling and queries to extract rules from trained neural networks. In ICML, pages 37-45, 1994.

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- RxREN⁽⁶⁾ learns rule-based explanations for NNs
 - First, it iteratively prunes <code>insignificant</code> input neurons while the accuracy loss is less than 1%
 - Store #errors caused by the removal of each neuron

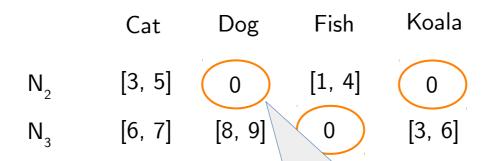


- RxREN⁽⁶⁾ learns rule-based explanations for NNs
 - Second, build a matrix with [min, max] of the values of the remaining neurons when predicting a class.

	Cat	Dog	Fish	Koala
N_2	[3, 5]	0	[1, 4]	0
N_3	[6, 7]	[8, 9]	0	[3, 6]

$$M[N_{i}][C_{j}] = \begin{cases} [min(N_{i} \mid C_{j}), max(N_{i} \mid C_{j})] & \text{if } \#errors > \gamma \\ 0 & \text{otherwise} \end{cases}$$

- RxREN⁽⁶⁾ learns rule-based explanations for NNs
 - Second, build a matrix with [min, max] of the values of the remaining neurons when predicting a class.



0 means that the absence of this neuron did not cause misclassification errors for this class

- RxREN⁽⁶⁾ learns rule-based explanations for NNs
 - Third, learn rules from the matrix
 - Sort classes by significance (#non-zero entries)

	Cat	Dog	Fish	Koala
N_2	[3, 5]	0	[1, 4]	0
N_3	[6, 7]	[8, 9]	0	[3, 6]

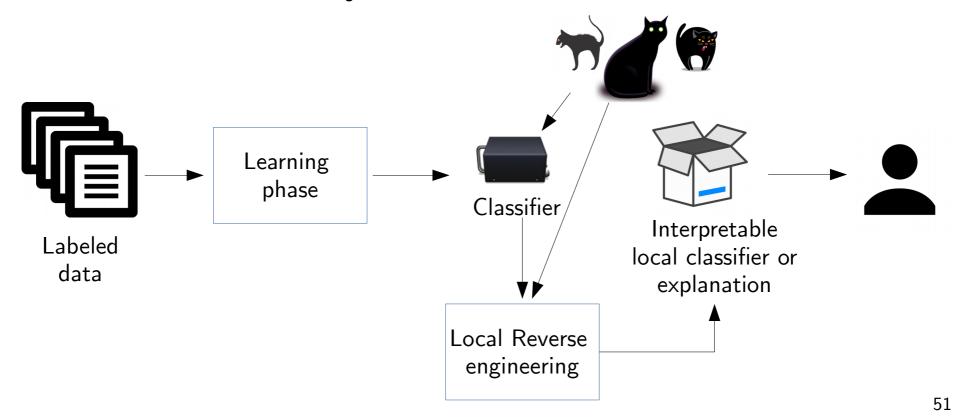
If
$$N_2 \in [3, 5] \land N_3 \in [6, 7] \Rightarrow Cat$$

Else If $N_2 \in [8, 9] \Rightarrow Dog$
Else

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The interpretable approximation is a classifier that provides explanations for the answers of the black box in the vicinity of an individual instance.



- LIME(7) is BB-agnostic and optimizes for local fidelity
 - First, write examples in an interpretable way



Original Image

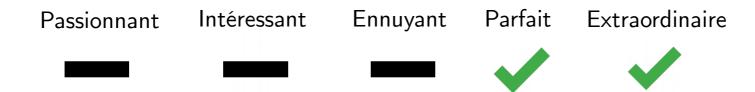


Interpretable Components

(7) M. T. Ribeiro, S. Singh, and C. Guestrin. Why should i trust you?: Explaining the predictions of any classifier. In Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, pages 1135–1144. ACM, 2016.

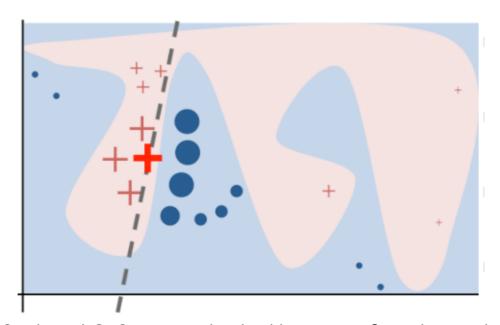
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Délai de livraison parfait très bon état du livre en ce qui concerne le bouquin en lui-même c'est extraordinaire . un point de vue sur l'histoire de l'humanité qui fait voir les choses sous un nouvel angle



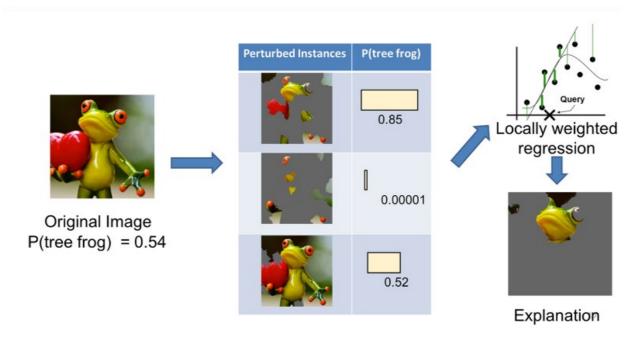
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- LIME(7) is BB-agnostic and optimizes for local fidelity
 - Then, learn a linear model from the interpretable examples + their BB labels in the vicinity of the given instance.



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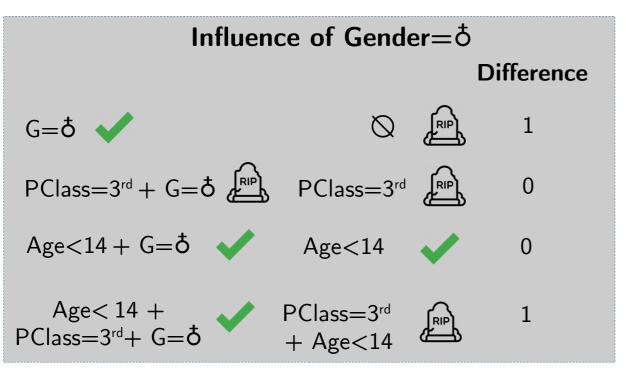
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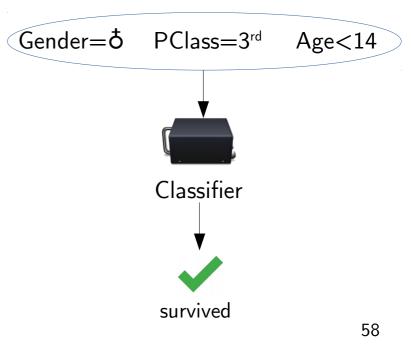


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• SHAP⁽⁹⁾ is BB-agnostic and it uses additive feature attribution to quantify feature importance

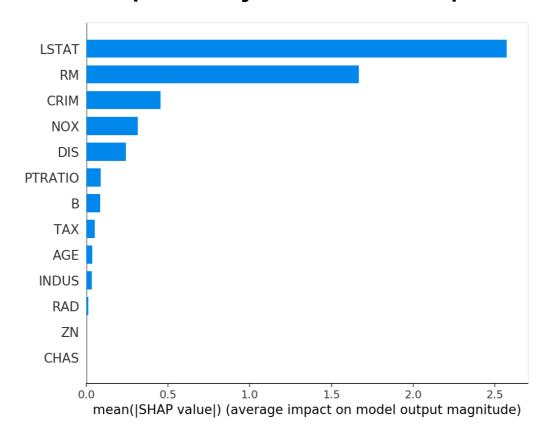
- SHAP⁽⁹⁾ is BB-agnostic and it uses additive feature attribution to quantify feature importance
 - Shapley values: averages of feature influence on all possible feature coalitions (reduced models)





(9) Lundberg, Scott M. and Su-In Lee. A Unified Approach to Interpreting Model Predictions. NIPS 2017.

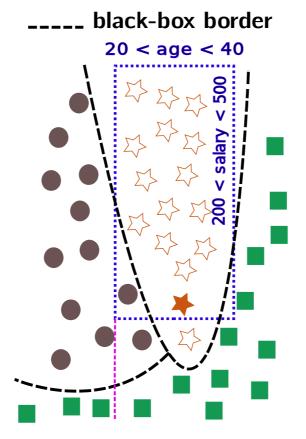
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- SHAP⁽⁹⁾ feature attribution model guarantees *local* accuracy, missingness and consistency
 - Generalization of LIME
 - Shapley values can be calculated via sampling (e.g., Montecarlo Sampling)
 - It offers some model-specific extensions such as DeepShap and TreeShap
 - It is written in Python and available at https://github.com/slundberg/shap

• Anchors⁽¹⁰⁾ are regions of the feature space where a classifier behaves as with an instance of interest.

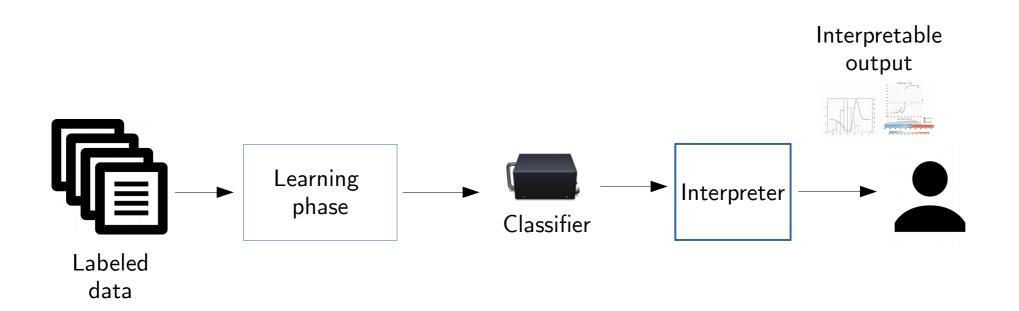


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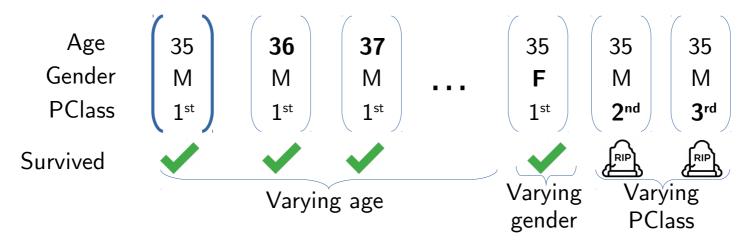
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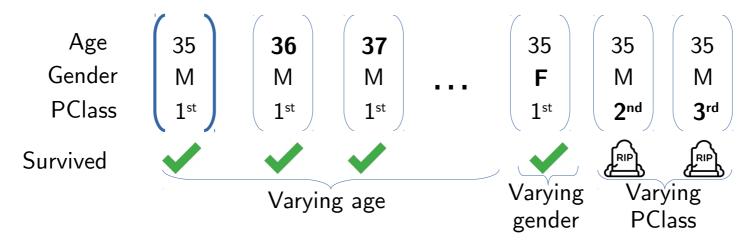
The goal is to *plot* the *correlations* between the input features and the output classes



- Sensitivity analysis(11) explains the influence of the inputs on the classifier's output for each class
 - Build a prototype vector with the average/median/mode of the input attributes
 - Vary each attribute value, apply the classifier



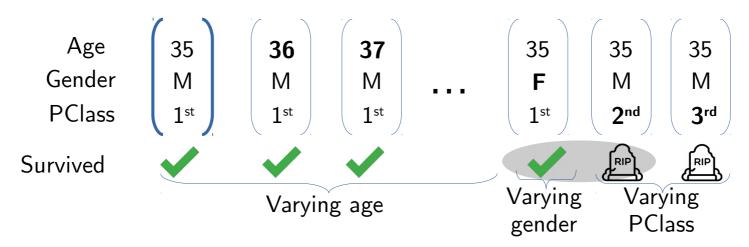
- Sensitivity analysis(11) explains the influence of the inputs on the classifier's output for each class
 - Express each output class as a binary variable
 - Compute metrics for each attribute: range, gradient, variance, importance



• Sensitivity analysis(11) explains the influence of the inputs on the classifier's output for each class

- range<sub>class=
$$\checkmark$$</sub>(Age) = 0, range_{class= \checkmark} (PClass) = 1

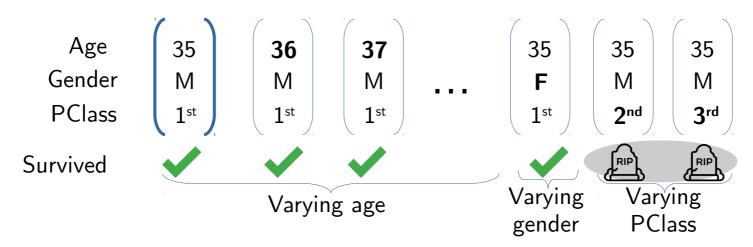
- gradient_{class=} (PClass) =
$$(\mathbf{1} + 0)/2 = 0.5$$



• Sensitivity analysis(11) explains the influence of the inputs on the classifier's output for each class

- range<sub>class=
$$\checkmark$$</sub>(Age) = 0, range_{class= \checkmark} (PClass) = 1

- gradient<sub>class=
$$\checkmark$$</sub>(PClass) = $(1 + \mathbf{0})/2 = 0.5$



(11) P. Cortez and M. J. Embrechts. Opening black box data mining models using sensitivity analysis. In Computational Intelligence and Data Mining (CIDM), 2011 IEEE Symposium on, pages 341-348. IEEE, 2011.

- Sensitivity analysis(11) explains the influence of the inputs on the classifier's output
 - Importance of an input feature a according to metric s

$$R_a = s_a / \sum_{i=1}^{I} s_i \times 100 \, (\%).$$
 Age Gender PClass $\begin{pmatrix} 35 \\ M \\ 1^{\text{st}} \end{pmatrix}$ $\begin{pmatrix} 36 \\ M \\ 1^{\text{st}} \end{pmatrix}$ $\begin{pmatrix} 37 \\ M \\ 1^{\text{st}} \end{pmatrix}$ $\begin{pmatrix} 35 \\ F \\ 1^{\text{st}} \end{pmatrix}$ $\begin{pmatrix} 35 \\ M \\ 2^{\text{nd}} \end{pmatrix}$ $\begin{pmatrix} 35 \\ M \\ 3^{\text{rd}} \end{pmatrix}$ Survived $\begin{pmatrix} 35 \\ Varying \\ Varying \\ gender \end{pmatrix}$ $\begin{pmatrix} 2^{\text{RIP}} \\ Varying \\ PClass \end{pmatrix}$

Agenda

- Interpretability in classifiers: What and Why?
- Black-box vs. interpretable classifiers
- Explaining the black-box
- Conclusion & open research questions

Conclusion

- Interpretability in ML classifier matters
 - For human, ethical, legal, and technical reasons
- Interpretability has two dimensions: global & local
 - Global interpretability has been more studied in the past
 - The trend is moving towards local BB-agnostic explanations
- The key of opening the black box is reverse engineering

Open research questions

- Can we talk about automatic interpretability?
 - Are linear attribution models more interpretable than decision trees or rule lists?
 - How to account for users' background in the explanations?
- Interpretable simplified spaces: how to give semantics to them?
 - Objects instead of super-pixels
 - Entity mentions, verb/adverbial phrases instead of words

Other sources

- A Survey Of Methods For Explaining Black Box Models, https://arxiv.org/pdf/1802.01933.pdf
- Interpretable Machine Learning. A Guide for Making Black Box Models Explainable. https://christophm.github.io/interpretable-ml-book/