Explainable Artificial Intelligence

Jorge Amaya
Research Expert
KU Leuven
AIDA Project

github.com/CmPA/AIDA-School

Who has already worked with ML/AI models?

Who has already published scientific results obtained using ML/AI models?

Would you agree to tie your salary to the accuracy of your ML/AI model?

A crisis in science

AAAS: Machine learning 'causing science crisis'

By Pallab Ghosh
Science correspondent, BBC News, Washington

16 February 2019

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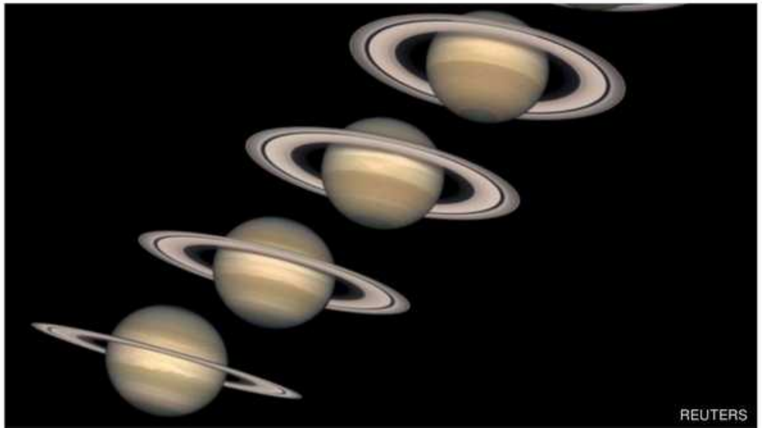
AAAS meeting



Astronomy is one of the many areas of science in which machine learning is used to make discoveries

Machine-learning techniques used by thousands of scientists to analyse data are producing results that are misleading and often completely wrong.

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- **Reproducibility:**
  - Patterns only in data sets and not in nature?

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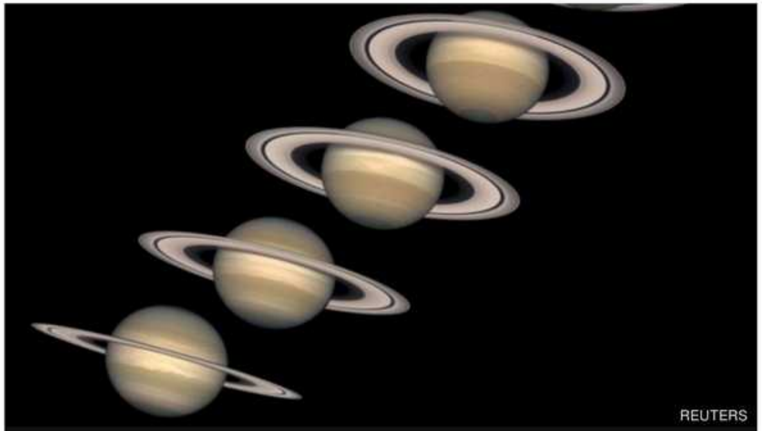

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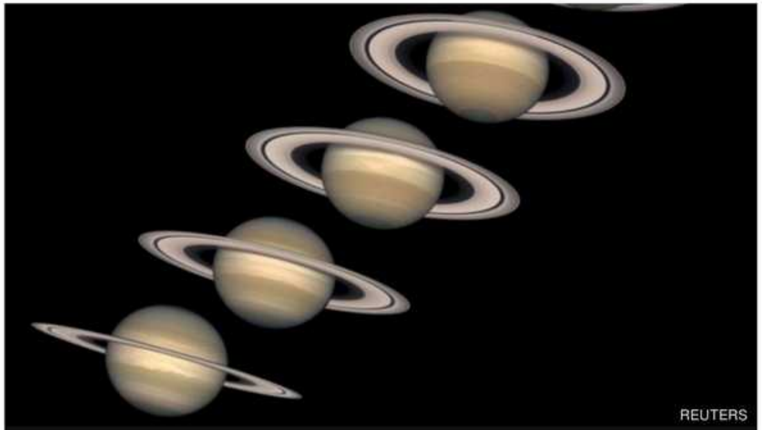

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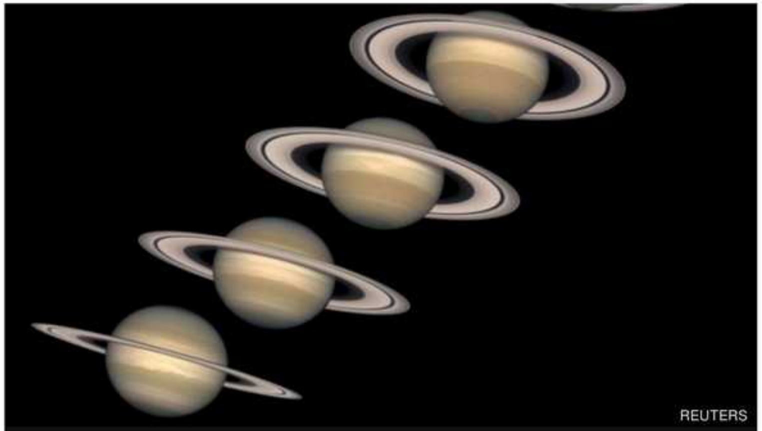

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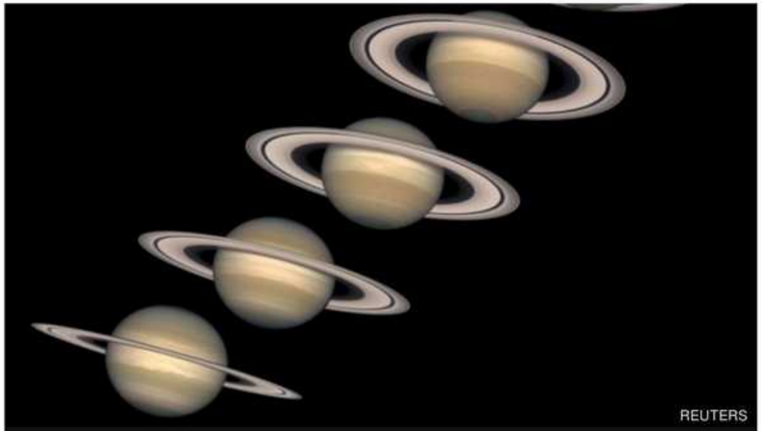

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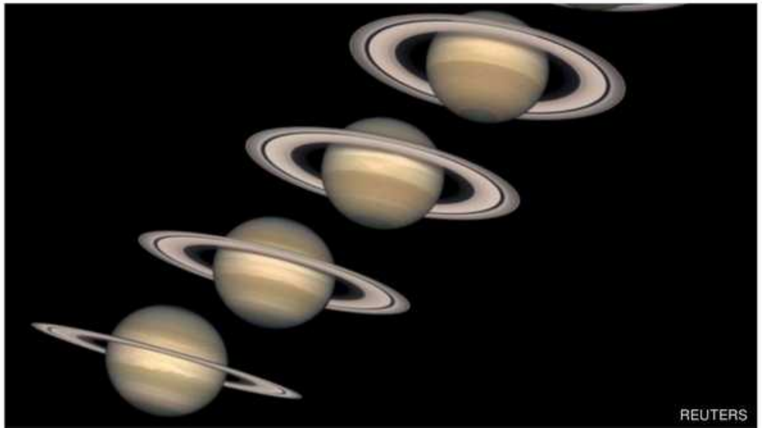

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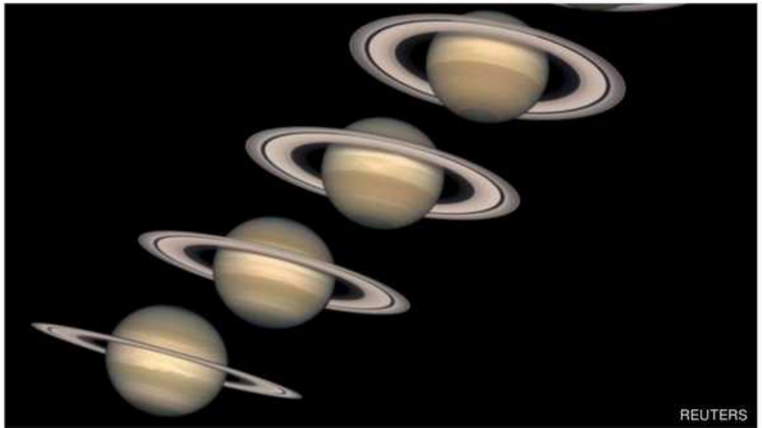
REUTERS

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- **Trust:**

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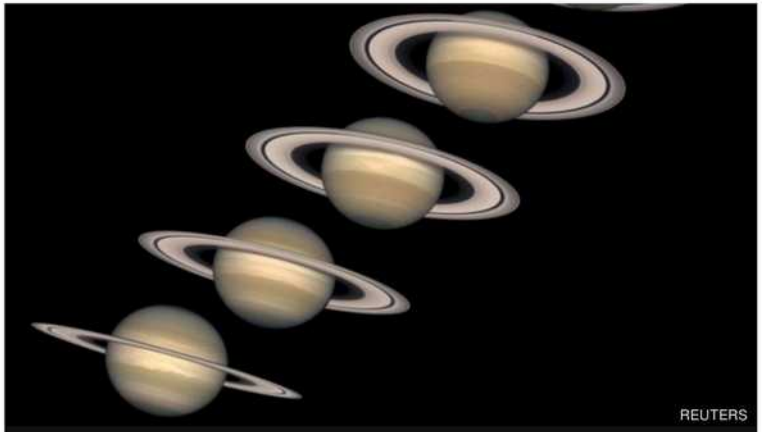

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  - Are you confident your model is accurate in all cases?

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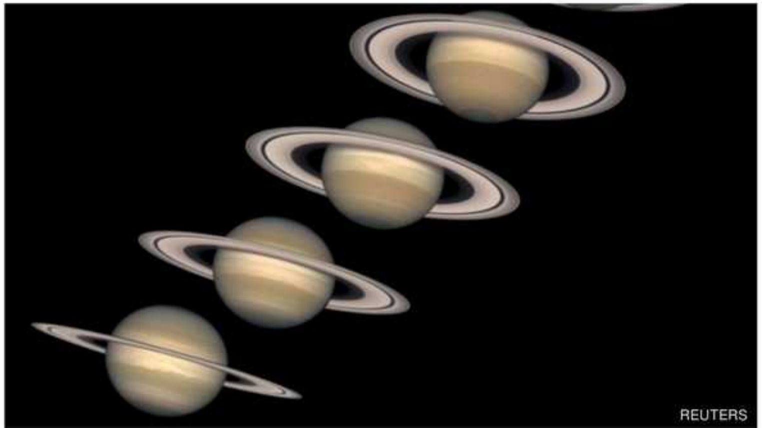

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- **Trust:**
  - Are you confident your model is accurate in all cases?
  - How does your model work internally?

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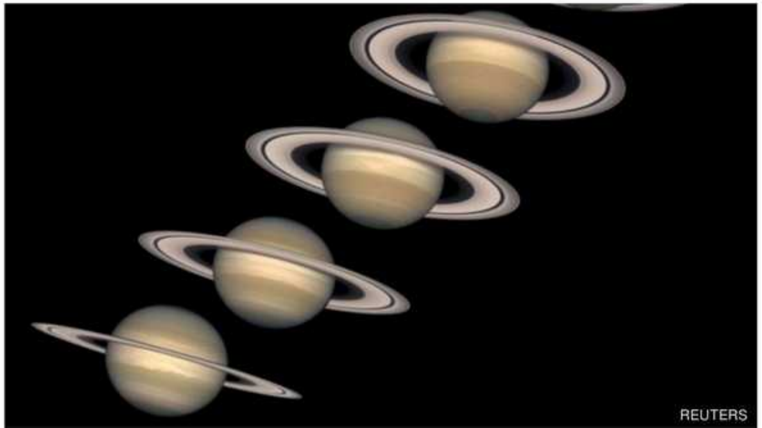

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- **Trust:**
  - Are you confident your model is accurate in all cases?
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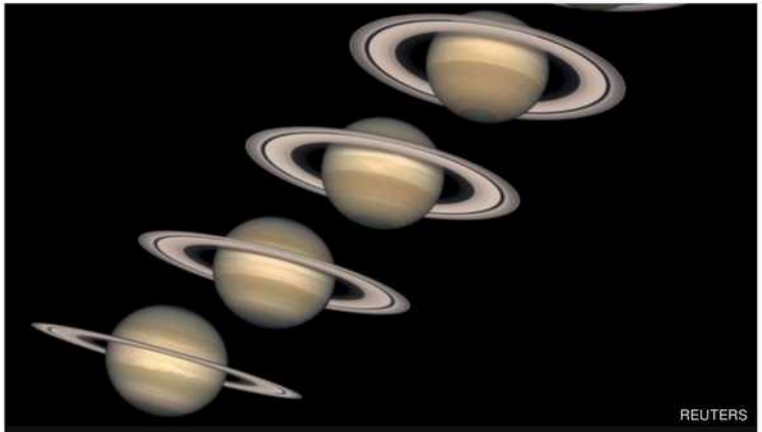

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- **Trust:**
  - Are you confident your model is accurate in all cases?
  - How does your model work internally?
  - Can you explain *why* an input gives an output?
  - Can a small change in the model (hyper- parameters, data, training time) lead to different results?

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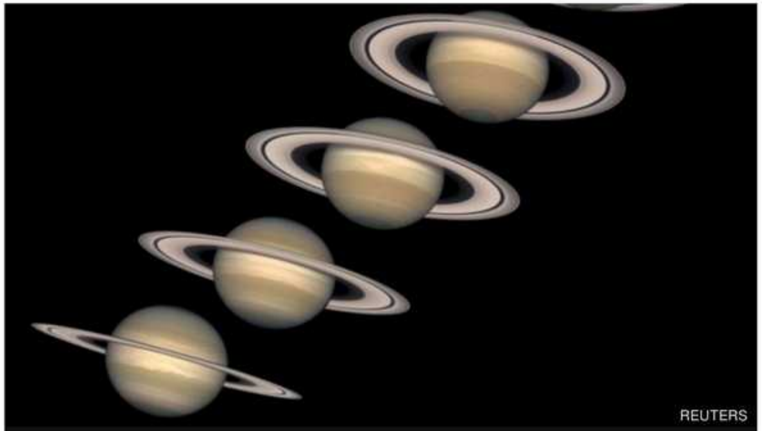

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ML data bias: horror stories

REUTERS

TECHNOLOGY NEWS OCTOBER 10, 2018 / 5:12 AM / A YEAR AGO

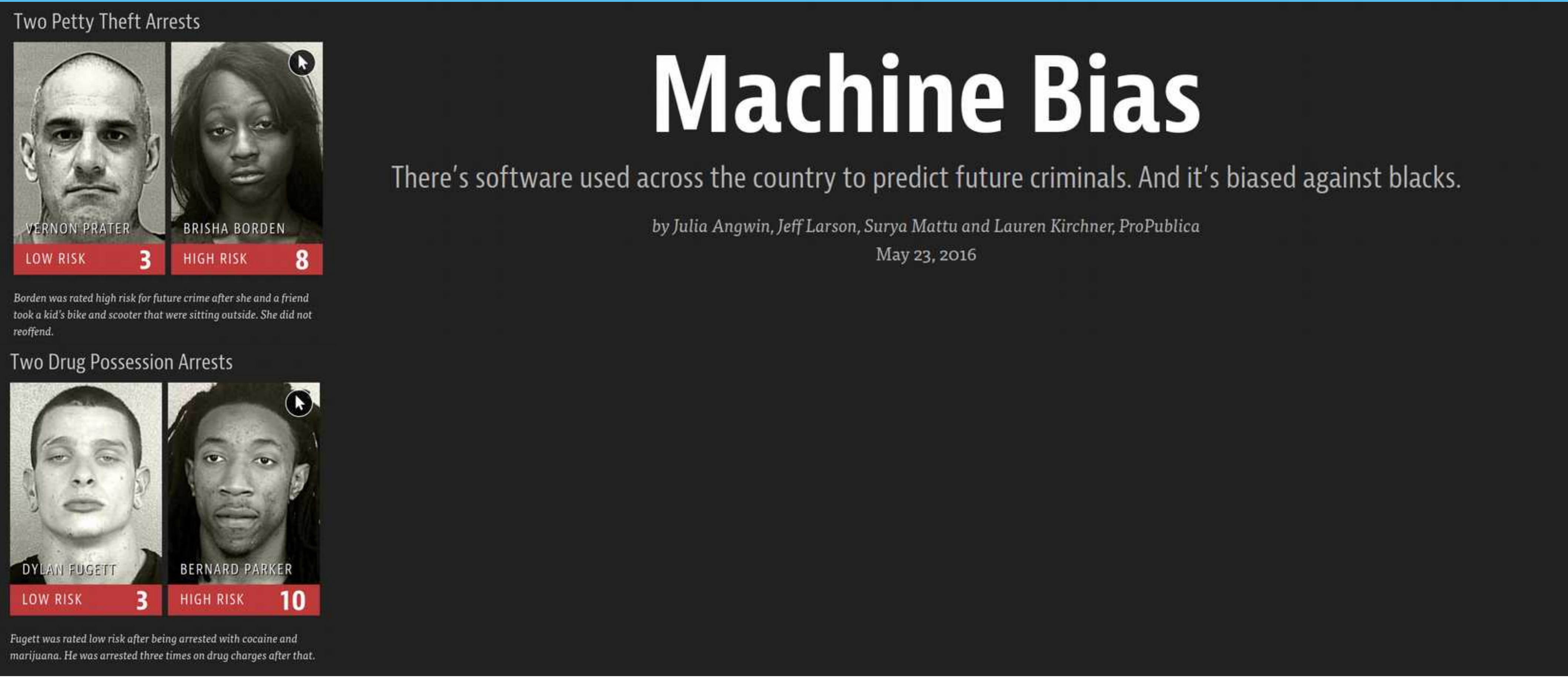
Amazon scraps secret AI recruiting tool that showed bias against women

Jeffrey Dastin

8 MIN READ

SAN FRANCISCO (Reuters) - Amazon.com Inc's (AMZN.O) machine-learning specialists uncovered a big problem: their new recruiting engine did not like women.

ML data bias: horror stories



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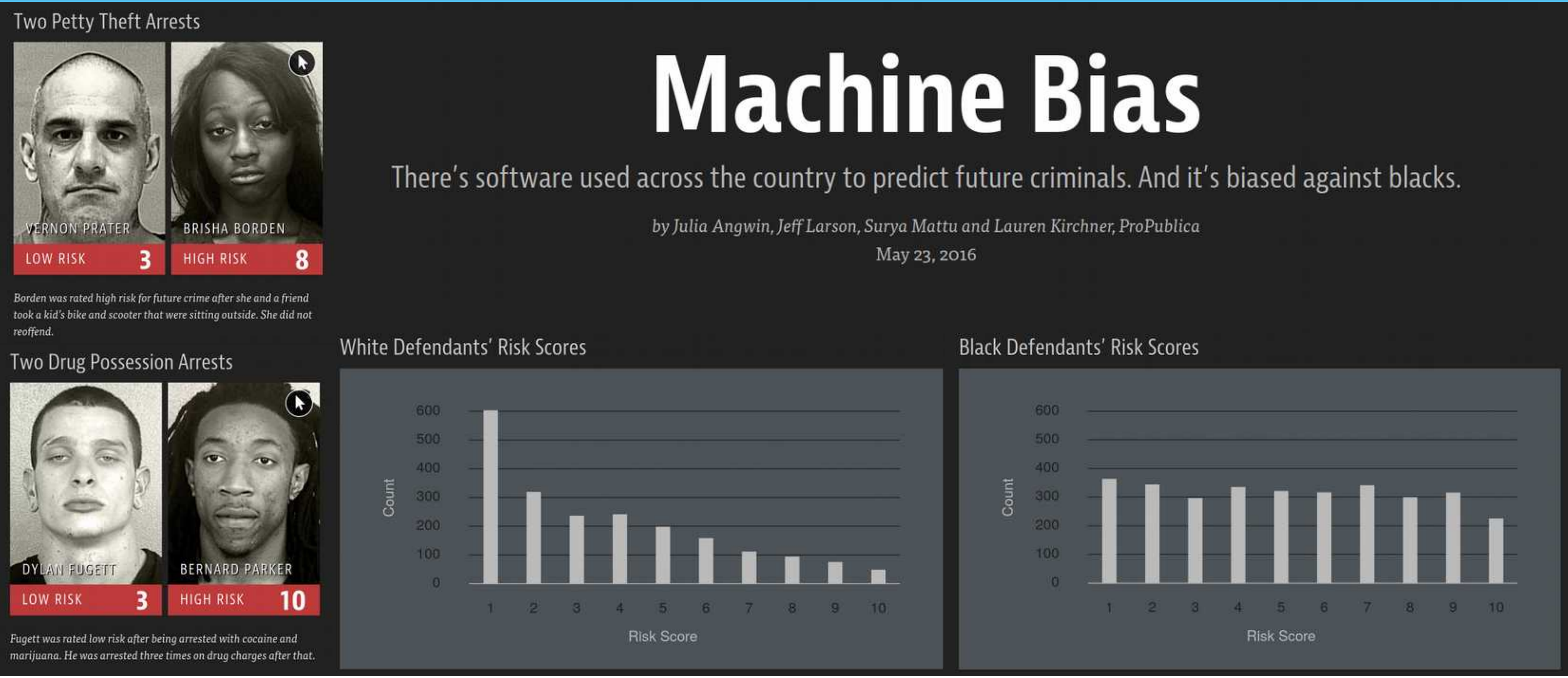
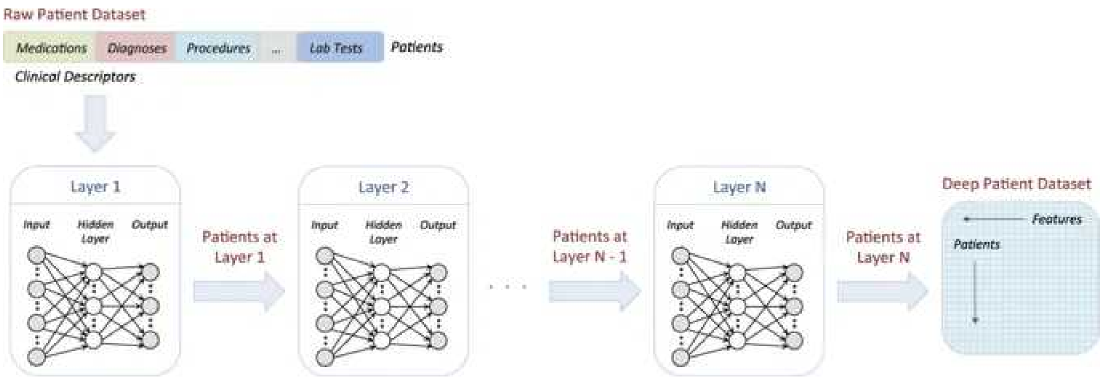


ML data bias: horror stories

Deep Patient (Mount Sinai Hospital in New York)



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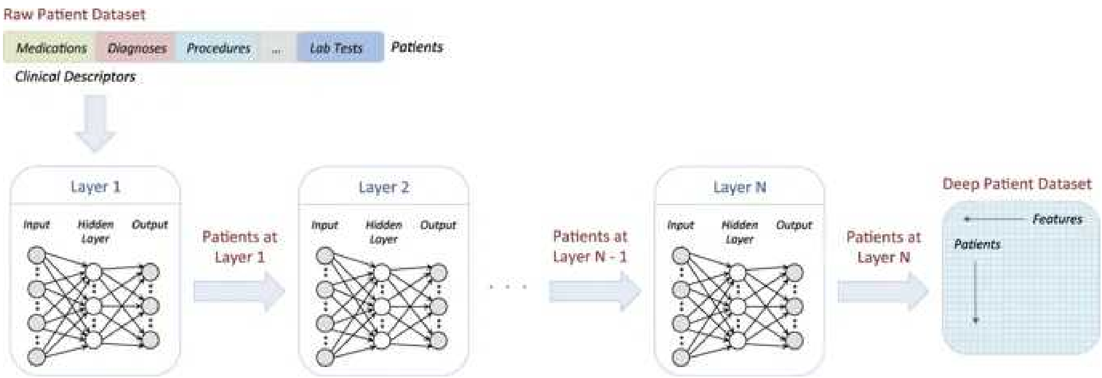

Joel Dudley, PhD

DIRECTOR, INSTITUTE FOR NEXT GENERATION HEALTHCARE
ASSOCIATE PROFESSOR | Genetics and Genomic Sciences
ASSOCIATE PROFESSOR | Population Health Science and Policy
ASSOCIATE PROFESSOR | Medicine

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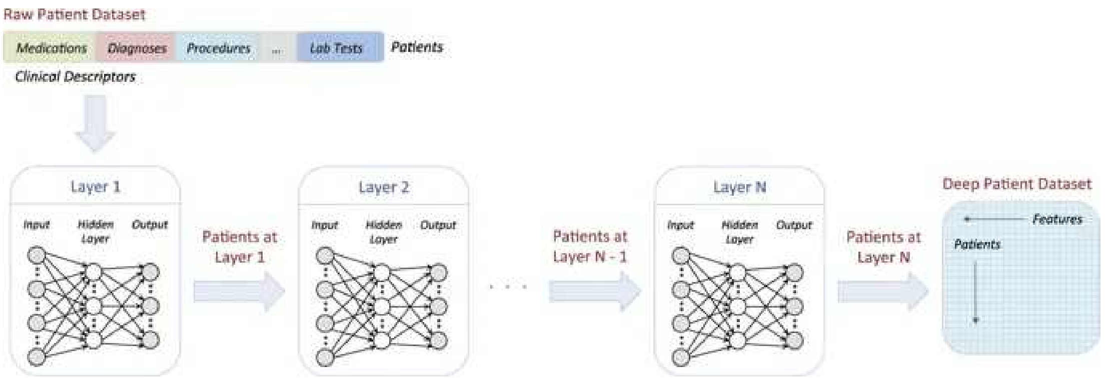

Artificial Intelligence / Machine Learning

The Dark Secret at the Heart of AI

No one really knows how the most advanced algorithms do what they do. That could be a problem.

by **Will Knight** Apr 11, 2017

Joel Dudley, PhD

DIRECTOR, INSTITUTE FOR NEXT GENERATION HEALTHCARE
ASSOCIATE PROFESSOR | Genetics and Genomic Sciences
ASSOCIATE PROFESSOR | Population Health Science and Policy
ASSOCIATE PROFESSOR | Medicine

"We can build these models, but we don't know how they work."

This story is part of our May/June 2017 issue

Facing the “science crisis” in ML

Facing the “science crisis” in ML

Reproducibility

How to reproduce the results of old experiments (from the literature)

Facing the “science crisis” in ML

Reproducibility

How to reproduce the results of old experiments (from the literature)

Trust

How to be confident in the results of my models and in the accuracy of my scientific discoveries

Reproducibility: the hell of ML

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ML technique used

Reproducibility: the hell of ML

ML technique used

Model architecture

Reproducibility: the hell of ML

ML technique used

Model architecture

Hyper-parameter selection

Reproducibility: the hell of ML

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Hyper-parameter selection

Data sources

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Data pre-processing methods

Reproducibility: the hell of ML

ML technique used	Model architecture	Hyper-parameter selection
Data sources	Data pre-processing methods	Computing resources

Reproducibility: the hell of ML

- ML technique used
- Model architecture
- Hyper-parameter selection
- Data sources
- Data pre-processing methods
- Computing resources
- Software

Reproducibility: the hell of ML

ML technique used	Model architecture	Hyper-parameter selection
Data sources	Data pre-processing methods	Computing resources
Software	Evaluation metrics	

Reproducibility: the hell of ML

ML technique used	Model architecture	Hyper-parameter selection
Data sources	Data pre-processing methods	Computing resources
Software	Evaluation metrics	Budget

Reproducibility: tools

Reproducibility: tools

GitHub

Keep a repository of your code

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GitHub

Keep a repository of your code

OSF

Keep a repository of your data

Reproducibility: tools

GitHub

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jupyter

Keep a clear track of your procedures

Reproducibility: tools

GitHub — Keep a repository of your code

binder — Allow your code to be openly examined by the community

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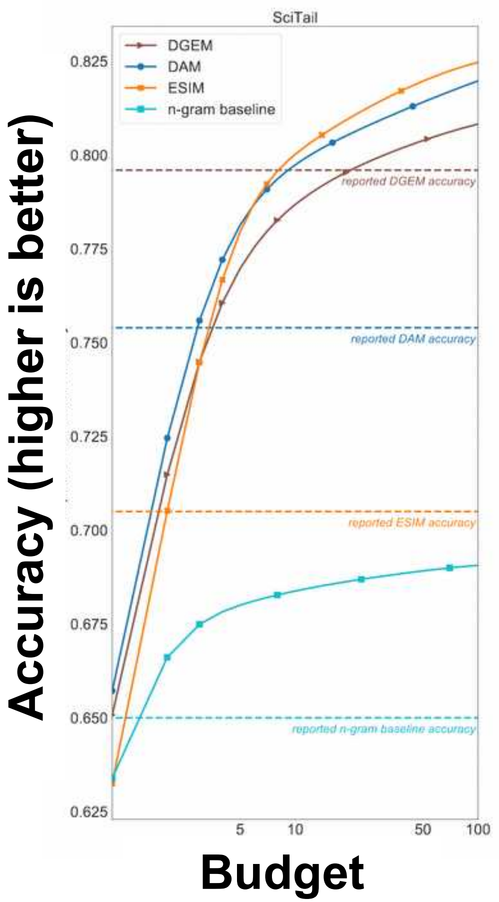
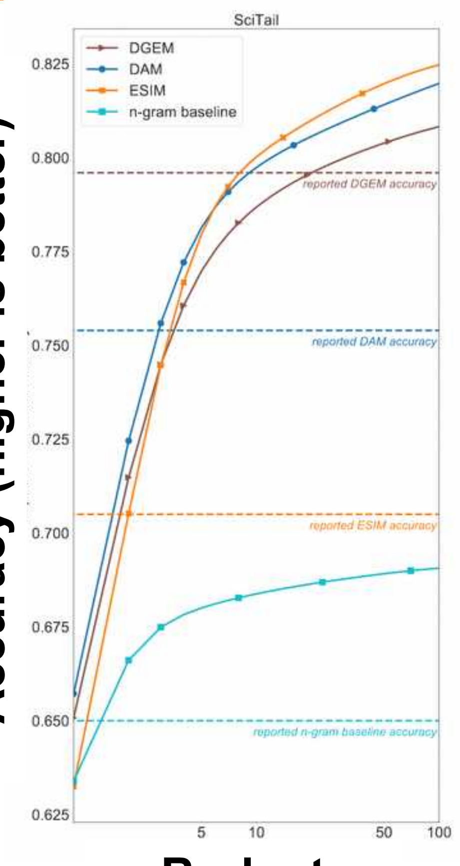
Even HPC/HPDA codes can be shared in containers

Reproducibility: budget



[1] Dodge, J., Gururangan, S., Card, D., Schwartz, R., & Smith, N. A. (2019). Show your work: Improved reporting of experimental results. arXiv preprint arXiv:1909.03004.

Reproducibility: budget



Accuracy (higher is better)

Budget

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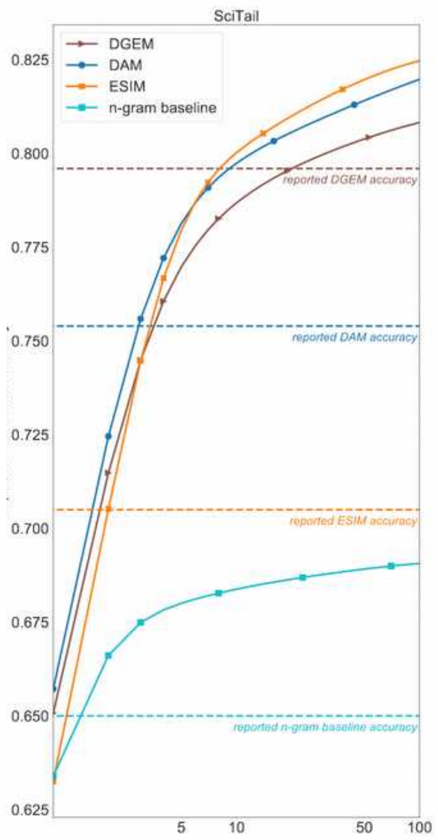

Budget

Budget:

- Training duration

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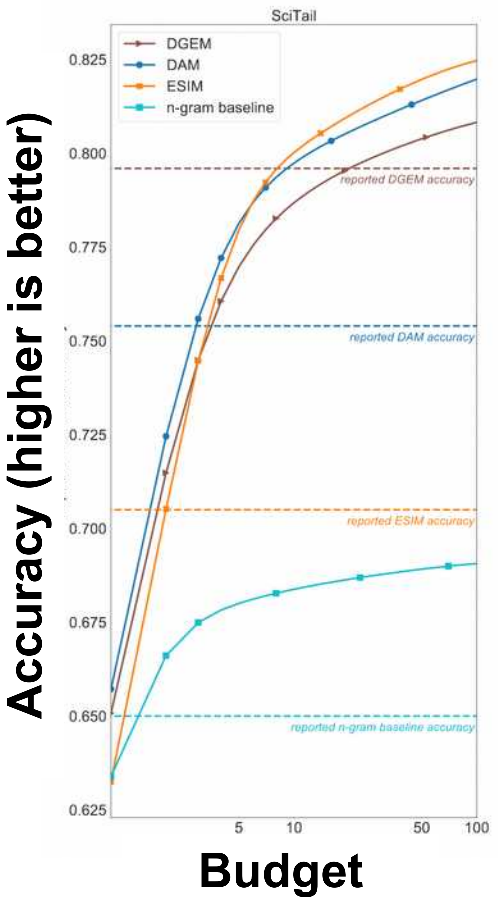

Budget:

- Training duration
- Persons month spent

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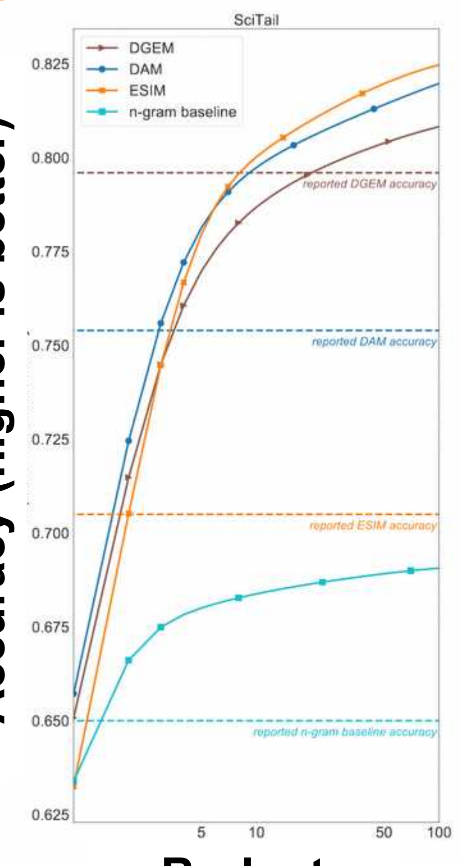

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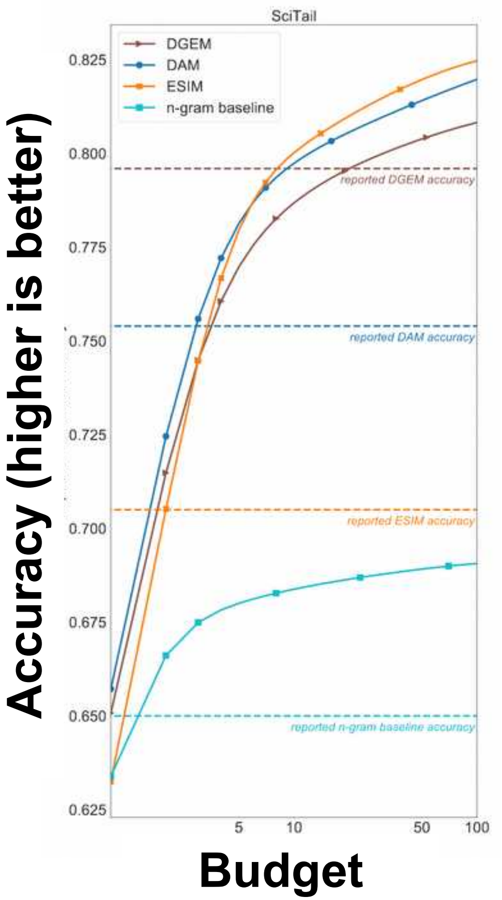

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Hyper-parameter search methods:

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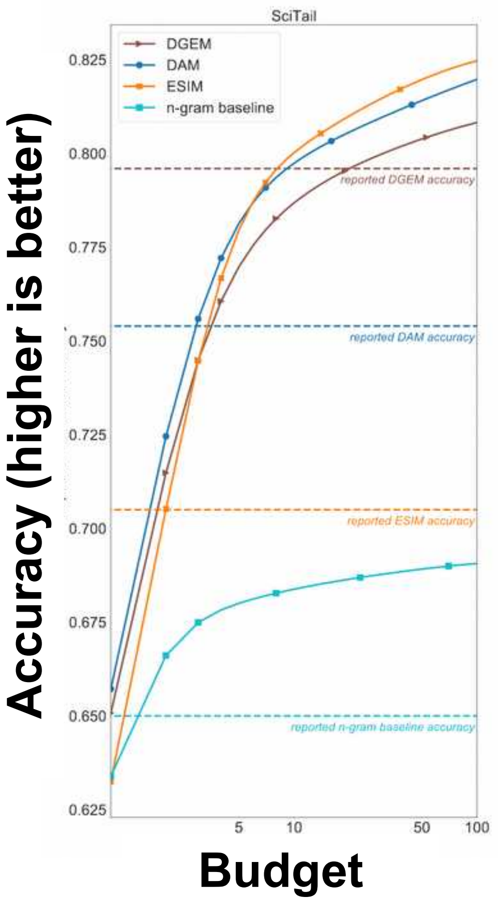

Budget:
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Hyper-parameter search methods:
- Manual

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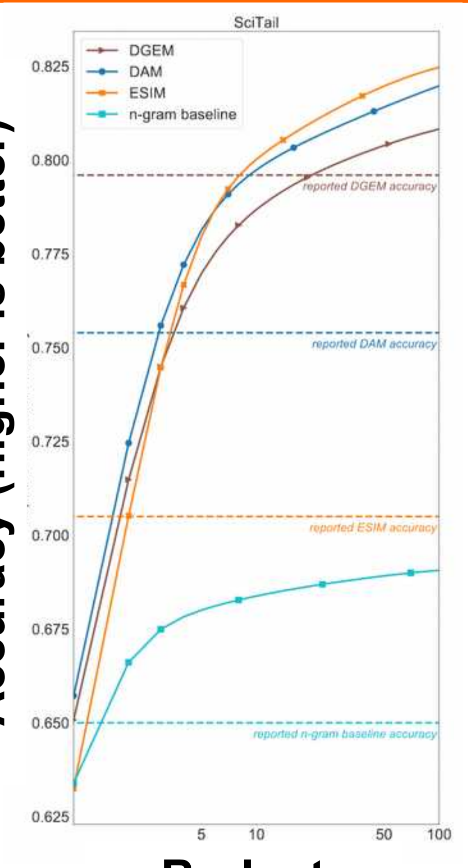

Budget

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Hyper-parameter search methods:
- Manual
- Grid search

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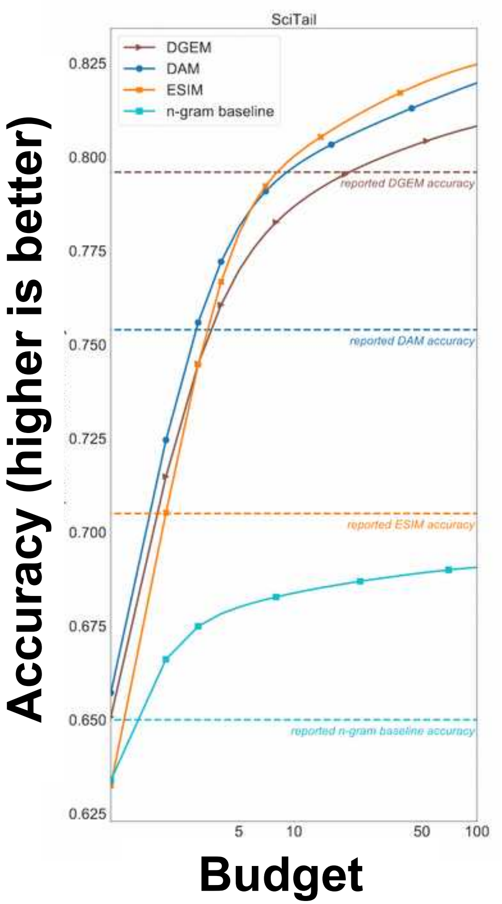

Budget:

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Hyper-parameter search methods:

- Manual
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- Uniform sampling

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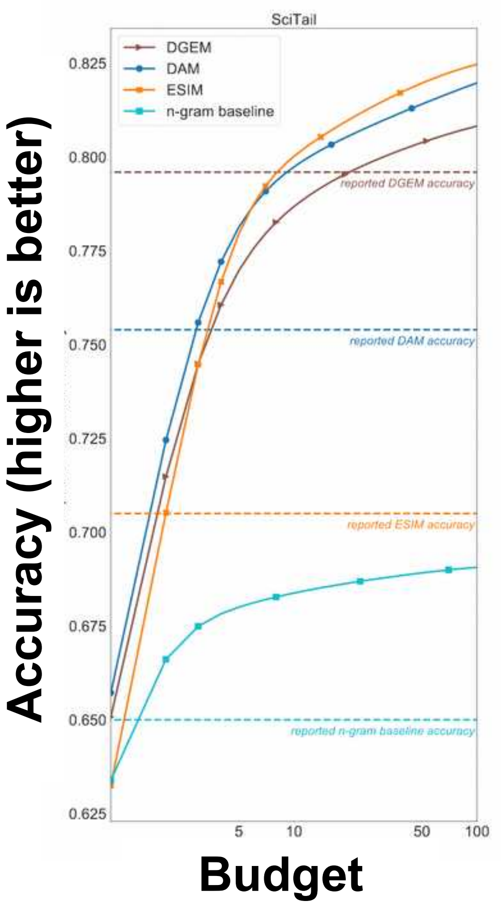

Budget:
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Hyper-parameter search methods:
- Manual
- Grid search
- Uniform sampling
- Bayesian selection

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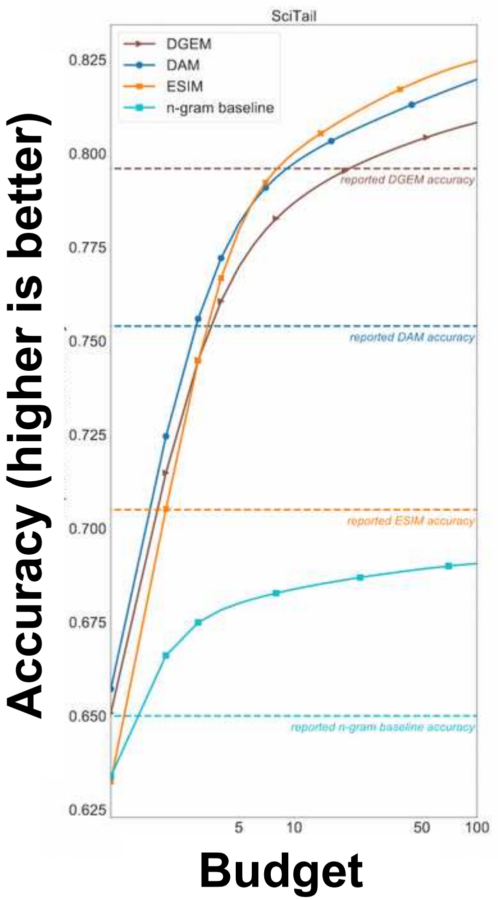

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Hyper-parameter search methods:

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- Evolutionary methods

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Reproducibility: minimal checklist

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Reproducibility: minimal checklist

For all reported experimental results

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For all reported experimental results

- ✔ Description of computing infrastructure

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For all reported experimental results

- ✓ Description of computing infrastructure
- ✓ Average runtime for each approach

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- ✔ Average runtime for each approach
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Reproducibility: minimal checklist

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- ✓ Description of computing infrastructure
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- ✓ Corresponding validation performance for each reported test result
- ✓ A link to implemented code

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For experiments with hyperparameter search:

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For experiments with hyperparameter search:

- Bounds for each hyperparameter

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- The criterion used to select among them
- Expected validation performance, or another measure of the mean and variance as a function of the number of hyperparameter trials.

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Give enough details so you and others can reproduce your exact same results with the same budget

Reproducibility is necessary but not sufficient to explain the results

Explainable AI (XAI)

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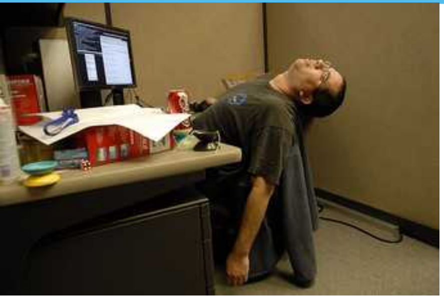

A fancy complex ML model
Clearly reproducible and traceable
Clean datasets

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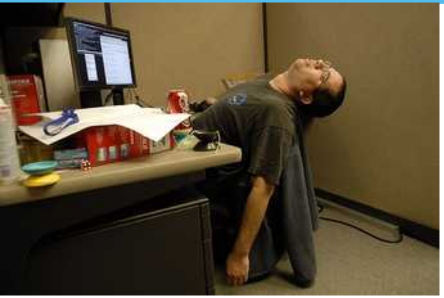

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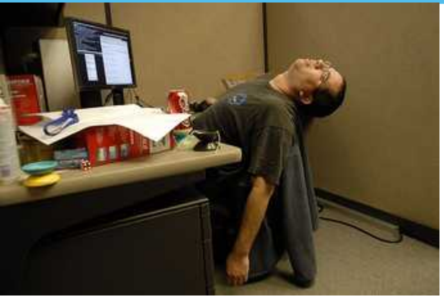

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Cool new scientific discovery
Write a paper
Present in a conference

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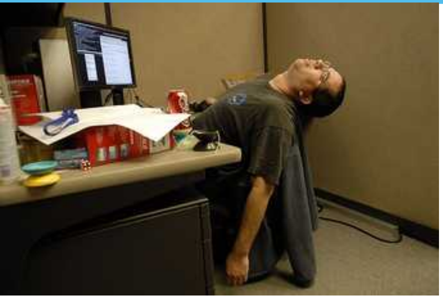

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“How do you know what you did is correct?”
“Why should I trust your results?”

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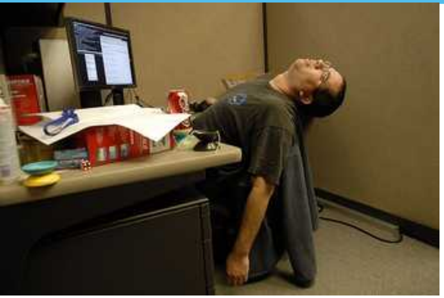

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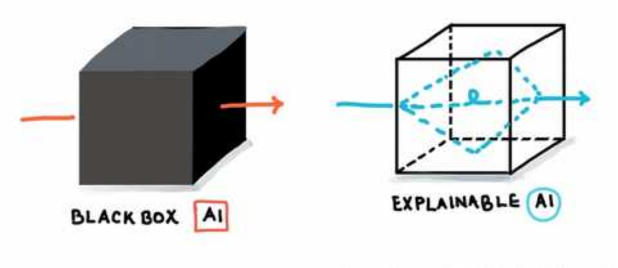

Your model might be behaving like a black box: you can not explain why it gives these results, you do not know its internal logic.

What is an explanation?

[1] Miller, T. (2019). Explanation in artificial intelligence: Insights from the social sciences. Artificial Intelligence, 267, 1-38.

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- Explanations refer to causes [1]

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Question	Reasoning	Description
What?	Associative	Reason about which unobserved events could have occurred given the observed events
How?	Interventionist	Simulate a change in the situation to see if the event still happens
Why?	Counterfactual	Simulating alternative causes to see whether the event still happens

Table 3: Classes of Explanatory Question and the Reasoning Required to Answer

[1] Miller, T. (2019). Explanation in artificial intelligence: Insights from the social sciences. Artificial Intelligence, 267, 1-38.

Explainability becomes an epistemological problem: this will not be a philosophy of science lecture!

Interpretability is the degree to which a human can understand the cause of a decision

[1] Miller, Tim. “Explanation in artificial intelligence: Insights from the social sciences.” arXiv Preprint arXiv:1706.07269. (2017)

Interpretability is the degree to which a human can consistently predict the model's result

[1] Kim, Been, Rajiv Khanna, and Oluwasanmi O. Koyejo. "Examples are not enough, learn to criticize! Criticism for interpretability." Advances in Neural Information Processing Systems (2016)

Explanation in AI

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Explanation in AI aims to create a suite of techniques that produce more explainable models, while maintaining a high level of searching, learning, planning, reasoning performance: optimization, accuracy, precision; and enable human users to understand, appropriately trust, and effectively manage the emerging generation of AI systems

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Guidelines

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Ethics guidelines for trustworthy AI

Guidelines

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Lawful

Ethical

Robust

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Lawful

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Robust

Human agency and oversight

Technical Robustness and safety

Privacy and data governance

Transparency

Diversity, non-discrimination and fairness

Societal and environmental well-being

Accountability

Explainable vs Interpretable AI

- Is it the same?

Explainable vs Interpretable AI

- Is it the same?

explanation
/ɛkspləˈneɪʃ(ə)n/

noun

a statement or account that makes something clear.
"the birth rate is central to any explanation of population trends"

Similar: clarification · simplification · description · report · version

- a reason or justification given for an action or belief.
  "Freud tried to make sex the explanation for everything"

  Similar: account · reason · justification · excuse · alibi · apologia

interpretation
/ɪntəːprɪˈteɪʃ(ə)n/

noun

the action of explaining the meaning of something.
"the interpretation of data"

Similar: explanation · elucidation · expounding · exposition · explication

- an explanation or way of explaining.
  plural noun: interpretations
  "this action is open to a number of interpretations"

  Similar: meaning · understanding · construal · connotation · reading

Explainable vs Interpretable AI

Explainable vs Interpretable AI

- Almost all the time used as synonyms
- **Explainable**: solutions can be understood by human experts. Black box
- **Interpretable**: solutions understood by anyone. Transparent models.

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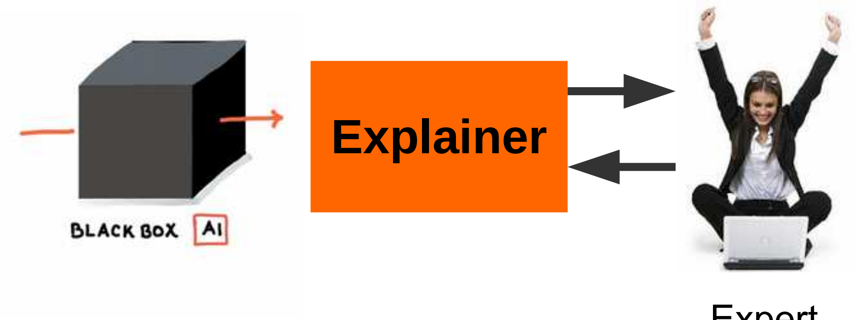

Expert

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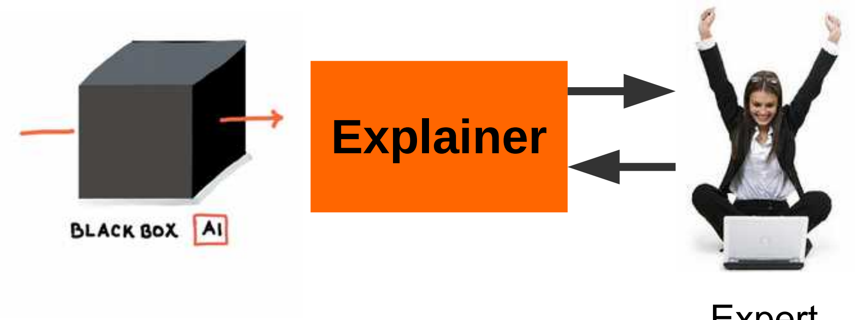
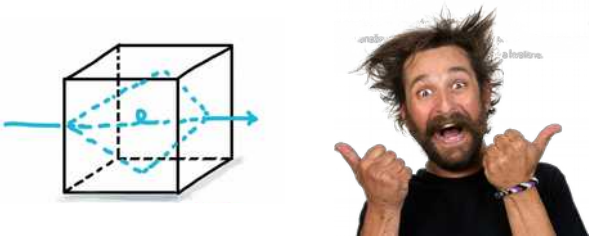


Expert



Anyone

Approaches to explain

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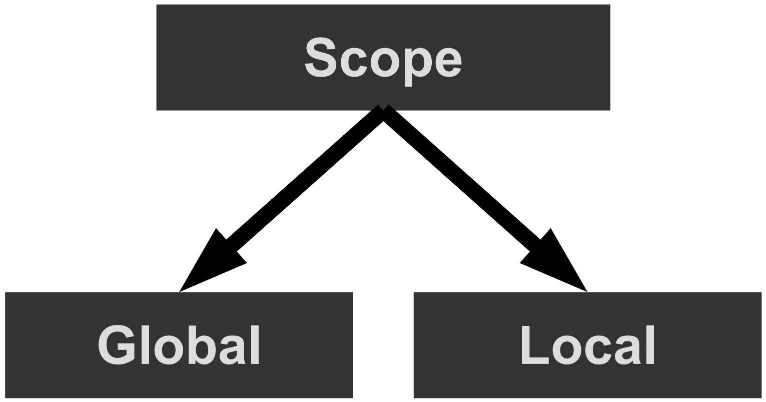
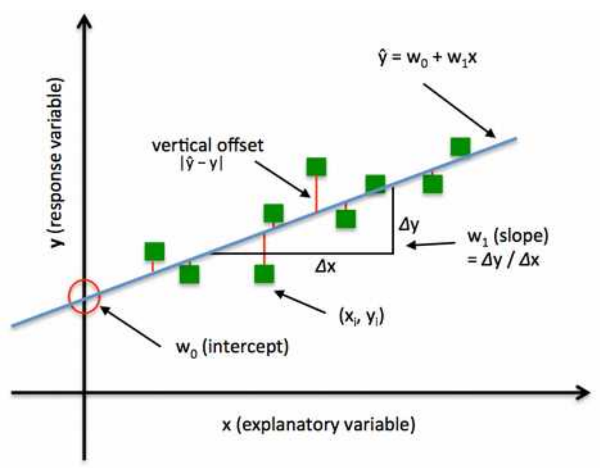


Approaches to explain

Interpretable models

Linear regression

Global | Local | **Specific**



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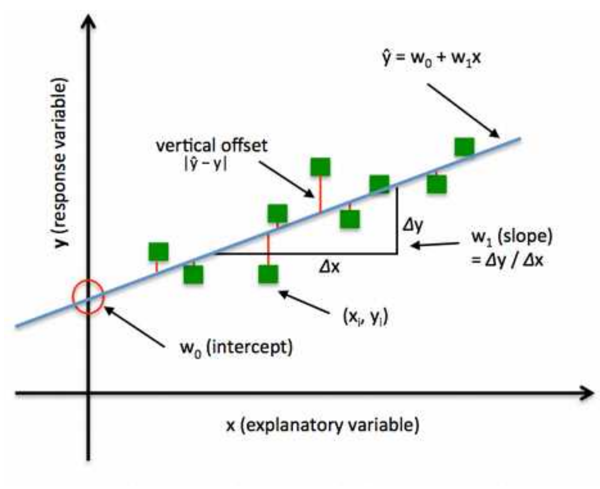

A linear model looks like this:

$$y = w_0 + w_1 * x_1 + w_2 * x_2$$

Interpretable models

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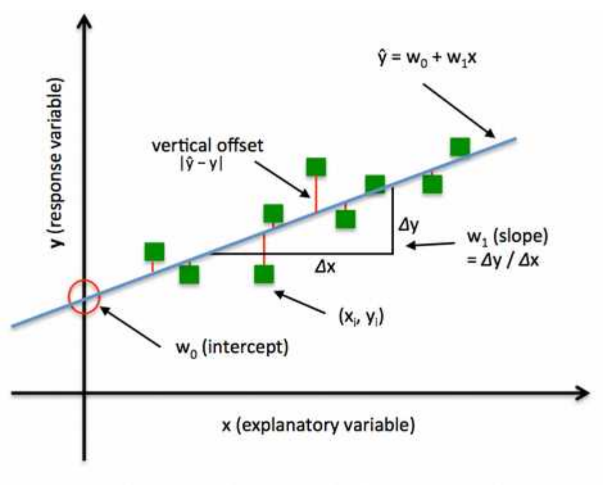

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Global explanation:

w_0 , w_1, w_2 Are the level of importance of each one of the features. They give a clear connection between ***x*** and ***y***

Interpretable models

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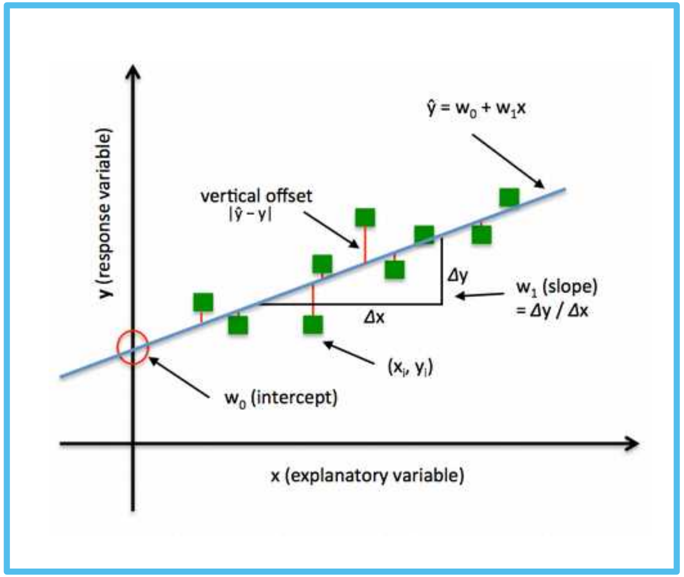

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w_0 , w_1, w_2 — Are the level of importance of each one of the features. They give a clear connection between ***x*** and ***y***

Local explanation:

$w_1 * x_1$, $w_2 * x_2$ — Give details about why the value of ***y*** was obtained

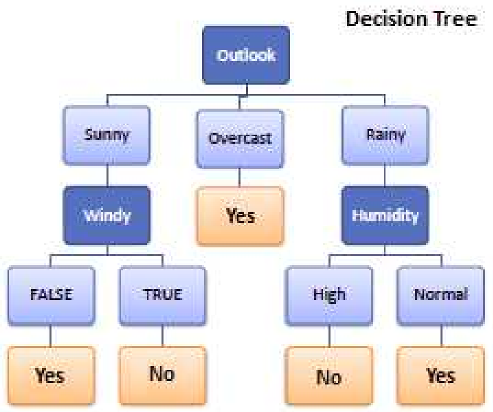
Interpretable models

Decision trees

Local

Specific

Golf today?



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In this model, I can insert a value of ***x***, and I can transparently follow the logic of the model down to the leaf containing ***y***

Interpretable models

Decision trees

Local

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x = (Sunny, Windy)

If Sunny → If Windy → No

y = (No)

Interpretable models

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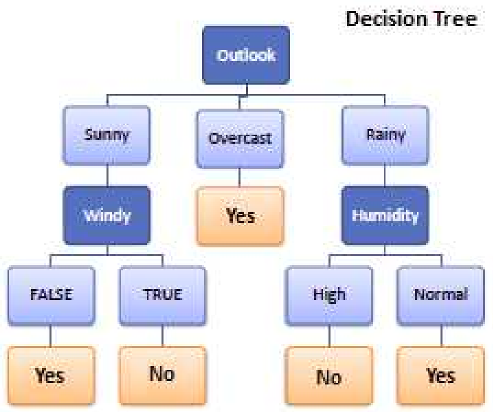

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x = (Sunny, Windy)
If Sunny → If Windy → No
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Why aren't you playing golf today?
Explanation: Because it is sunny and windy.

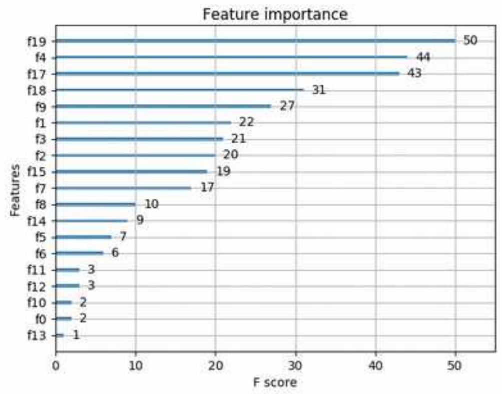
Interpretable models

Feature importance

Global

Specific

Built from decision trees



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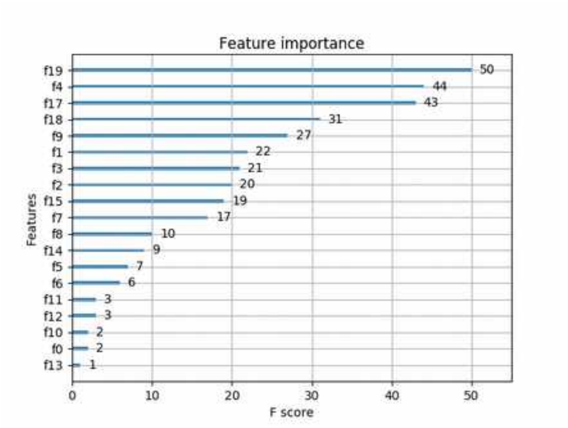

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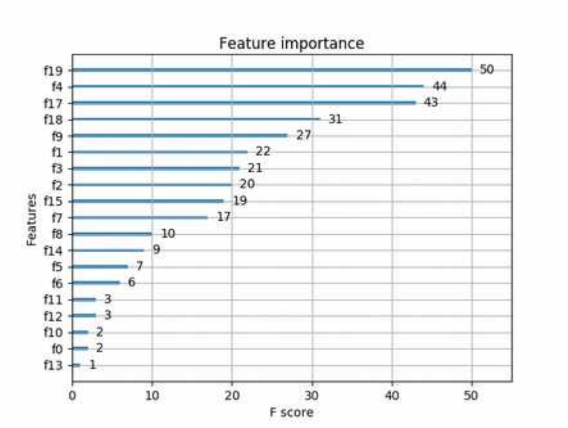

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How many times a particular feature has been used to make a decision in the tree.

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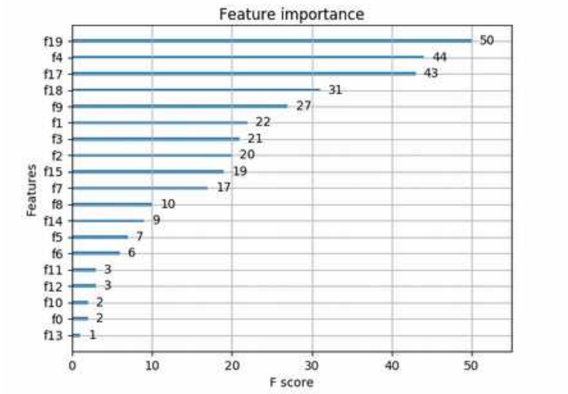

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Feature importance in decision trees indicates how much each feature has been used to make a decision.

Interpretable models

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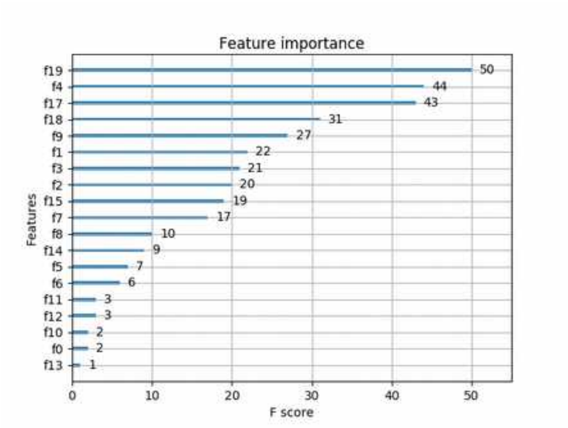

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Interpretable models

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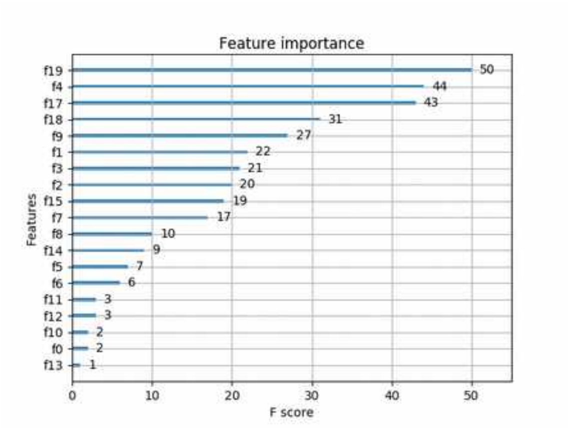

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How many times a particular feature has been used to make a decision in the tree.

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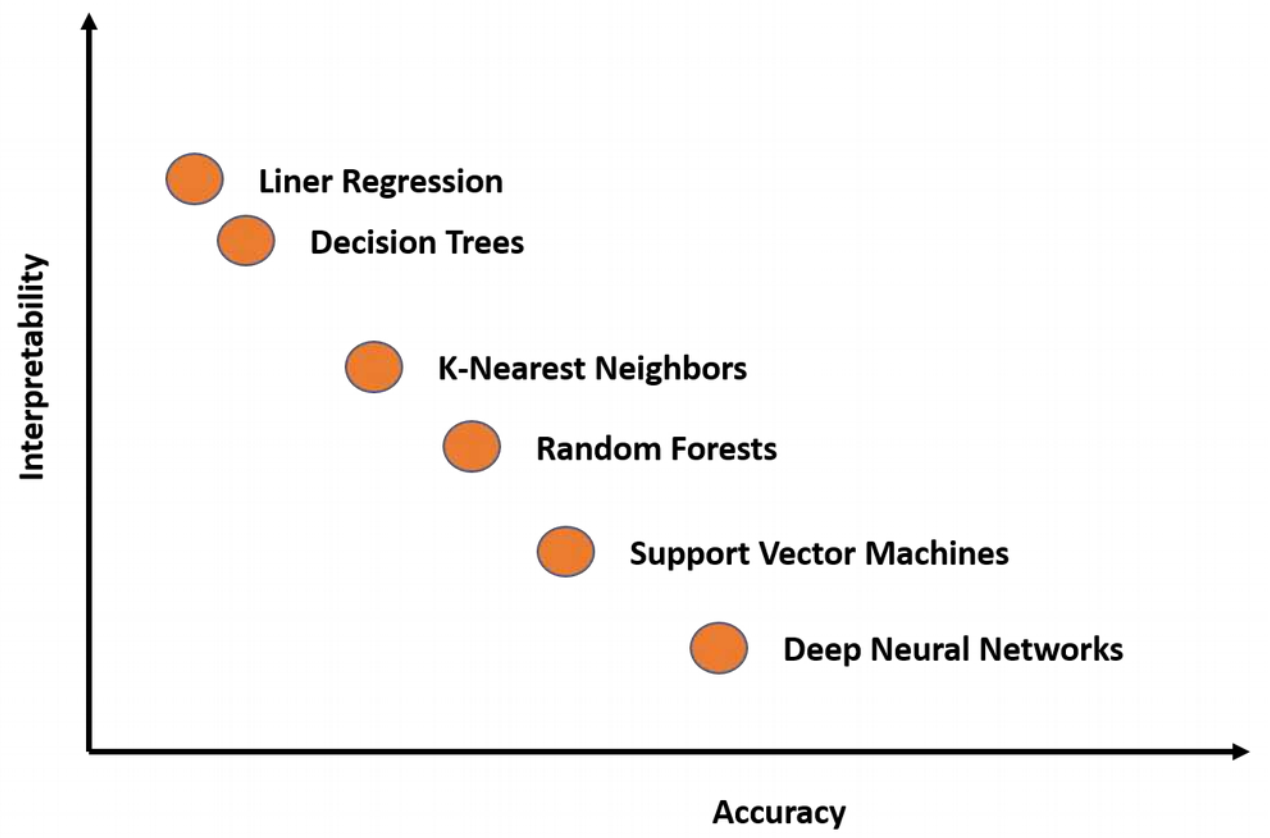
Explanation: Sunny is the most important feature and tomorrow is not sunny

Interpretable models

Algorithm	Linear	Monotone	Interaction	Task
Linear regression	Yes	Yes	No	regr
Logistic regression	No	Yes	No	class
Decision trees	No	Some	Yes	class,regr
RuleFit	Yes	No	Yes	class,regr
Naive Bayes	No	Yes	No	class
k-nearest neighbors	No	No	No	class,regr

Interpretability challenge



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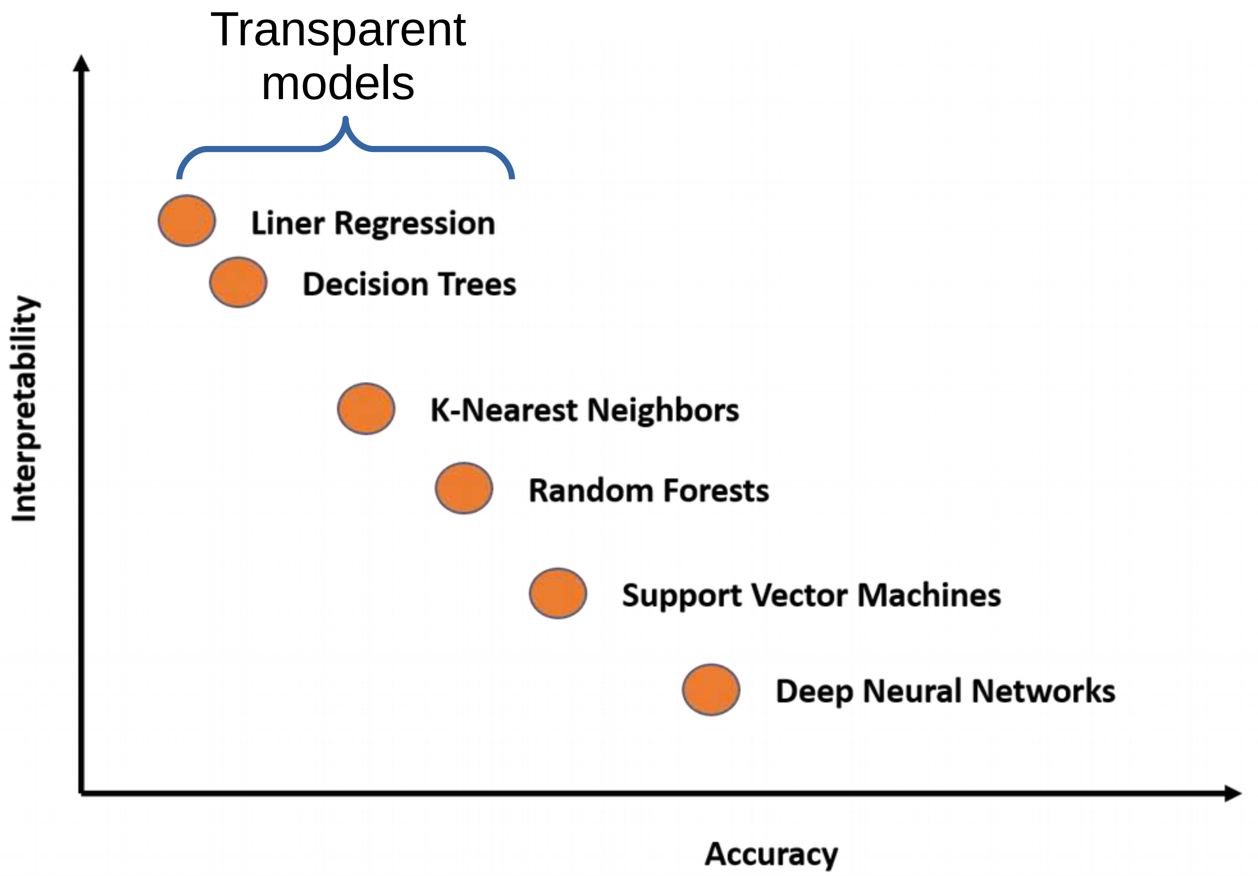

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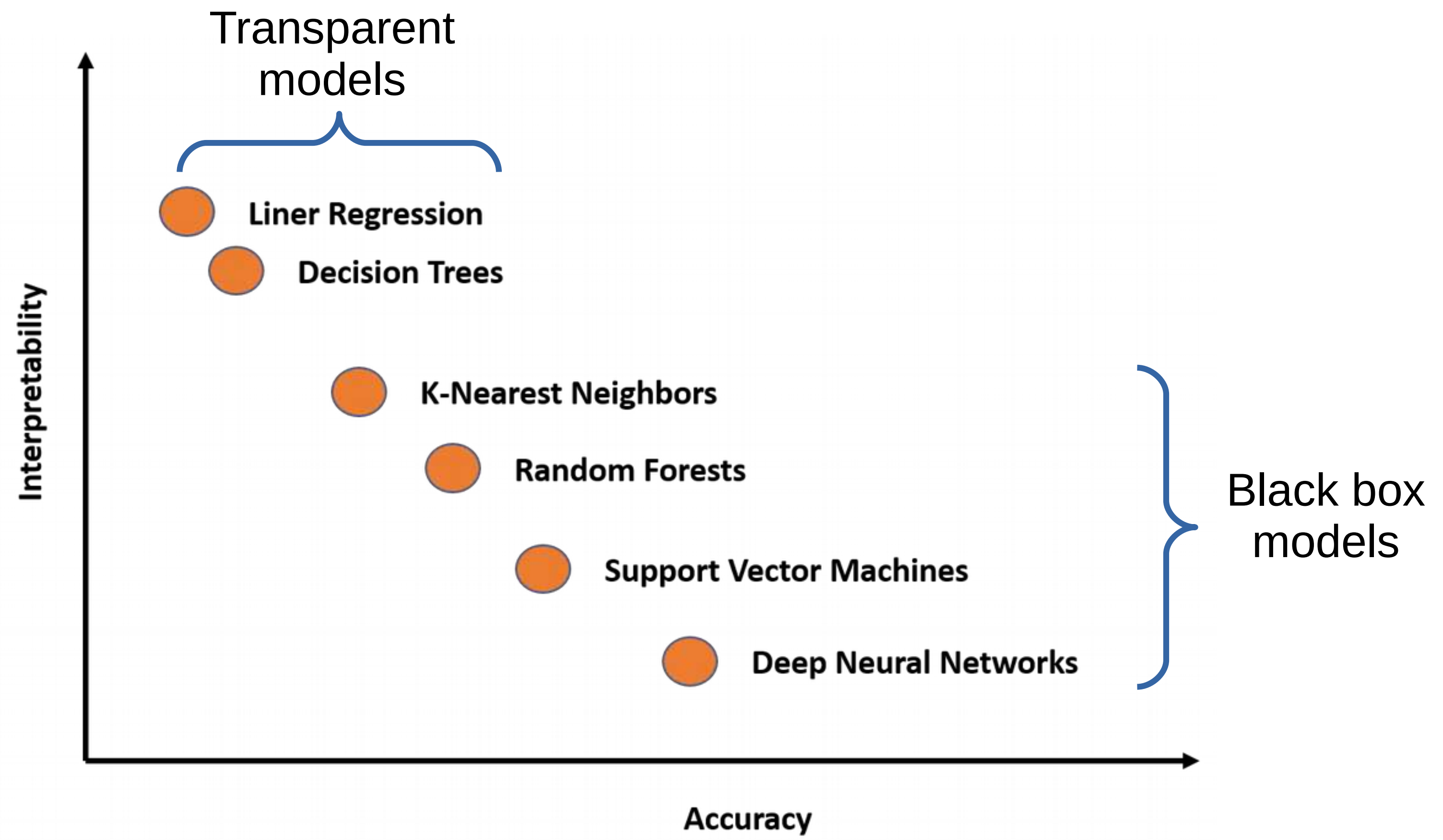

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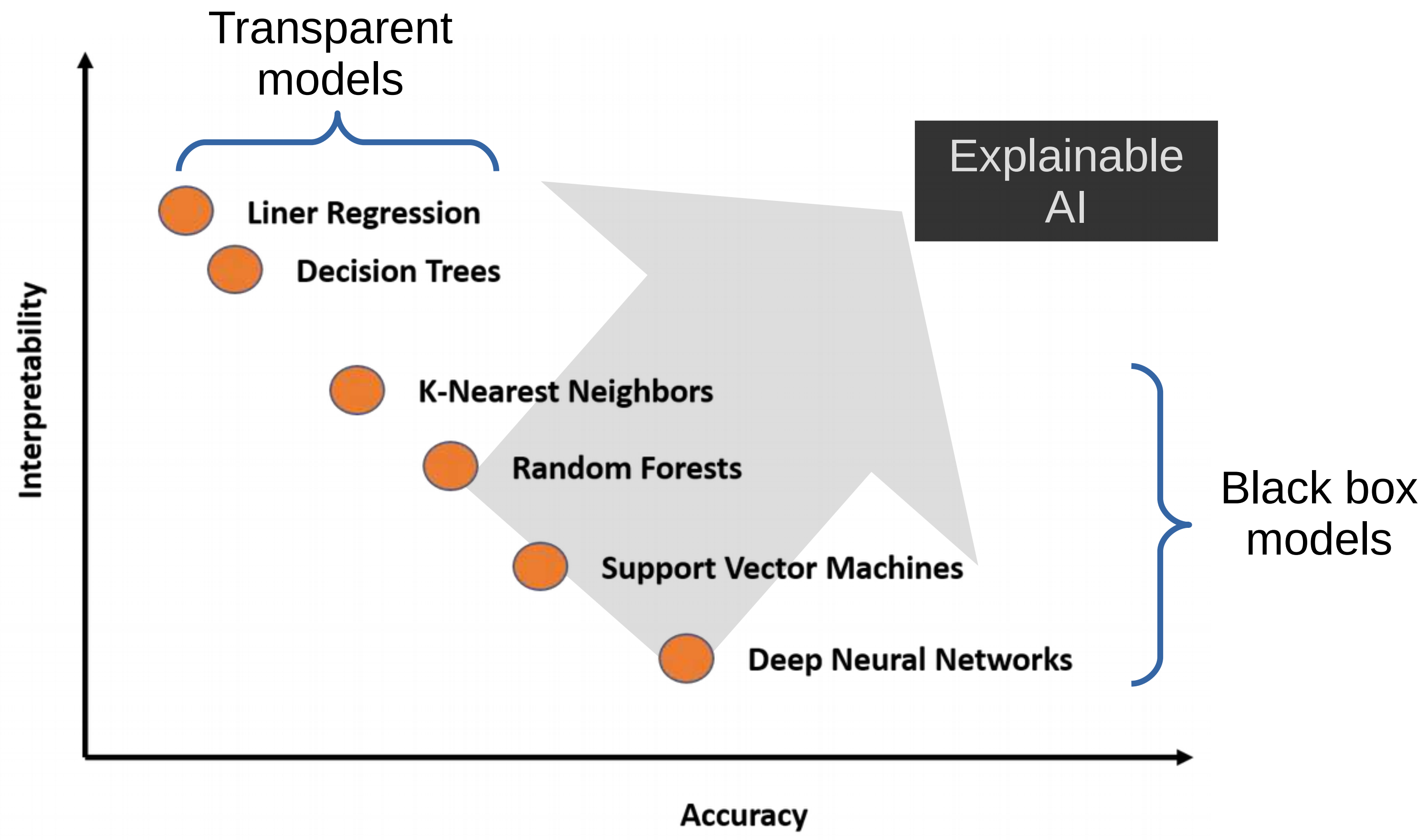

Two main techniques

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Feature sensitivity

Test how changes in the inputs affect the outputs.

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Test how changes in the inputs affect the outputs.

Surrogate models

Use transparent, explainable models, to interpret black box models

Feature sensitivity

Permutation Importance

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Idea: shuffle data in one column. How much does the output change?

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Permutation Importance

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Large change: feature is more “important”

X_A	X_B	X_C	Y
xa1	xb1	xc1	y1
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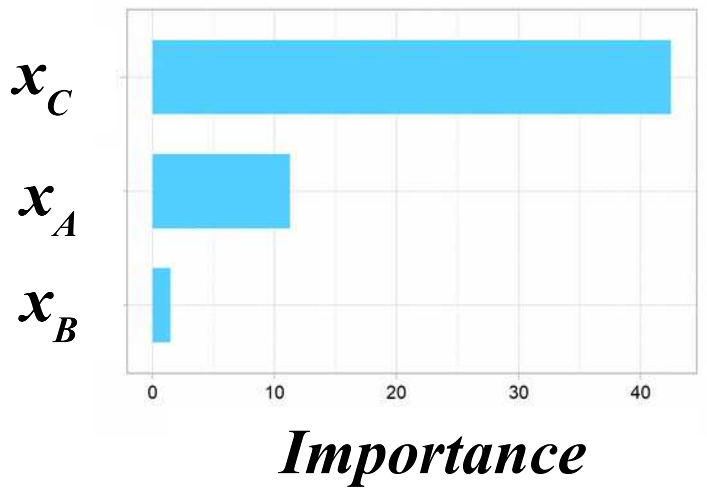
xa3	xb3	xc3	y3
xa4	xb4	xc4	y4
xa5	xb5	xc5	y5
xa6	xb6	xc6	y6



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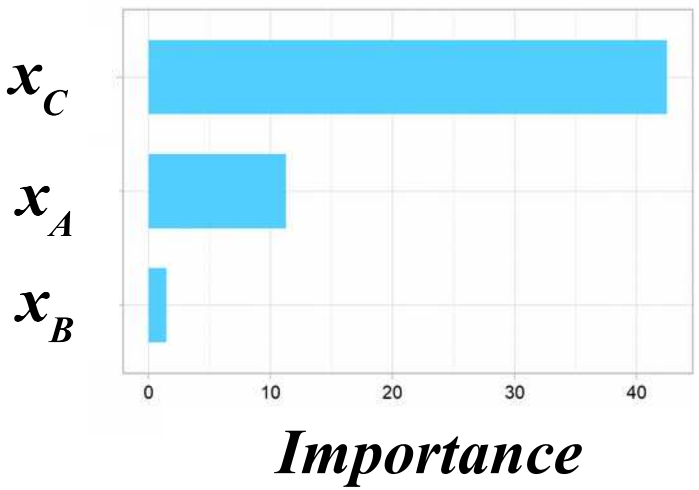

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Agnostic **Global**

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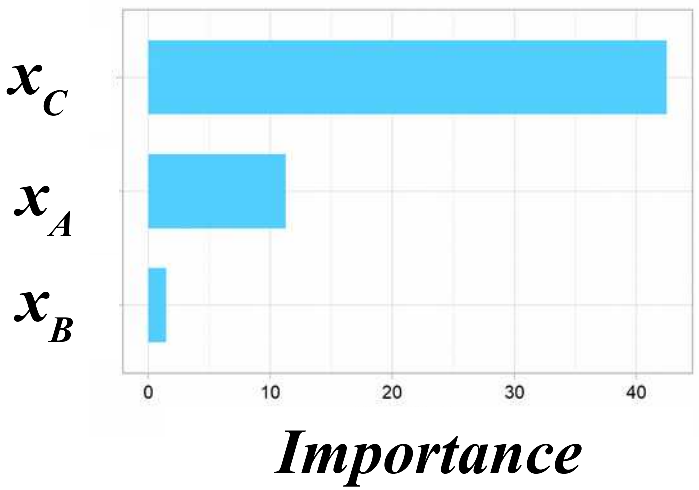


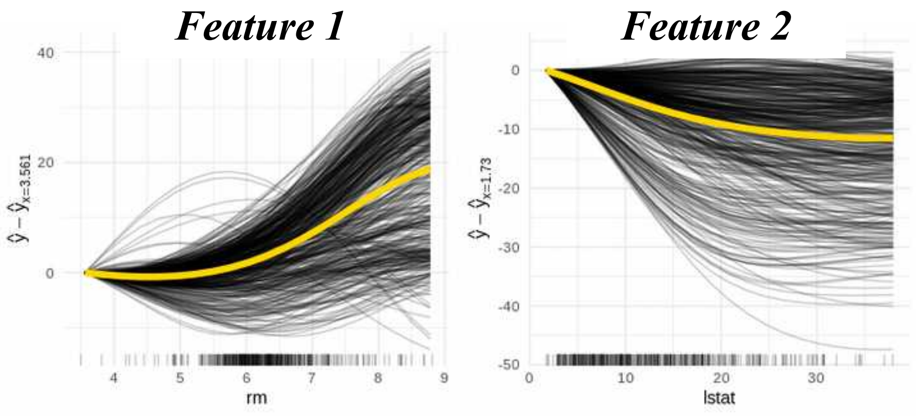
Feature sensitivity

Individual Conditional Expectation curves (ICE) and Partial Dependence Plots (PDP)

Feature sensitivity

Individual Conditional Expectation curves (ICE) and Partial Dependence Plots (PDP)

Idea: Continuously change the value of one feature. Do so for each one of the entries in the data set. This creates an error in the output, compared to what the trained model is expected to show.



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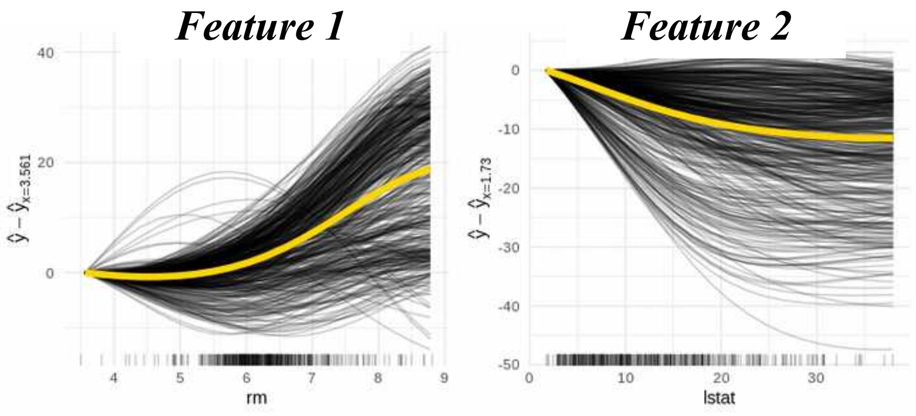

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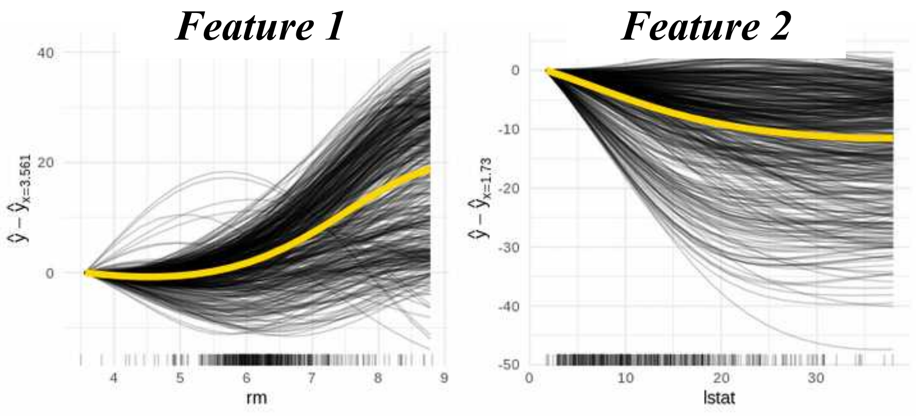

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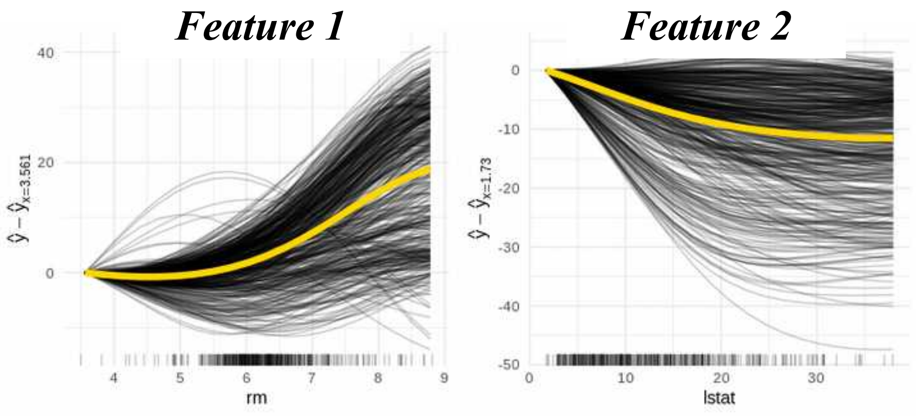

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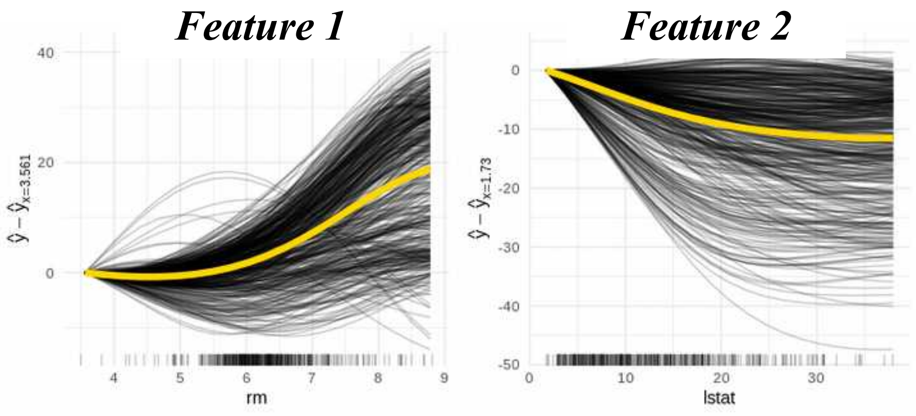

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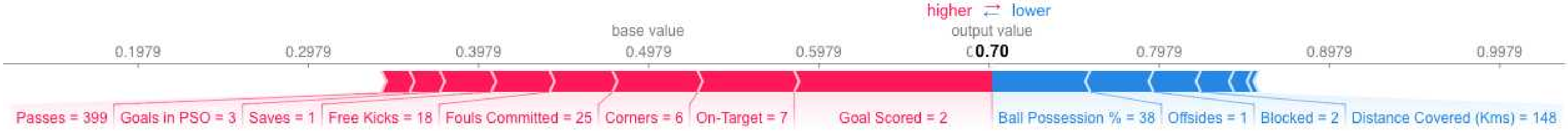

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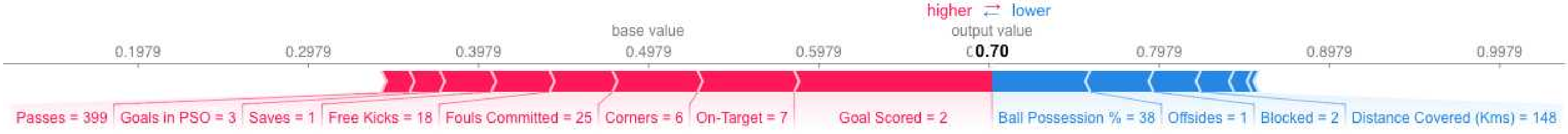

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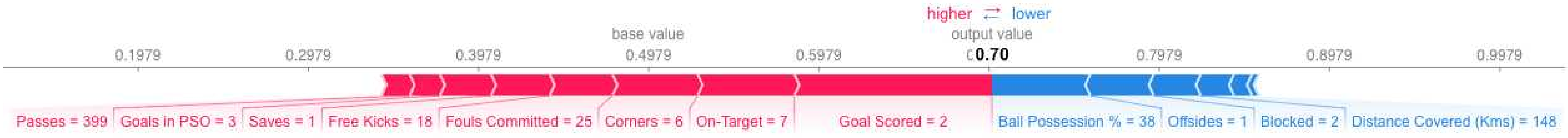

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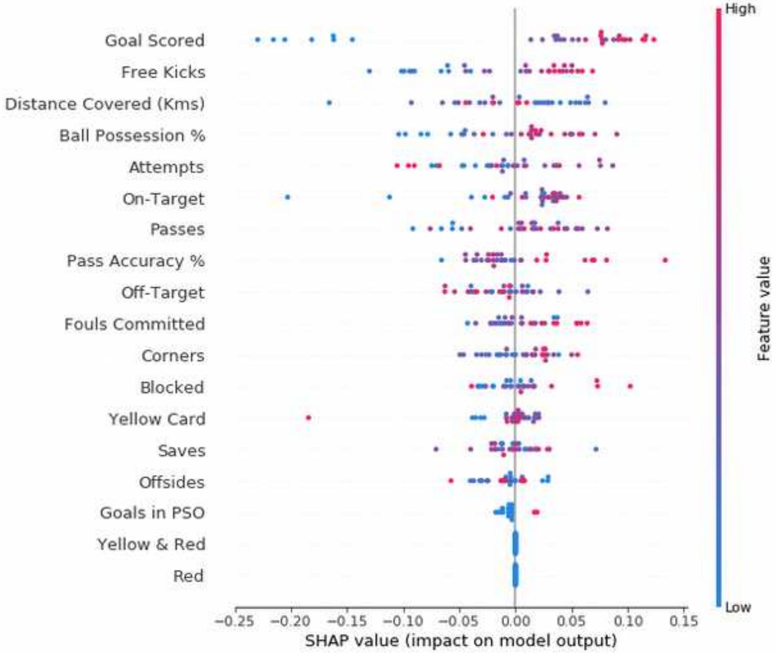

Surrogate models

Agnostic

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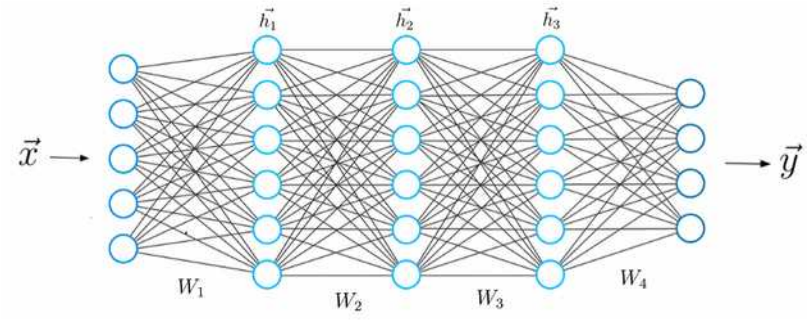

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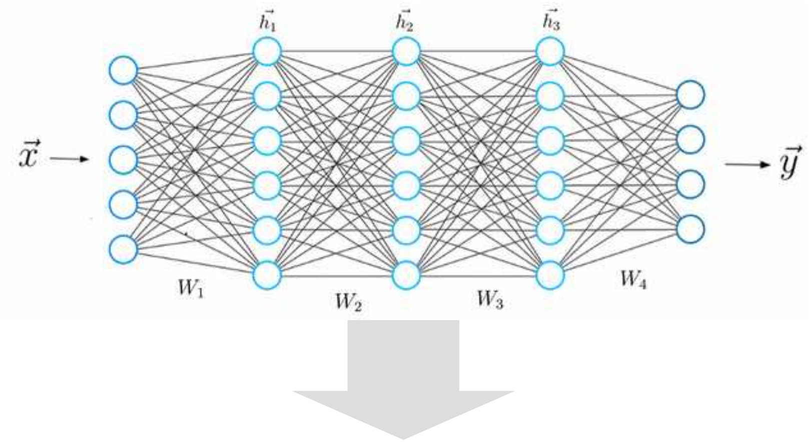

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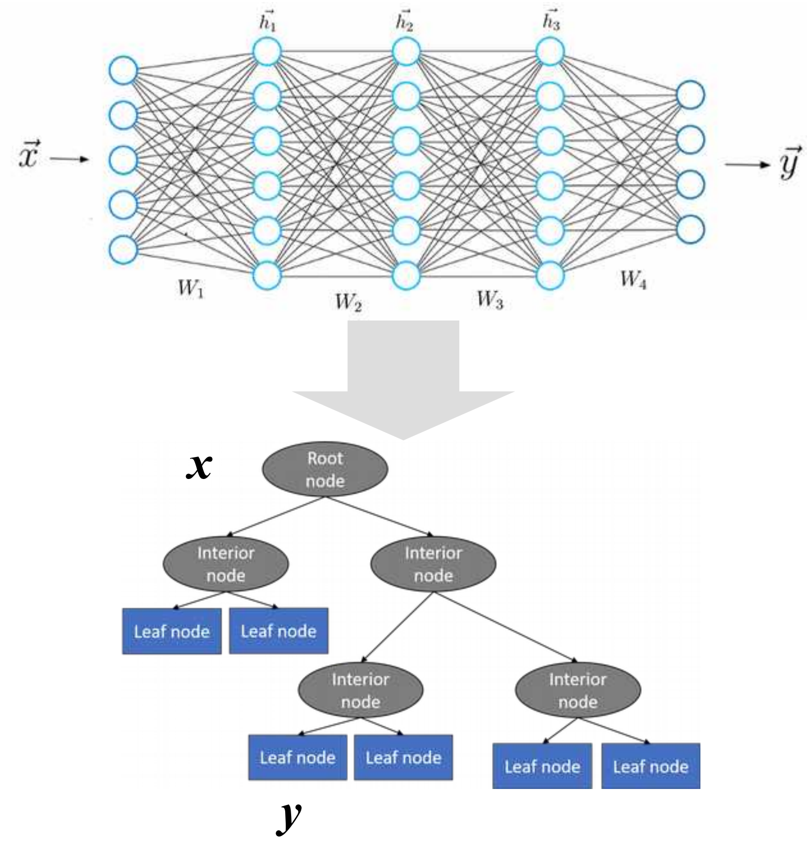

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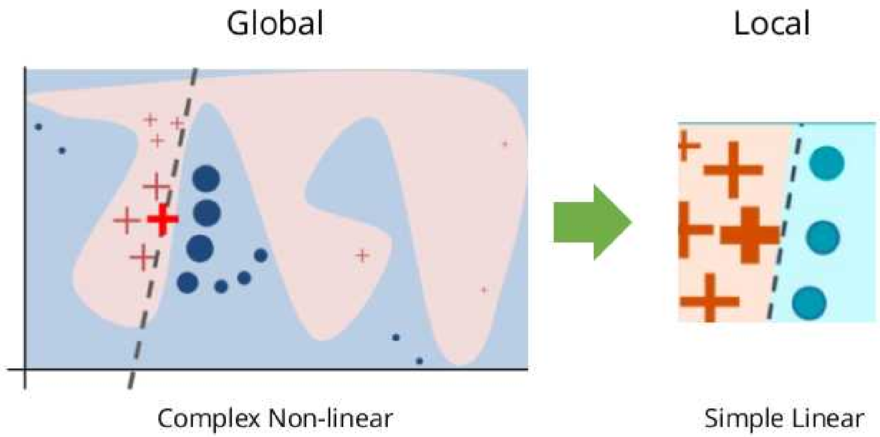

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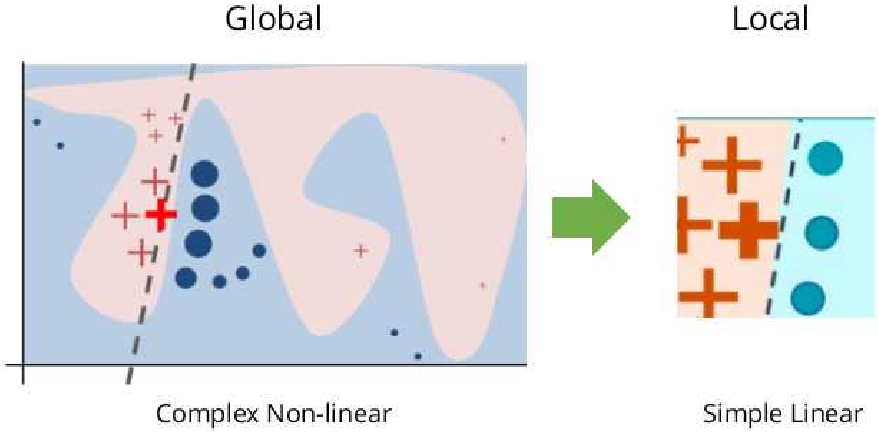

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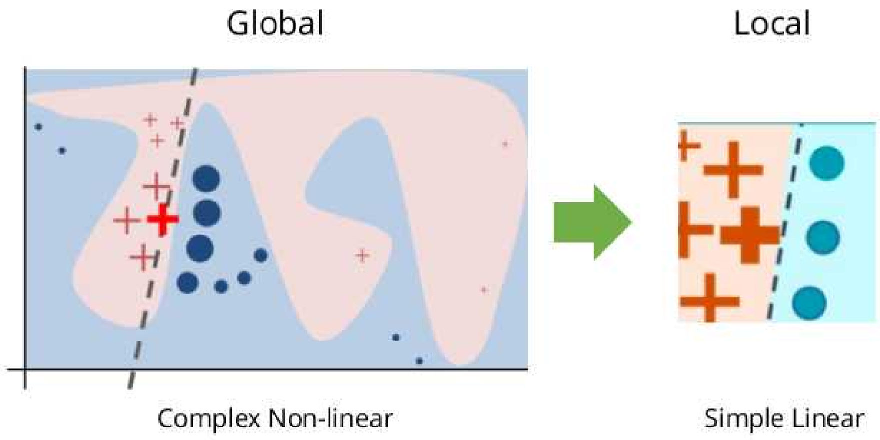

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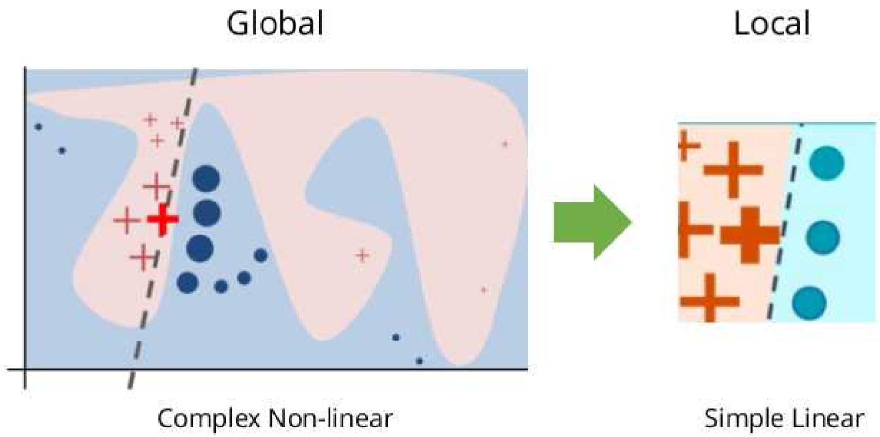

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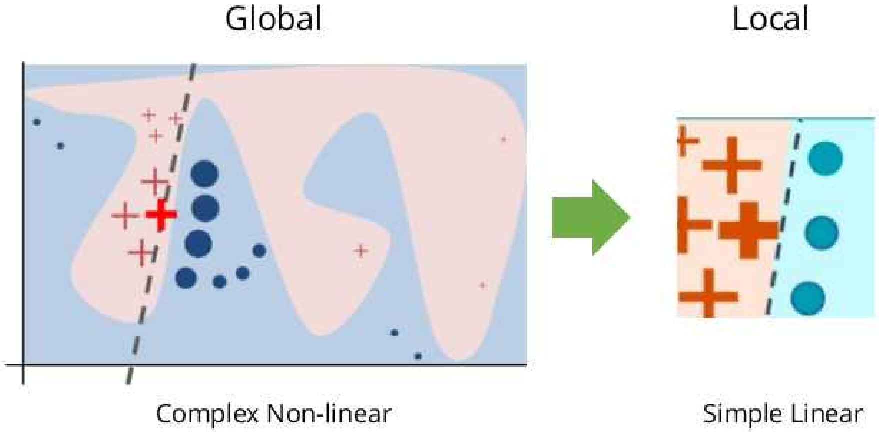

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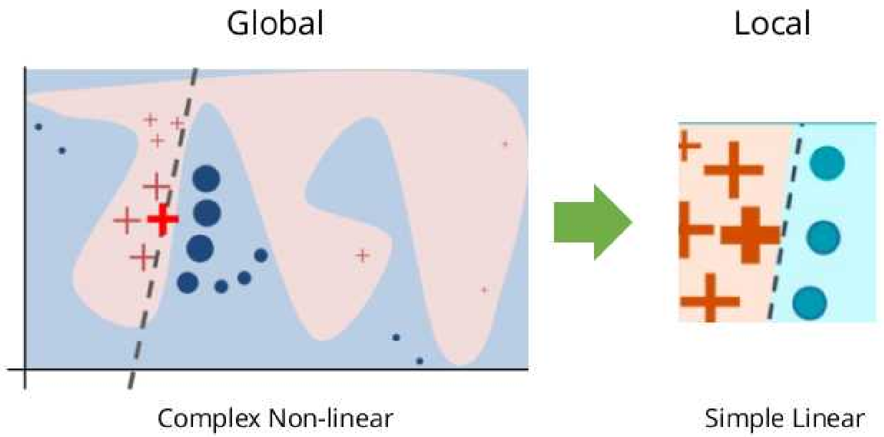
- **Interpretation**: the linear model explains why the original point belongs to one class or the other



Software tools for XAI

Permutation importance with ELI5

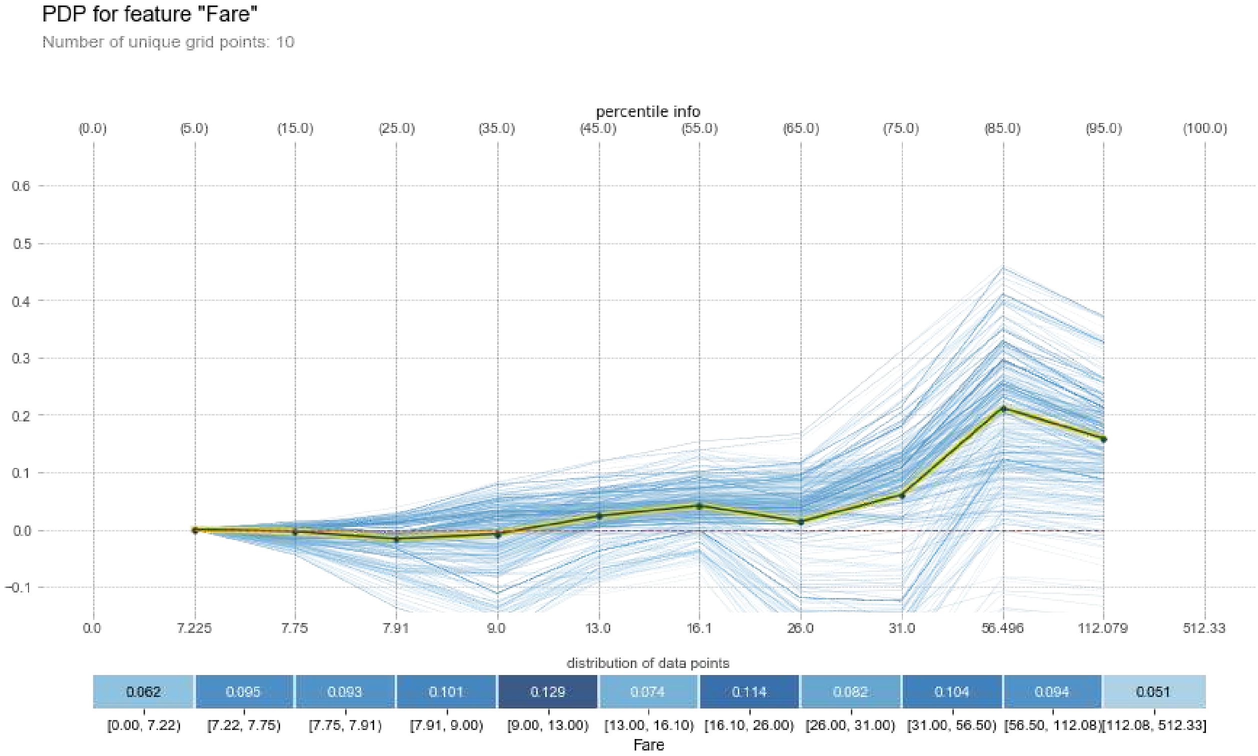
```
import eli5
from eli5.sklearn import PermutationImportance

perm = PermutationImportance(my_model, random_state=1).fit(val_X,
val_y)
eli5.show_weights(perm, feature_names = val_X.columns.tolist())
```

Weight	Feature
0.0750 ± 0.1159	Goal Scored
0.0625 ± 0.0791	Corners
0.0437 ± 0.0500	Distance Covered (Kms)
0.0375 ± 0.0729	On-Target
0.0375 ± 0.0468	Free Kicks
0.0187 ± 0.0306	Blocked
0.0125 ± 0.0750	Pass Accuracy %
0.0125 ± 0.0500	Yellow Card
0.0063 ± 0.0468	Saves
0.0063 ± 0.0250	Offsides
0.0063 ± 0.1741	Off-Target
0.0000 ± 0.1046	Passes
0 ± 0.0000	Red
0 ± 0.0000	Yellow & Red
0 ± 0.0000	Goals in PSO
-0.0312 ± 0.0884	Fouls Committed
-0.0375 ± 0.0919	Attempts
-0.0500 ± 0.0500	Ball Possession %

Software tools for XAI

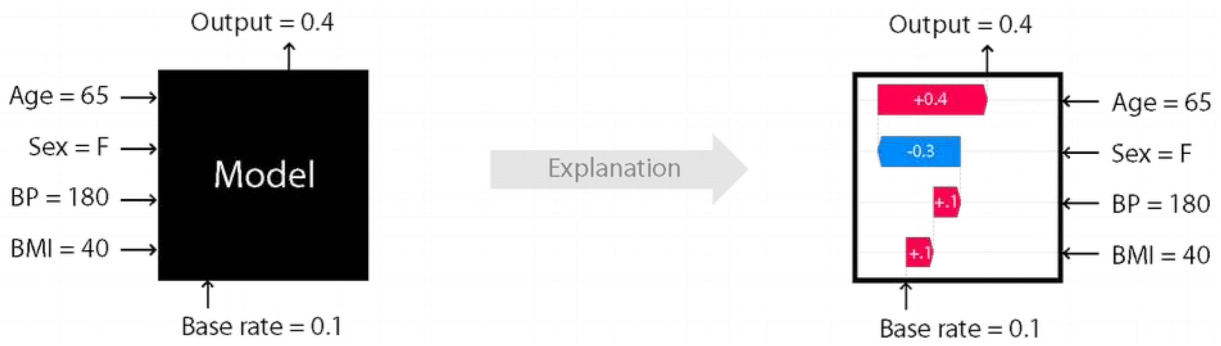
Partial Dependence Plots with PDPbox



Software tools for XAI

SHAP values with the Shap library:

SHAP



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- Multiple new and interesting techniques

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- XAI is currently under constant evolution; keep an eye on the latest results and tools.

XAI: one little more layer to worry about...
...but an important one!

Enjoy XAI
Thank you!

This school has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 776262 (AIDA, www.aida-space.eu)