

What and How of Machine Learning Transparency

Building Bespoke Explainability Tools
with Interoperable Algorithmic
Components

Kacper Sokol and Peter Flach

Outline

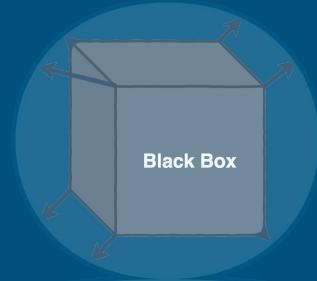
- What is Explainability?
- Post-hoc Explainability: Modular Surrogates
- Surrogates for Text Data
- Surrogates for Image Data
- Surrogates for Tabular Data
- Conclusions
- Break (5–10 minutes)
- Hands-on
- Closing Remarks

What is Explainability?

What is Explainability?

No universally accepted definition.

- Simulability
 - Lipton, 2018. *The mythos of model interpretability*.
- The Chinese Room Theorem
 - Searle, 1980. *Minds, brains, and programs*.
- Mental Models:
Kulesza et al., 2013. Too much, too little, or just right? Ways explanations impact end users' mental models.
 - Functional -- operationalisation without understanding;
 - Structural -- appreciation of the underlying mechanism.



What is Explainability?

Explainability = $\underbrace{\text{Reasoning}(\text{Transparency} \mid \text{Background Knowledge})}_{\text{understanding}}$

- Transparency -- **insight** (of arbitrary complexity) into operation of a system.
- Background Knowledge -- implicit or explicit **exogenous** information.
- Reasoning -- **algorithmic** or **mental** processing of information.

Explainability → **explainee** walking away with **understanding**.

Explaining AI with Exemplars

Transparent insights:

- [humidity=**low**, temperature=23, rain=no] → like
- [humidity=**medium**, temperature=23, rain=no] → dislike
- [humidity=**high**, temperature=23, rain=no] → dislike

With **23°C** and **clear sky**,
the person *enjoys* the
weather when the **humidity**
is low.

Human-centred Explainability



Artificial Intelligence
Volume 267, February 2019, Pages 1-38



Explanation in artificial intelligence: Insights from the social sciences

Tim Miller✉

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<https://doi.org/10.1016/j.artint.2018.07.007>

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Abstract

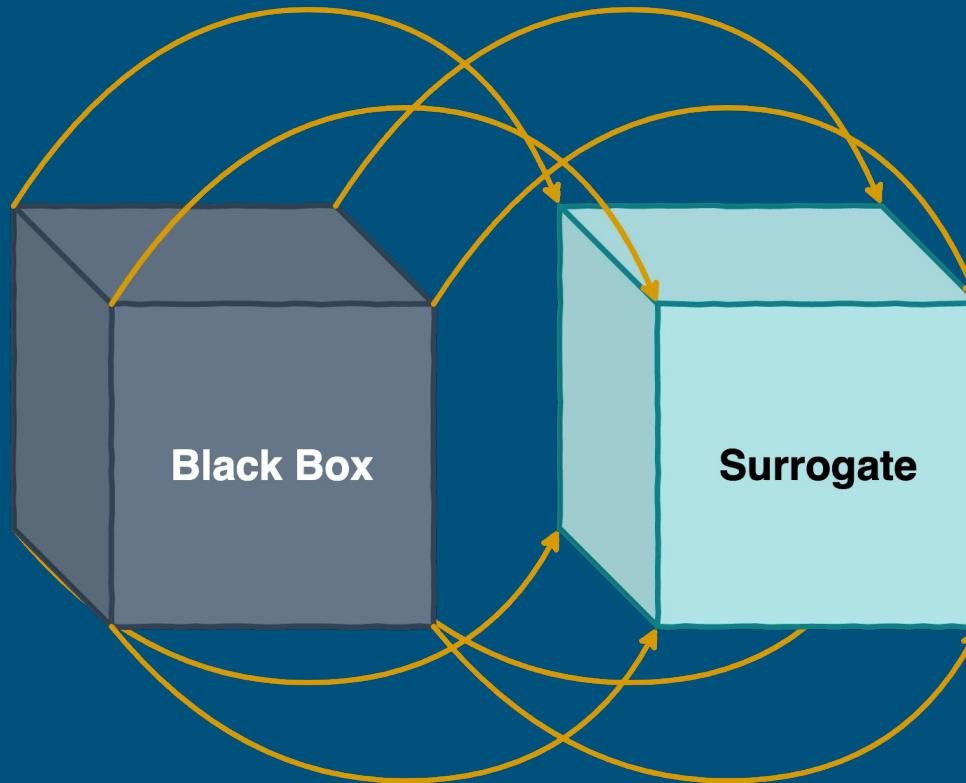
There has been a recent *resurgence* in the area of explainable artificial intelligence as researchers and practitioners seek to provide more transparency to their algorithms. Much of this research is focused on explicitly explaining decisions or actions to a human observer, and it should not be controversial to say that looking at how humans explain to each other can serve as a useful starting point for explanation in artificial intelligence. However, it is fair to say that most work in explainable artificial intelligence uses only the researchers' intuition of what constitutes a 'good' explanation. There exist vast and valuable bodies of research in philosophy, psychology, and cognitive science of how people define, generate, select, evaluate, and present explanations, which argues that people employ certain

Human-centred explanations:

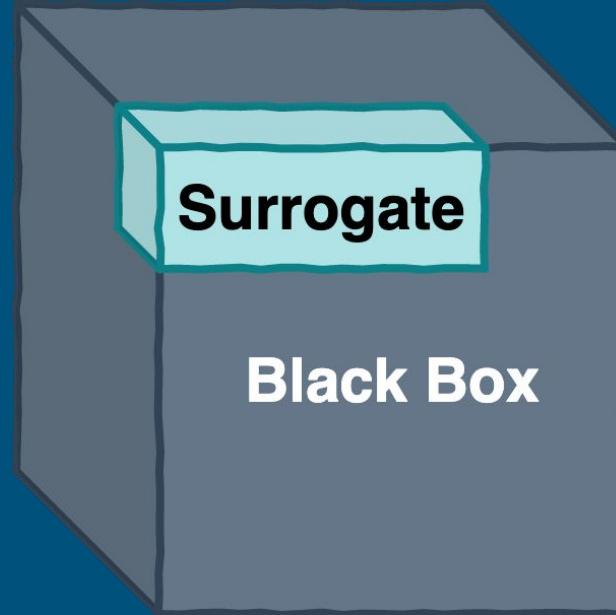
- **interactive dialogue (bi-directional);**
- **contrastive statements.**

Modular Surrogate Explainability

Scope: Global Surrogates

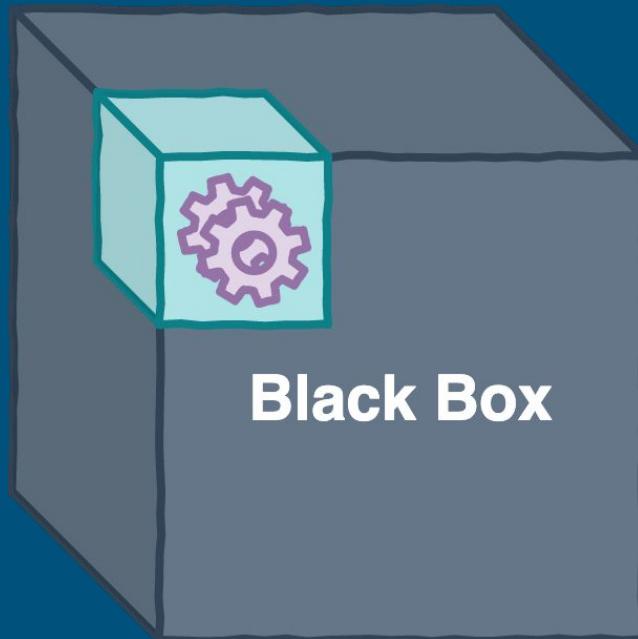


Scope: Local Surrogates



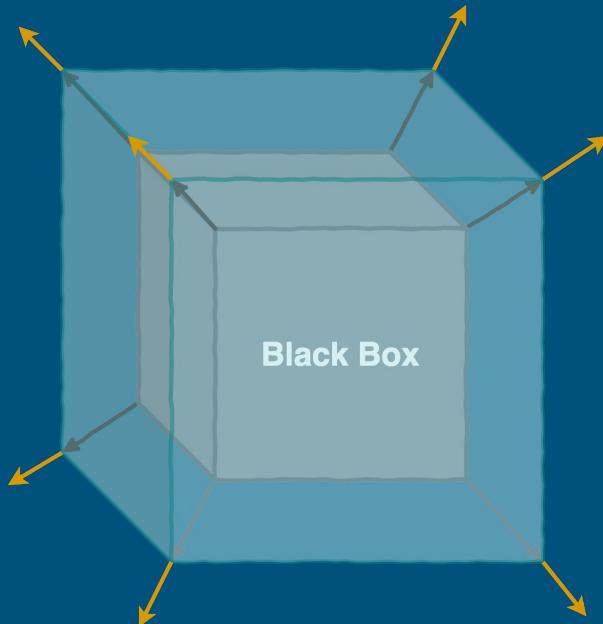
Mimicry Source: Structural Surrogate

(model)

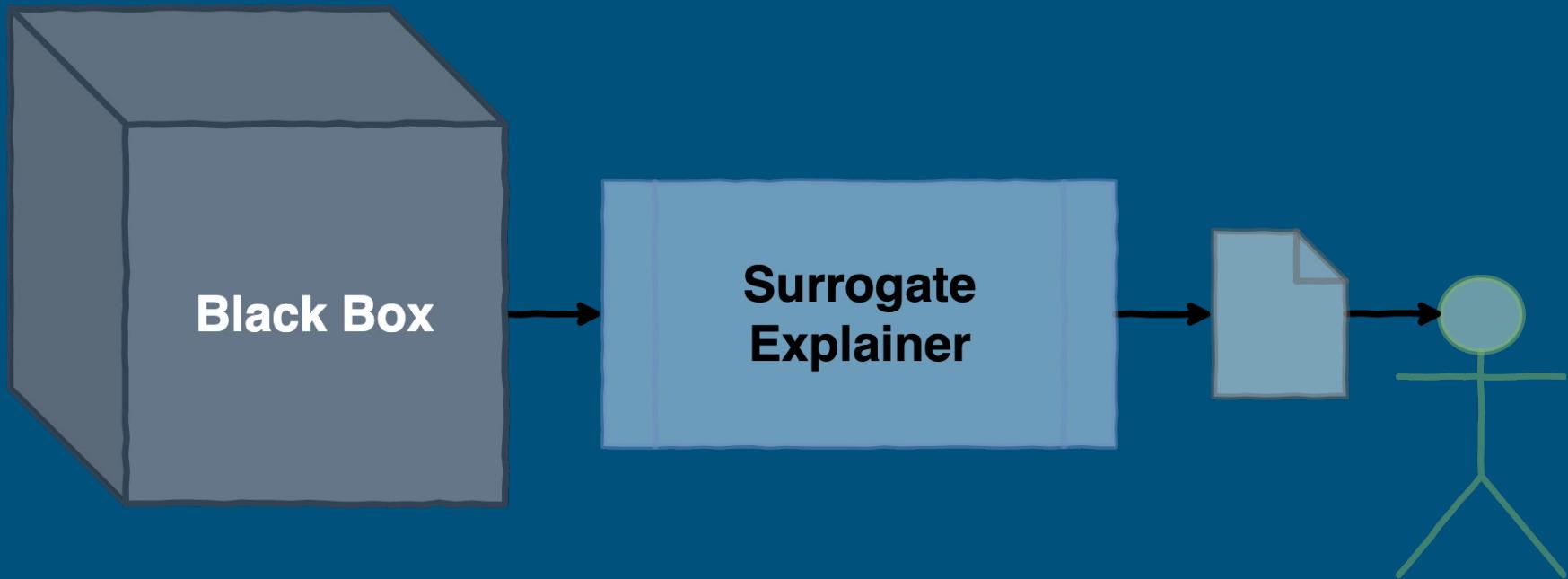


Mimicry Source: Behavioural Surrogate

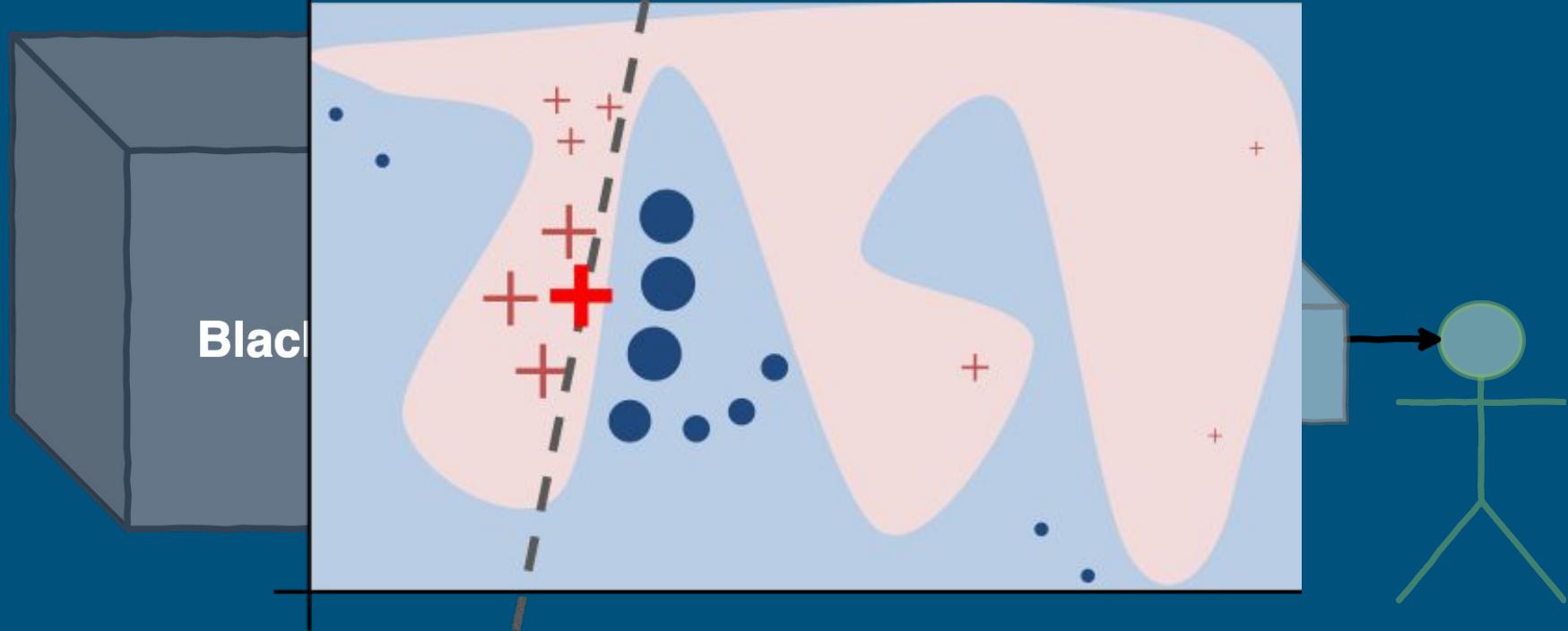
(predictions)



Surrogate Explainability in AI and ML



Surrogate Explainability in AI and ML



Ribeiro et al., 2016. "Why should I trust you?" Explaining the predictions of any classifier.

The Benefits of Surrogates

- **Model-agnostic** -- work with *any* black box.
- **Post-hoc** -- can be retrofitted into pre-existing predictors.
- **Data-universal** -- work with image, tabular and text data because of *interpretable data representations*.

Actual Surrogate Explainers

- Local Interpretable Model-agnostic Explanations (LIME)
 - *Ribeiro et al., 2016. "Why should I trust you?" Explaining the predictions of any classifier.*
- Anchor
 - *Ribeiro et al., 2018. Anchors: High-Precision Model-Agnostic Explanations.*
- SHapley Additive exPlanations (SHAP)
 - *Lundberg and Lee, 2017. A unified approach to interpreting model predictions.*
- RuleFit
 - *Friedman and Popescu, 2008. Predictive learning via rule ensembles.*

Universally Applicable Explainers



Surrogate
Explainers

Caveat: The No Free Lunch Theorem



Post-hoc Explainers have Poor Fidelity

The screenshot shows a white page with a dark blue header. The header contains the text "nature machine intelligence" and two dropdown menus: "Explore our content" and "Journal information". Below the header, the URL "nature > nature machine intelligence > perspectives > article" is visible. The main content area features a large title "Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead" in bold black font. Below the title, the author's name "Cynthia Rudin" is listed with an envelope icon. Further down, the journal details "Nature Machine Intelligence 1, 206–215(2019) | Cite this article" and metrics "23k Accesses | 151 Citations | 233 Altmetric | Metrics" are shown. At the bottom, there is a section titled "Abstract" with a descriptive paragraph.

nature machine intelligence

Explore our content ▾ Journal information ▾

nature > nature machine intelligence > perspectives > article

Perspective | Published: 13 May 2019

Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead

Cynthia Rudin

Nature Machine Intelligence 1, 206–215(2019) | Cite this article

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Abstract

Black box machine learning models are currently being used for high-stakes decision making throughout society, causing problems in healthcare, criminal justice and other domains. Some people hope that creating methods for explaining these black box models will alleviate some of the problems, but trying to explain black box models, rather than creating models that are interpretable in the first place, is likely to perpetuate bad practice and can potentially cause great harm to society. The way forward is to design models that

Post-hoc Explainers have Poor Fidelity

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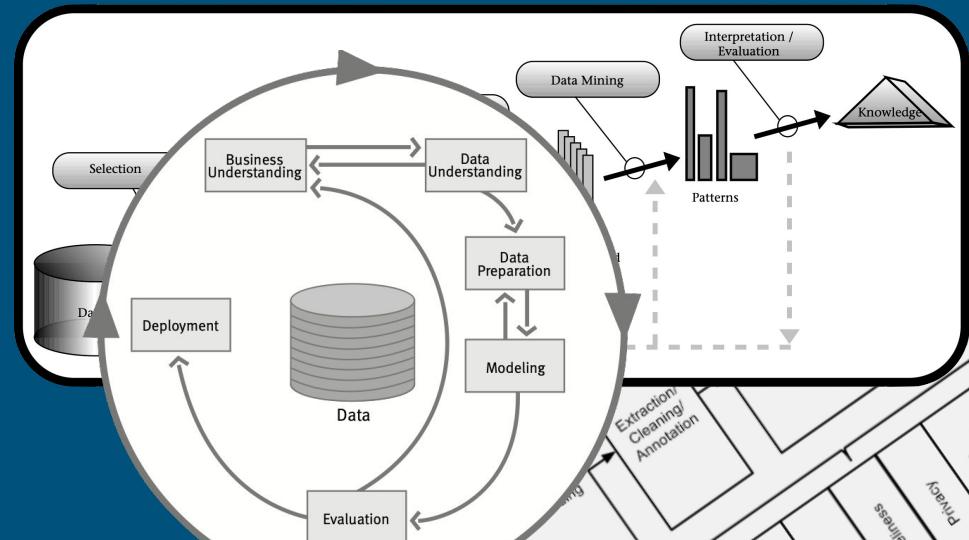
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- Explainability needs a process similar to: **KDD**, **CRISP-DM** or **BigData**.



Post-hoc Explainers have Poor Fidelity

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nature machine intelligence

Explore our content ▾ Journal information ▾

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- Explainability needs a process similar to: KDD, CRISP-DM or BigData.
- Engineers should spend time creating **informative features** and building **inherently transparent models**.

Bottom Line: It requires effort.

XAI Process

- A **generic** eXplainable Artificial Intelligence Process is beyond our reach at the moment.
- Attempts:
 - XAI Taxonomy spanning social and technical desiderata.
 - *Sokol and Flach, 2020. Explainability Fact Sheets: A Framework for Systematic Assessment of Explainable Approaches.*
 - Generic framework for black-box explainers.
 - *Henin and Le Métayer, 2019. Towards a generic framework for black-box explanations of algorithmic decision systems.*



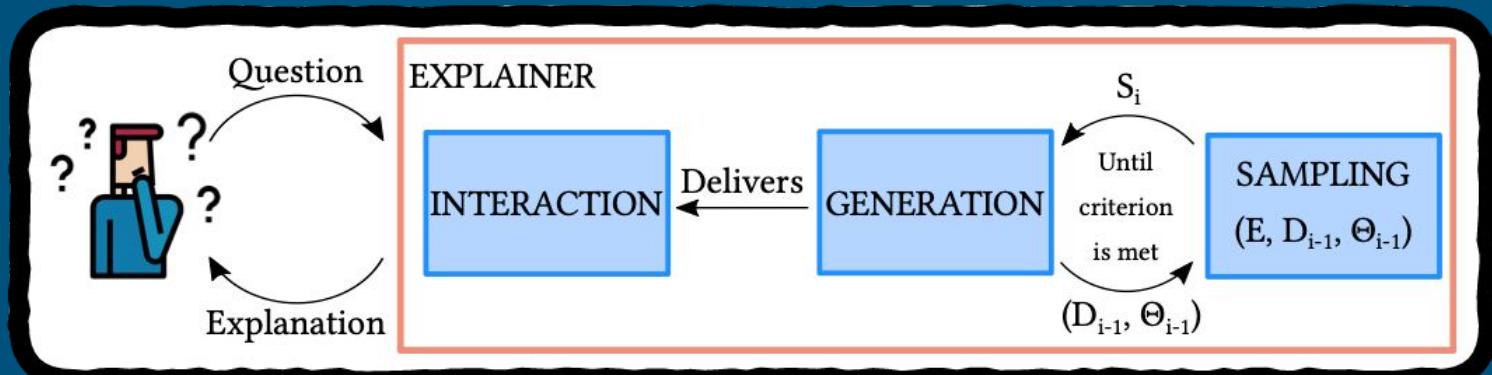
XAI Process

XAI Taxonomy spanning **social** and **technical** desiderata.

Functional	Operational	Usability	Safety	Validation
...



Generic framework for black-box explainers.



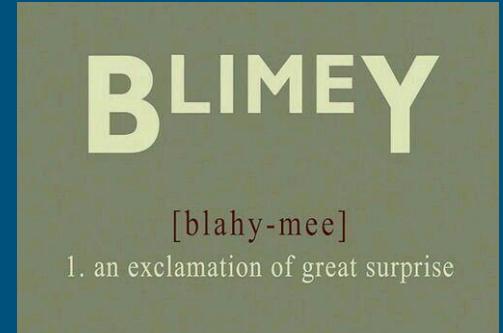
bLIMEy, there has to be a better way...

bLIMEy → build LIME yourself

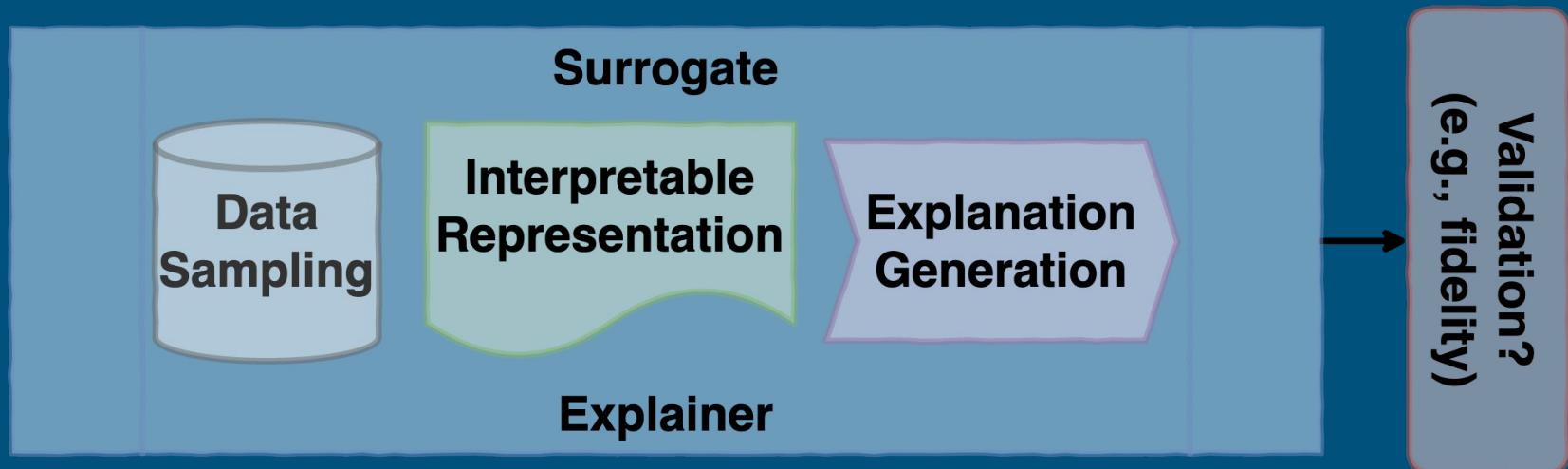
- *Framework* for building surrogate explainers.
- *Meta-algorithm* for operationalising them.
- Accompanied by analysis of surrogate building blocks (akin to a user guide).
- Practical recommendations.

Good news: A means to build flexible, faithful, interactive, ... surrogates.

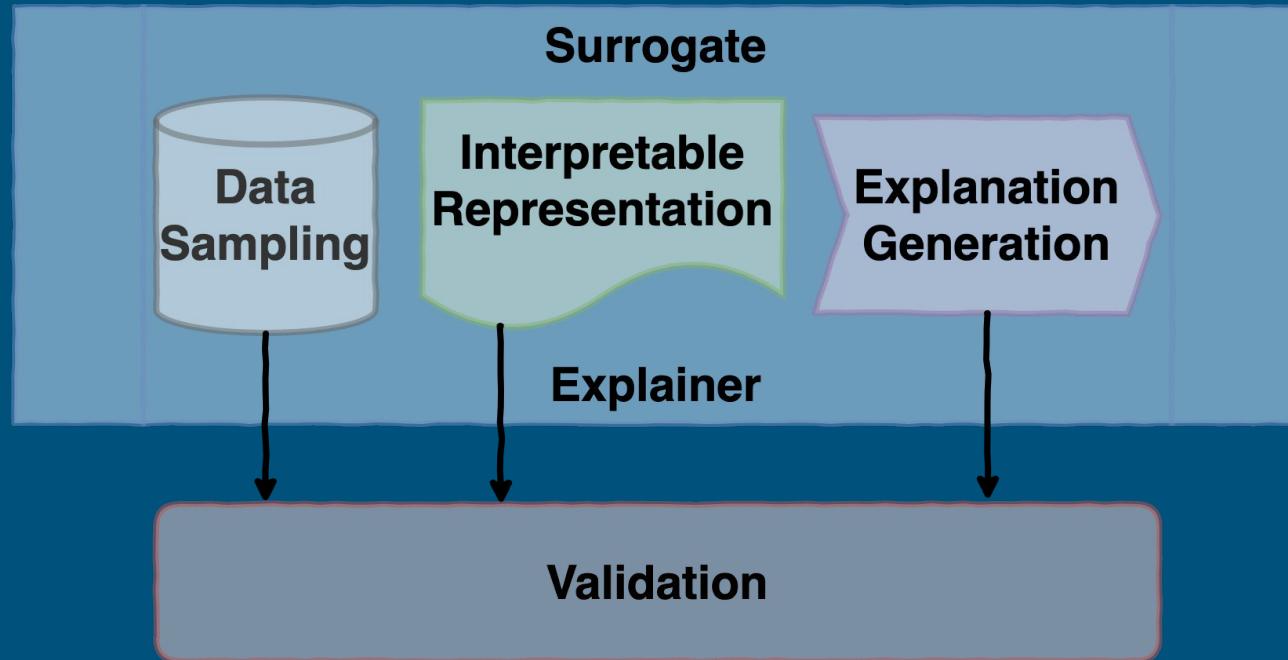
Not so good news: It requires **effort**.



Building Blocks of Surrogate Explainers



bLIMEy Framework



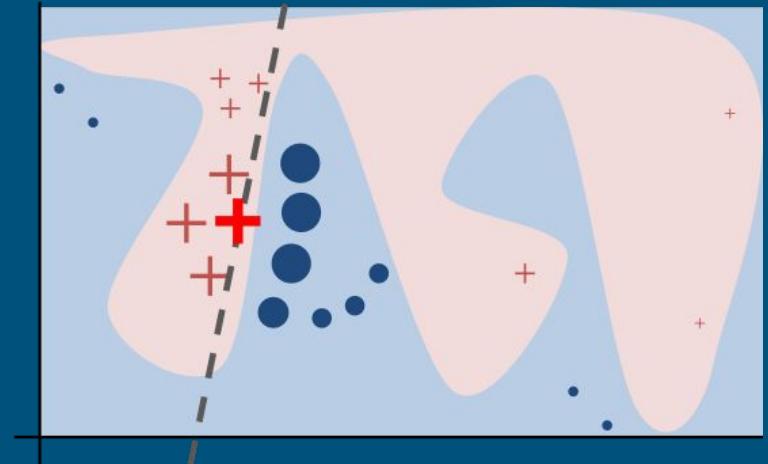
Operationalising Surrogates

We need to:

- Understand where surrogates come from.
- Know how to (correctly) interpret their explanations.

Then we should:

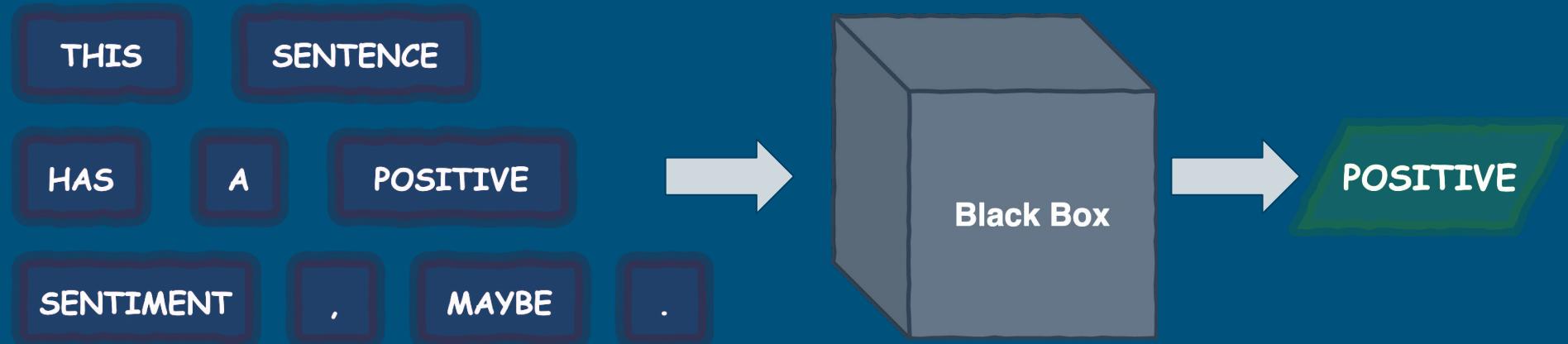
- Analyse needed components and choose suitable algorithms.
- Evaluate and validate them.



Ribeiro et al., 2016. "Why should I trust you?"
Explaining the predictions of any classifier.

Surrogates for Text Data

Black-box Prediction



Interpretable Data Representation



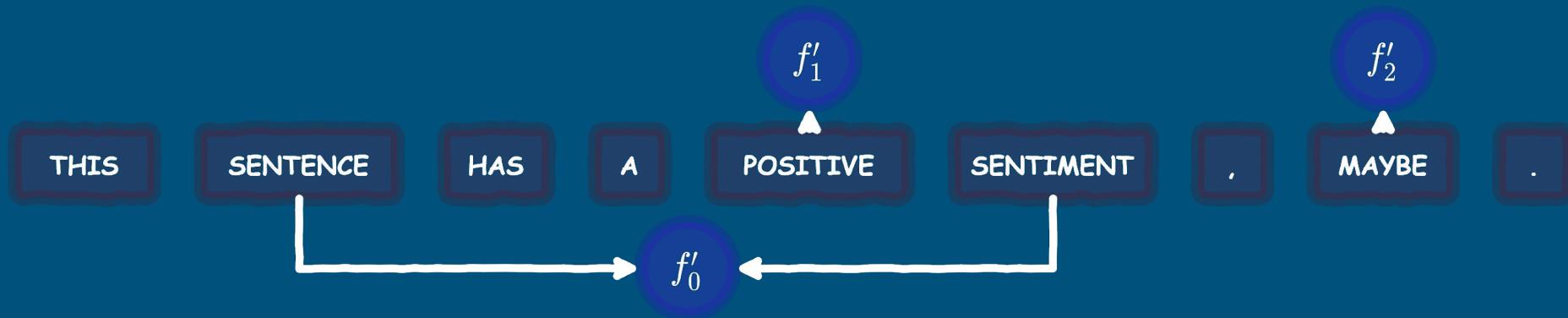
$$\mathring{x}' = [1, 1, 1, 1, 1, 1, 1, 1, 1]$$

Interpretable Data Representation[★]



$$\mathring{x}' = [1, 1, 1, 1]$$

Interpretable Data Representation*



$$\mathring{x}' = [1, 1, 1]$$

Data Sampling

- Sampling from the original data domain is ill-defined.
- We have to sample from the interpretable representation.

```
randint(low=0, high=1, shape=(3, 4))
```

$$x'_0 = [1, 0, 0, 1] \quad x'_2 = [0, 0, 0, 1]$$
$$x'_1 = [1, 0, 1, 0]$$

Explanation Generation -- Restoring Sample

$$x'_0 = [1, 0, 0, 1]$$



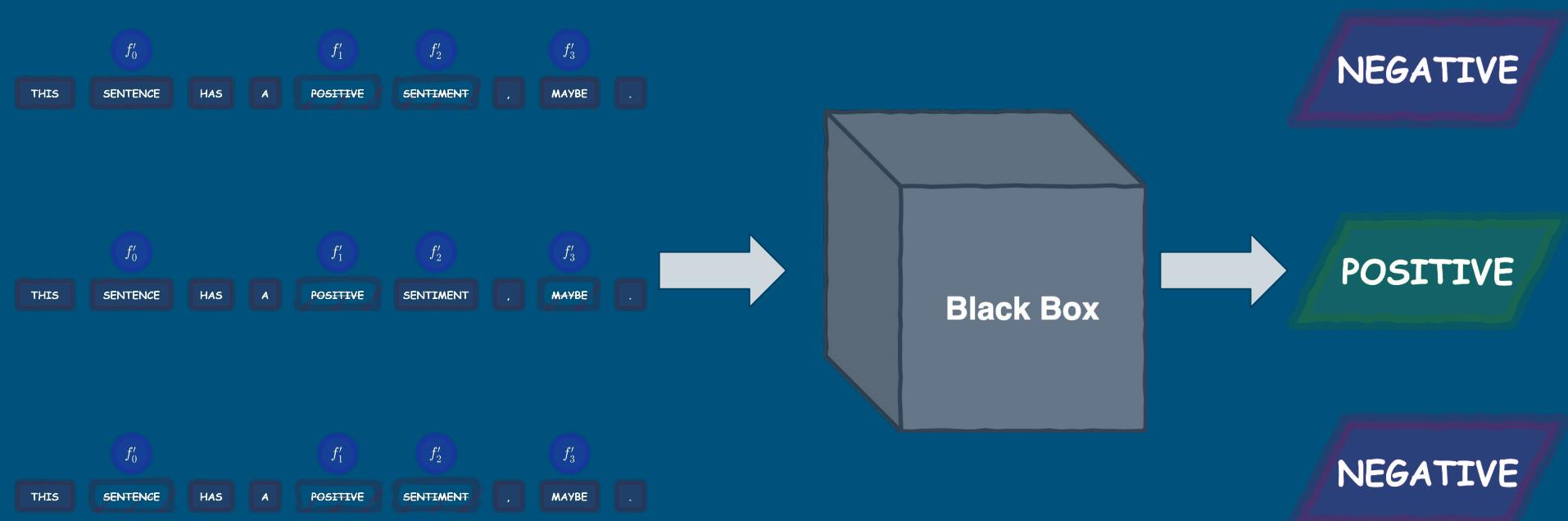
$$x'_1 = [1, 0, 1, 0]$$



$$x'_2 = [0, 0, 0, 1]$$



Explanation Generation -- Predicting Sample



Explanation Generation -- Weighting Sample

		Distance	Similarity
$\ddot{x}' = [1, 1, 1, 1]$	$x'_0 = [1, 0, 0, 1]$	d=2	s=0.62
	$x'_1 = [1, 0, 1, 0]$	d=2	s=0.62
	$x'_2 = [0, 0, 0, 1]$	d=3	s=0.23

Explanation Generation -- Fitting Surrogate

- Fit a sparse linear classifier.
- Use the binary vectors as data.
- Use the black box-predictions for the sampled and reversed data as labels:
 - 0 -- negative sentiment;
 - 1 -- positive sentiment.
- Weight instances according to the similarity scores.
- Extract model coefficients as importance scores (explanation).



Explanation Generation -- Fitting Surrogate

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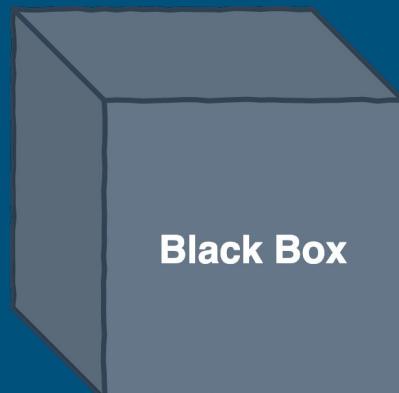


Surrogates for Image Data

Black-box Prediction



husky/eskimo/malamute
dog



HUSKY

Interpretable Data Representation



$$\mathring{x}' = [1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1]$$

Interpretable Data Representation[★]



$$\mathring{x}' = [1, 1, 1, 1, 1, 1, 1]$$

Data Sampling

- Sampling from the original data domain is ill-defined.
- We have to sample from the interpretable representation.

```
randint(low=0, high=1, shape=(3, 7))
```

$$x'_0 = [0, 0, 0, 1, 1, 1, 1] \quad x'_1 = [0, 1, 1, 1, 0, 1, 0]$$

$$x'_2 = [1, 1, 1, 0, 1, 1, 1]$$

Explanation Generation -- Restoring Sample

How to remove super-pixels?
Using occlusion.

$$x'_0 = [0, 0, 0, 1, 1, 1, 1] \quad x'_1 = [0, 1, 1, 1, 0, 1, 0]$$

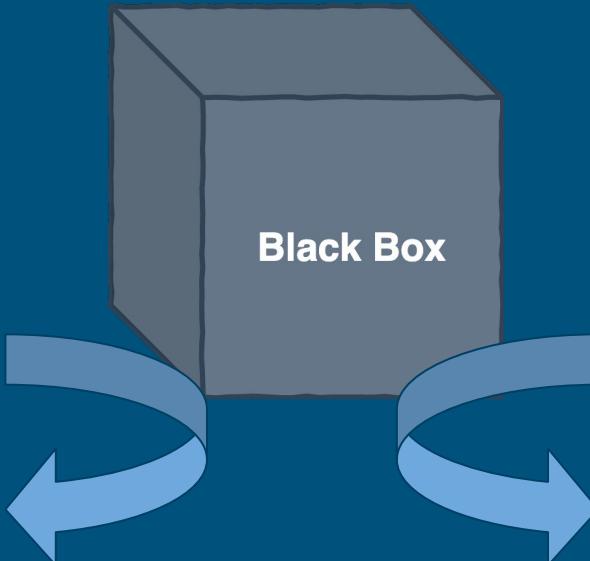


Explanation Generation -- Restoring Sample

What occlusion colour to use?



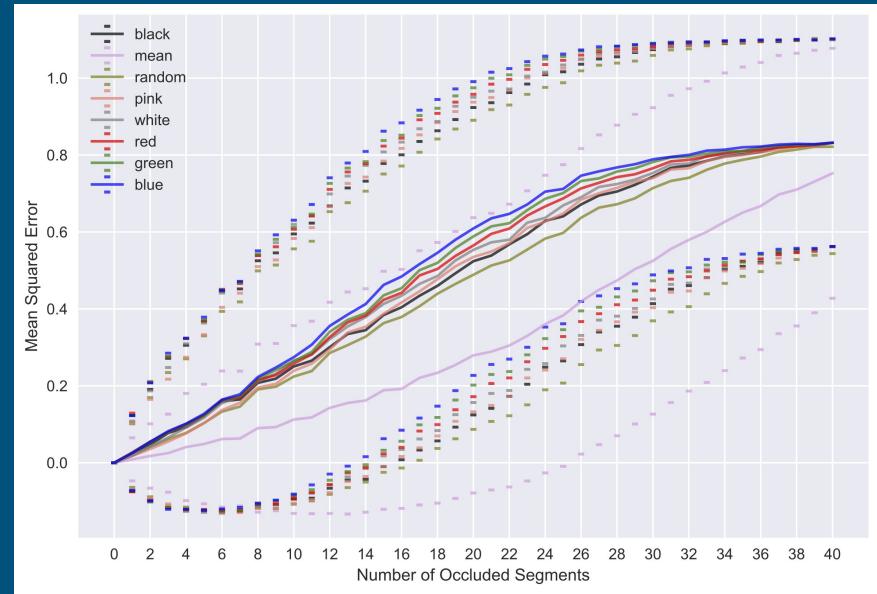
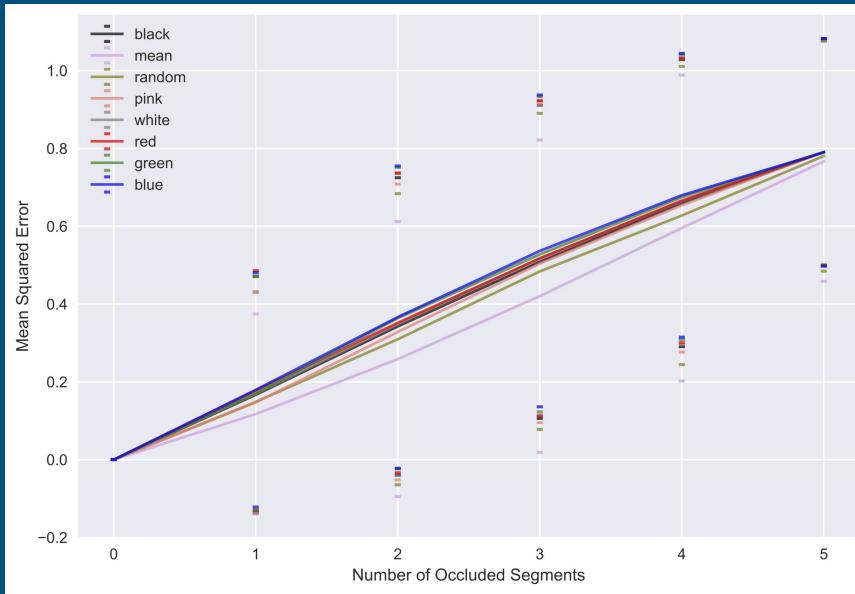
MALAMUTE



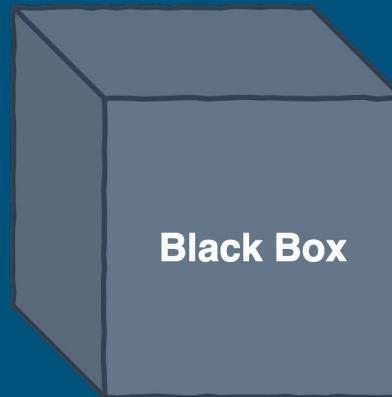
HUSKY

Explanation Generation -- Restoring Sample

What occlusion colour and segmentation granularity to use?



Explanation Generation -- Predicting Sample



MALAMUTE

HUSKY

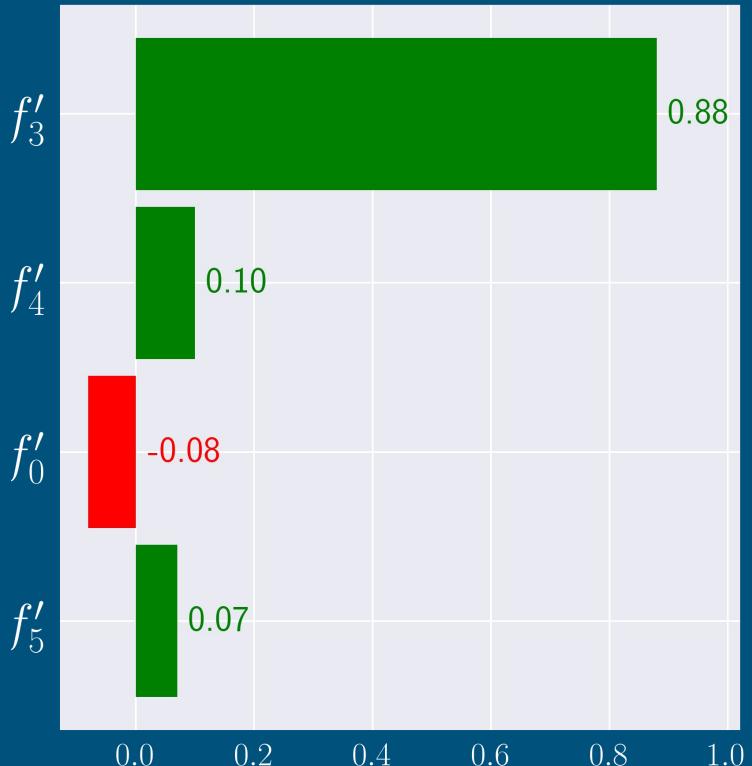
ESKIMO

Explanation Generation -- Weighting Sample

	Distance	Similarity
$x'_0 = [0, 0, 0, 1, 1, 1, 1]$	d=3	s=0.57
$\mathring{x}' = [1, 1, 1, 1, 1, 1, 1]$ $x'_1 = [0, 1, 1, 1, 0, 1, 0]$	d=3	s=0.57
$x'_2 = [1, 1, 1, 0, 1, 1, 1]$	d=1	s=0.09

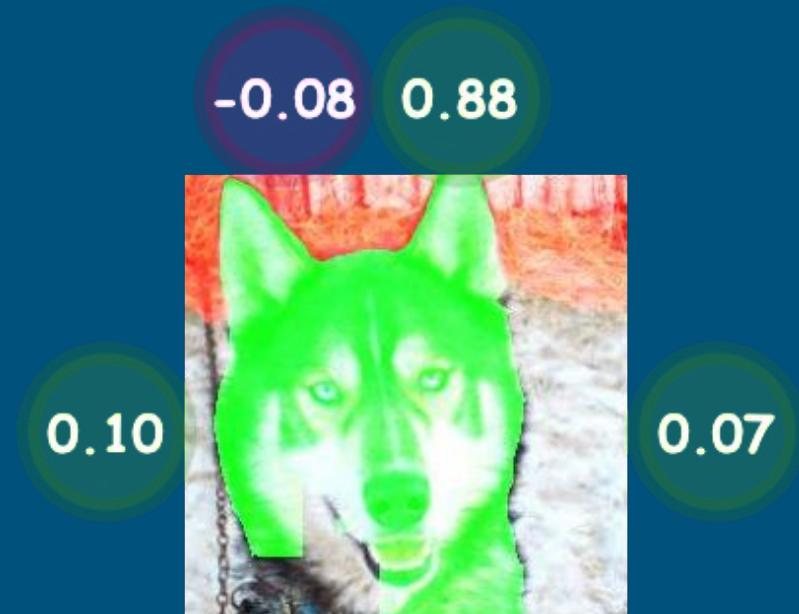
Explanation Generation -- Fitting Surrogate

- Fit a sparse linear classifier.
- Use the binary vectors as data.
- Use the black box-predictions for the sampled and reversed data as labels:
 - What about multi-class problems?
- Weight instances according to the similarity scores.
- Extract model coefficients as importance scores (explanation).



Explanation Generation -- Fitting Surrogate

- Fit a sparse linear classifier.
- Use the binary vectors as data.
- Use the black box-predictions for the sampled and reversed data as labels:
 - What about multi-class problems?
- Weight instances according to the similarity scores.
- Extract model coefficients as importance scores (explanation).



Explanation Generation -- Fitting Surrogate



Black box is a multi-class classifier.
Surrogate is a (linear) binary classifier.



MALAMUTE

HUSKY

ESKIMO

ESKIMO

HUSKY

Explained Class:

HUSKY

0

1

0

0

1

Explanation Generation -- Fitting Surrogate



Black box is a probabilistic multi-class classifier.
Surrogate is a (linear) regressor.



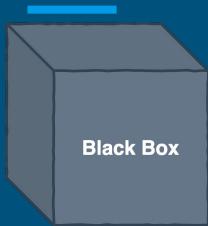
.97 MALAMUTE	.01 HUSKY	.02 ESKIMO
.06 MALAMUTE	.88 HUSKY	.06 ESKIMO
.13 MALAMUTE	.23 HUSKY	.64 ESKIMO
.11 MALAMUTE	.10 HUSKY	.79 ESKIMO
.42 MALAMUTE	.58 HUSKY	.00 ESKIMO

Explained Class:

HUSKY

.01 HUSKY
.88 HUSKY
.23 HUSKY
.10 HUSKY
.58 HUSKY

Explanation Generation -- Fitting Surrogate



Black box is a probabilistic multi-class classifier.
Surrogate is a (linear) regressor.



.97 MALAMUTE	.01 HUSKY	.02 ESKIMO
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.42 MALAMUTE	.58 HUSKY	.00 ESKIMO

Explained Class:

HUSKY

.01 HUSKY
.88 HUSKY
.23 HUSKY
.10 HUSKY
.58 HUSKY

Explanation Generation -- Fitting Surrogate



Black box is a probabilistic multi-class classifier.
Surrogate is a multi-output regressor (tree).

.97 MALAMUTE	.01 HUSKY	.02 ESKIMO
.06 MALAMUTE	.88 HUSKY	.06 ESKIMO
.13 MALAMUTE	.23 HUSKY	.64 ESKIMO
.11 MALAMUTE	.10 HUSKY	.79 ESKIMO
.42 MALAMUTE	.58 HUSKY	.00 ESKIMO

Explained
Classes:
HUSKY
ESKIMO

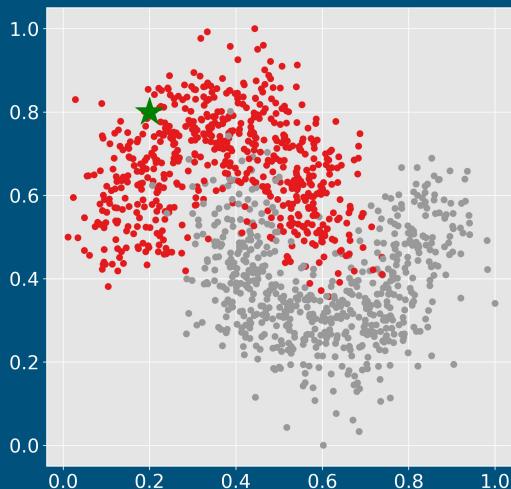
.01 HUSKY	.02 ESKIMO
.88 HUSKY	.06 ESKIMO
.23 HUSKY	.64 ESKIMO
.10 HUSKY	.79 ESKIMO
.58 HUSKY	.00 ESKIMO

DEMO

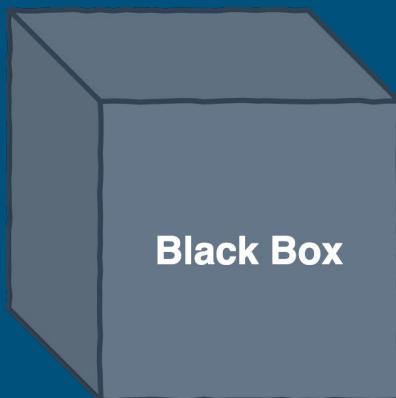
Surrogates for Tabular Data

Black-box Prediction

$$\ddot{x} = [0.2, 0.8]$$

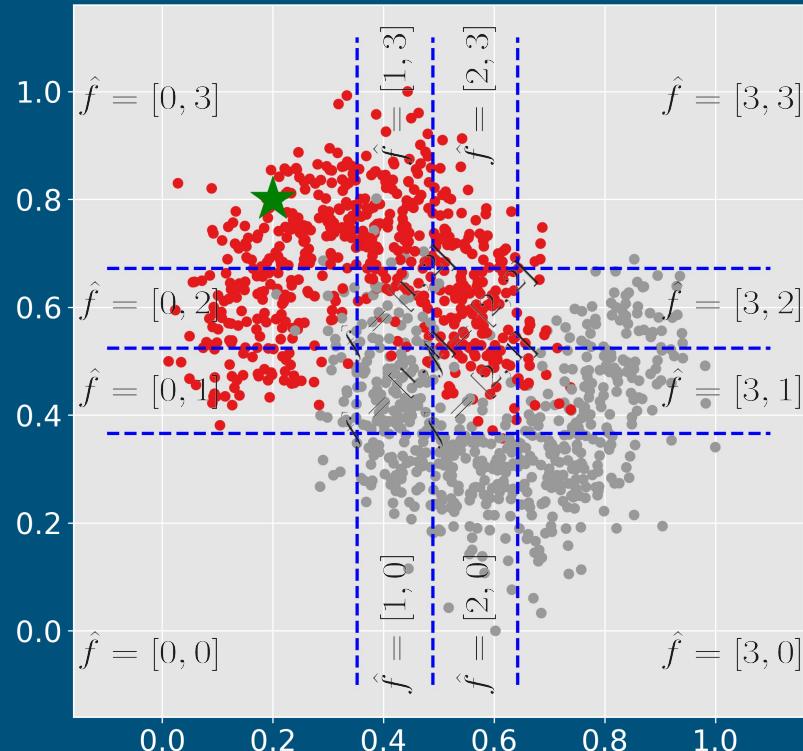


red/grey



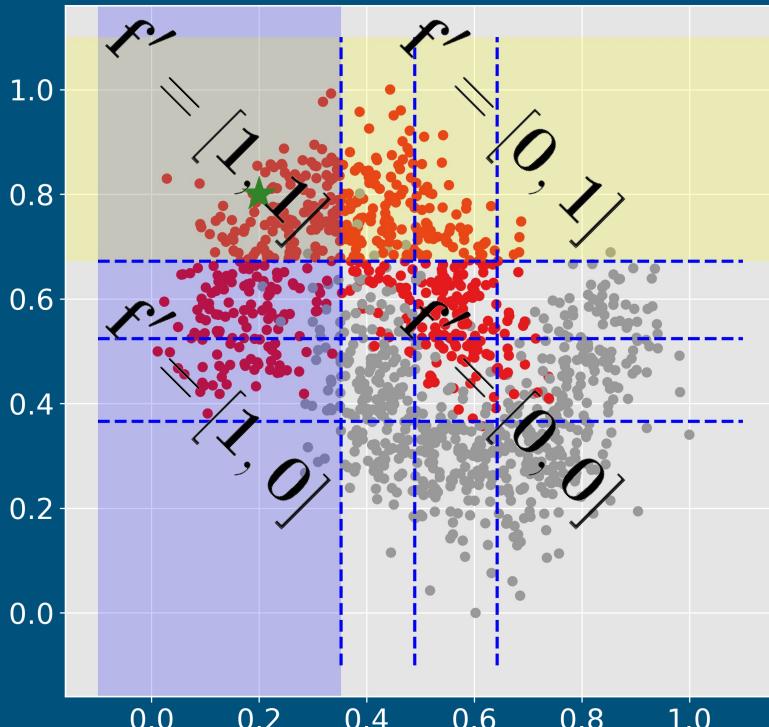
Interpretable Representation: (Q) Discretisation

$$\hat{\mathring{x}} = [0, 3]$$



Interpretable Representation: (Q) Binarisation

$$\mathring{x}' = [1, 1]$$



Interpretable Representation: (Q) Complexity

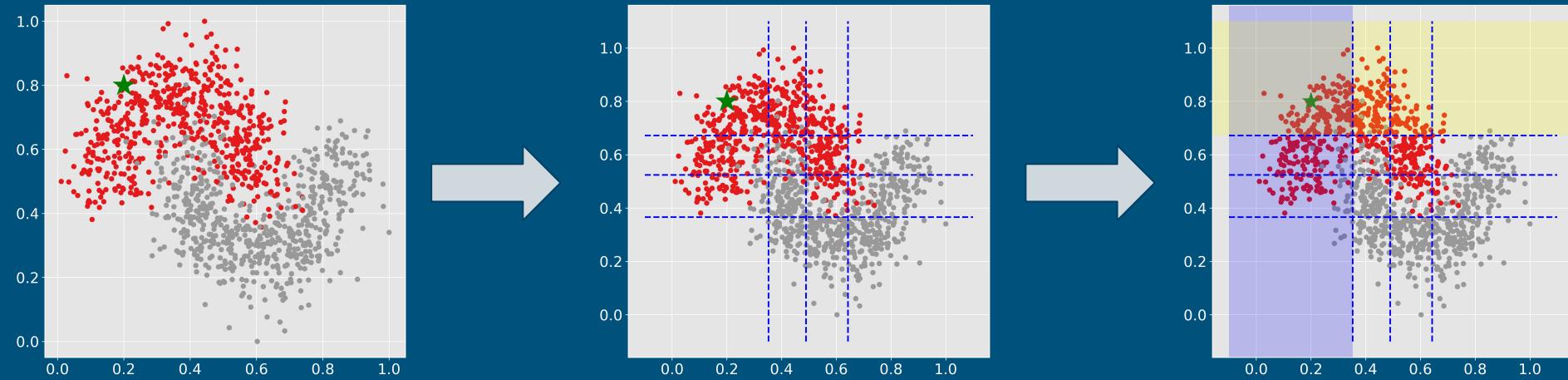
What happens in higher dimensions?

- **Discrete** → exponential growth of partitions -- n^d , e.g., $4^2=16$ for quartile discretisation in our toy example.
 - Original data with d numerical features.
 - Each numerical feature split into n sectors.
 - Categorical attributes not affected.
- **Binary** → reduces this number to 2^d , e.g., $2^2=4$ for binarisation of our toy example.

Sparsity problem -- 11 numerical features yield $4^{11}=4,194,304$ hyper-rectangles and $2^{11}=2,048$ binary encodings.

Interpretable Representation: (★) Purity

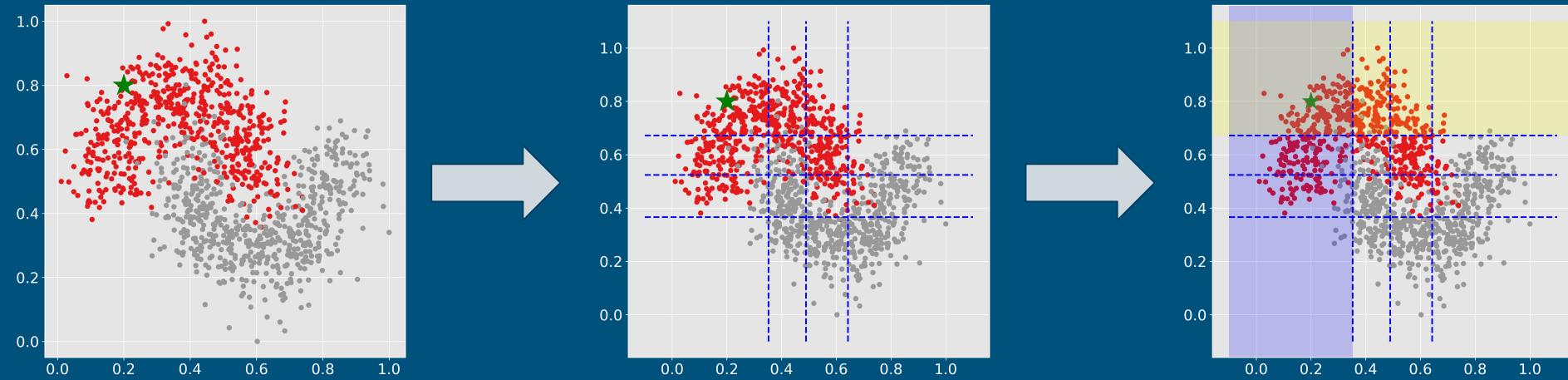
- Imagine this is a **sample around the explained data point**.
- The colour of markers encodes a **class predicted by a black box**.
- **Pure hyper-rectangles** imply good approximation of a black-box boundary.



Interpretable Representation: (★) Purity

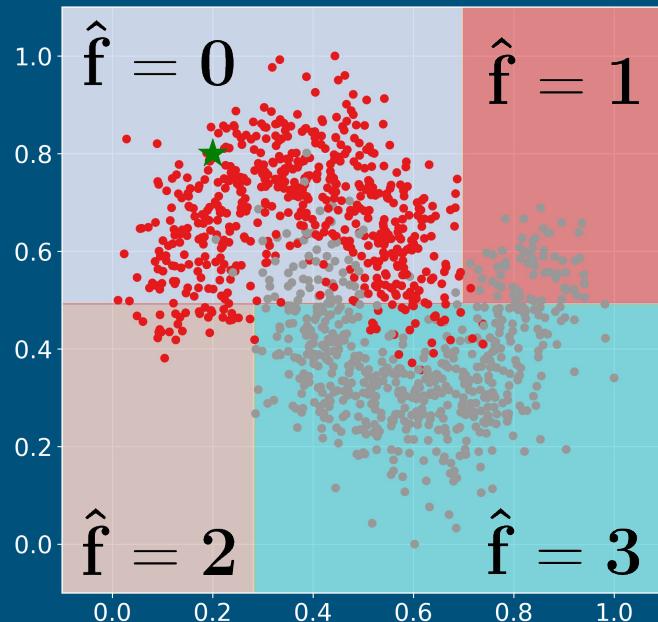
Purity score weighted by the number of instances in each partition:

- crisp classification → **Gini Index/Impurity**;
- probabilistic classification or regression → **Mean Squared Error**.



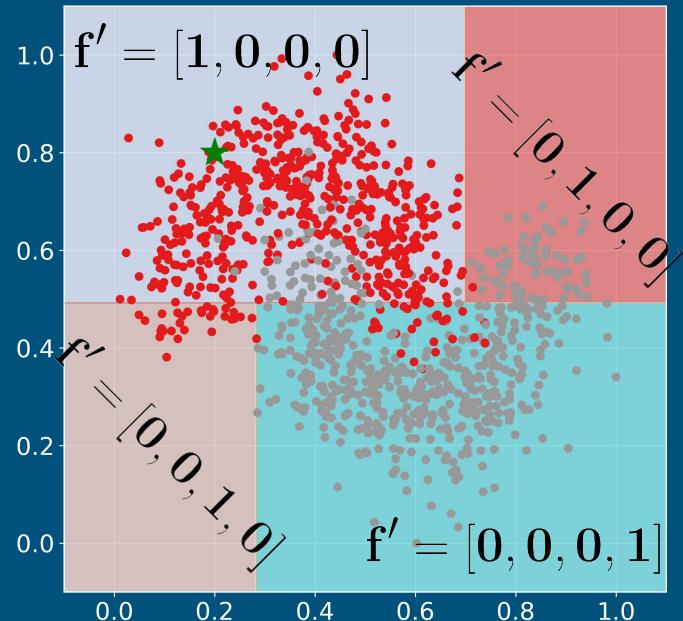
Interpretable Representation: (T) Discretisation

$\hat{\vec{x}} = 0$



Interpretable Representation: (T) Binarisation

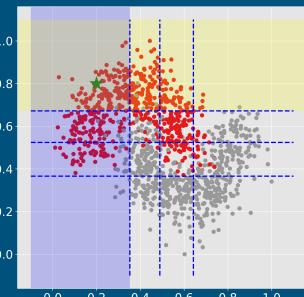
$$\mathring{x}' = [1, 0, 0, 0]$$



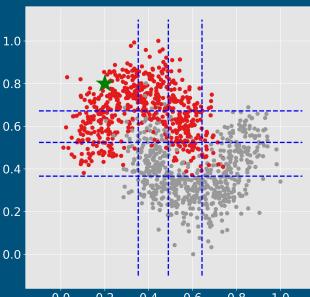
Data Sampling

Sample from:

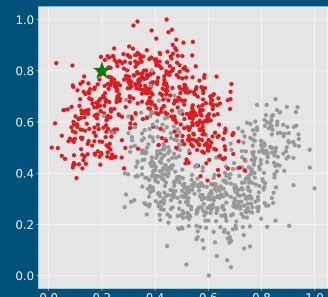
binary interpretable
representation



discrete intermediate
representation



original data
domain

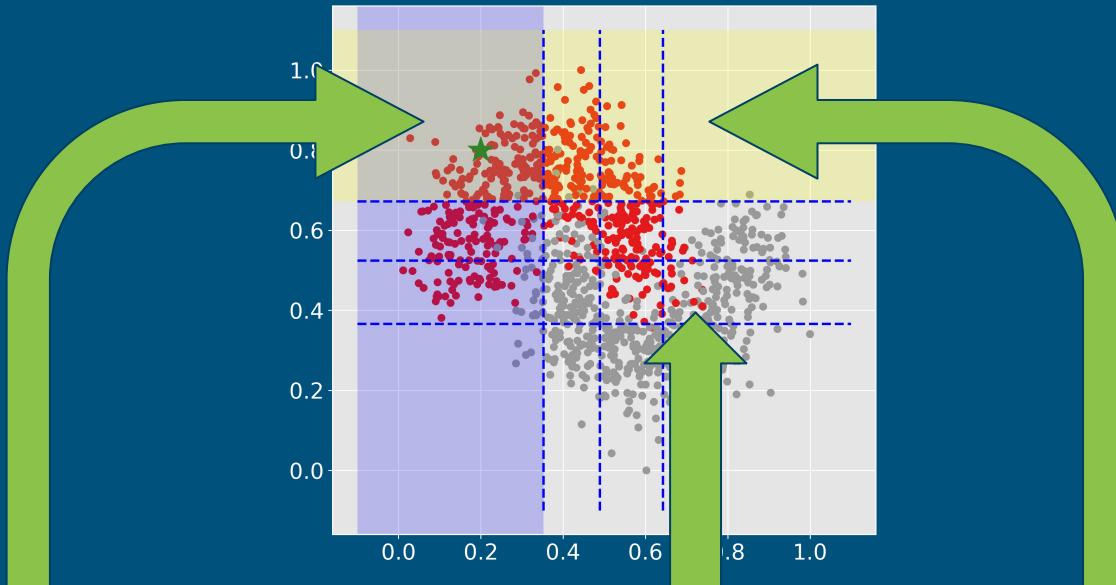


`randint(low=0, high=1,
shape=(3, 2))`

`randint(low=0, high=3,
shape=(3, 2))`

...

Data Sampling: Interpretable (Binary)

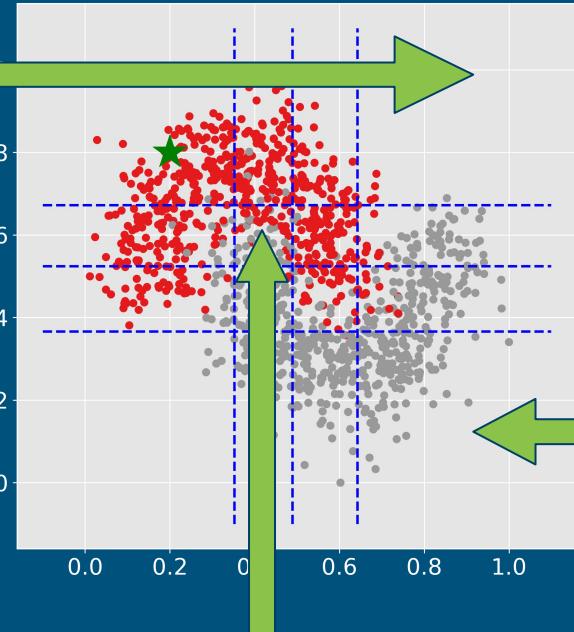


$$x'_0 = [1, 1]$$

$$x'_1 = [0, 0]$$

$$x'_2 = [0, 1]$$

Data Sampling: Intermediate (Discrete)



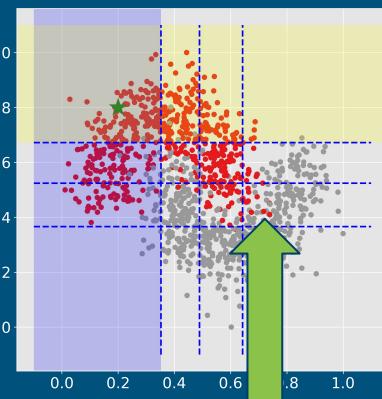
$$\hat{x}_0 = [3, 3]$$

$$\hat{x}_1 = [1, 2]$$

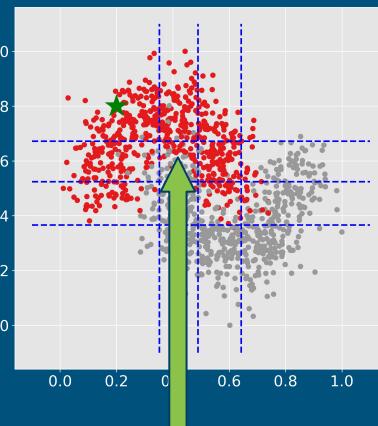
$$\hat{x}_2 = [3, 0]$$

Explanation Generation -- Restoring Sample

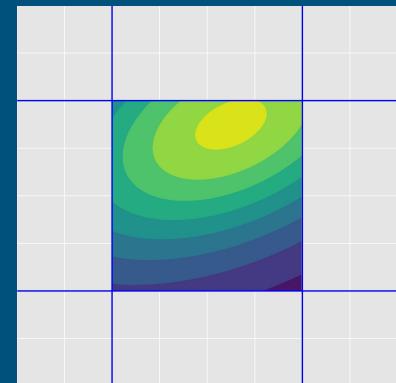
Only required for binary and discrete sampling.



$$x'_1 = [0, 0]$$

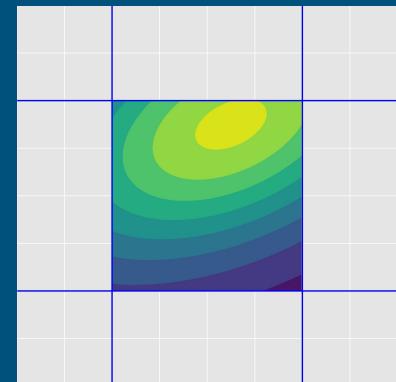
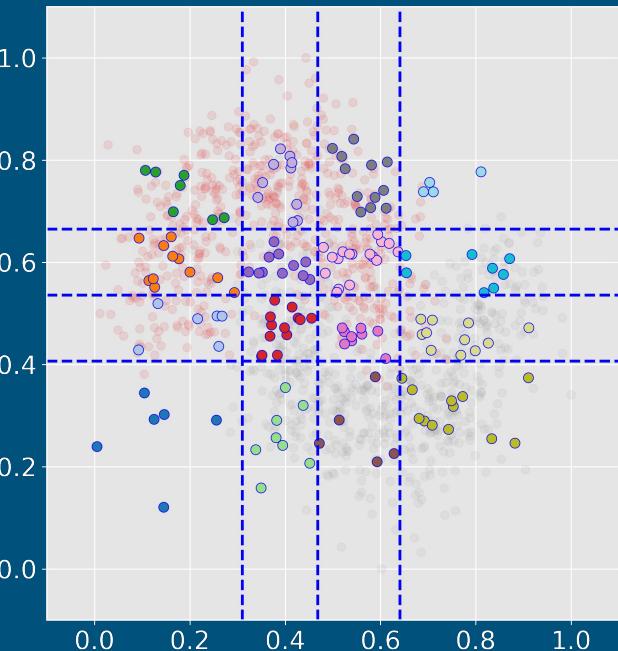


$$\hat{x}_1 = [1, 2]$$



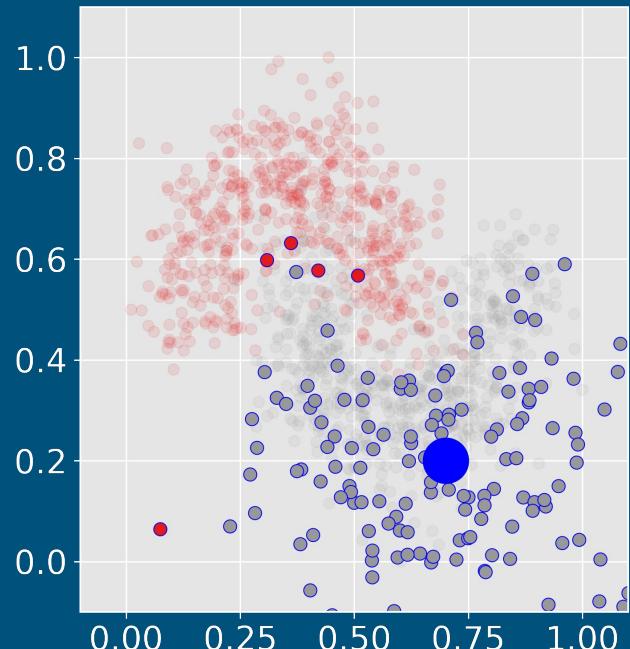
Explanation Generation -- Restoring Sample

Only required for binary and discrete sampling.

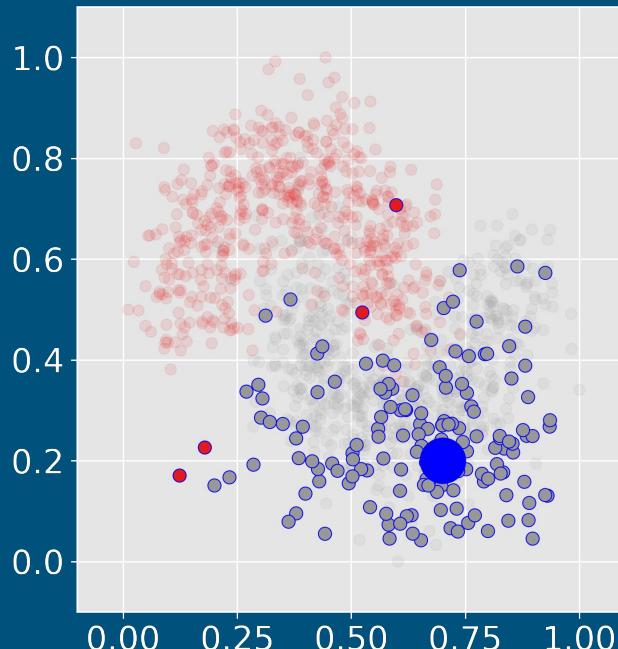


Data Sampling: Original

Normal

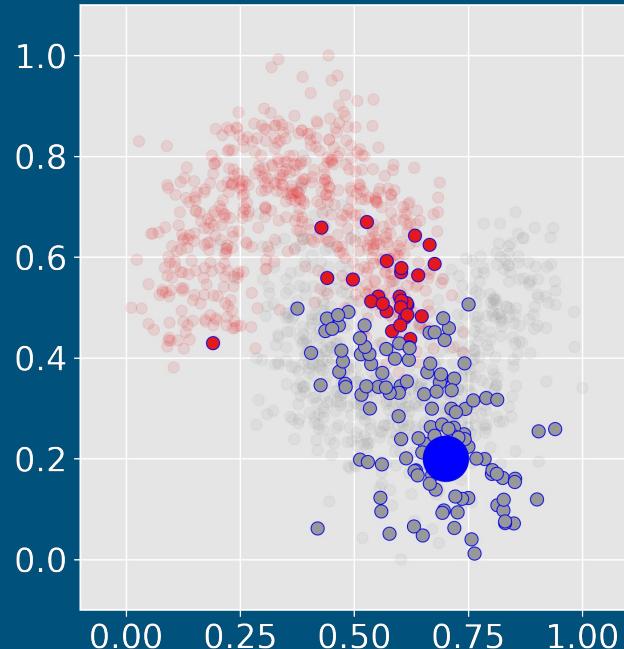


Truncated Normal

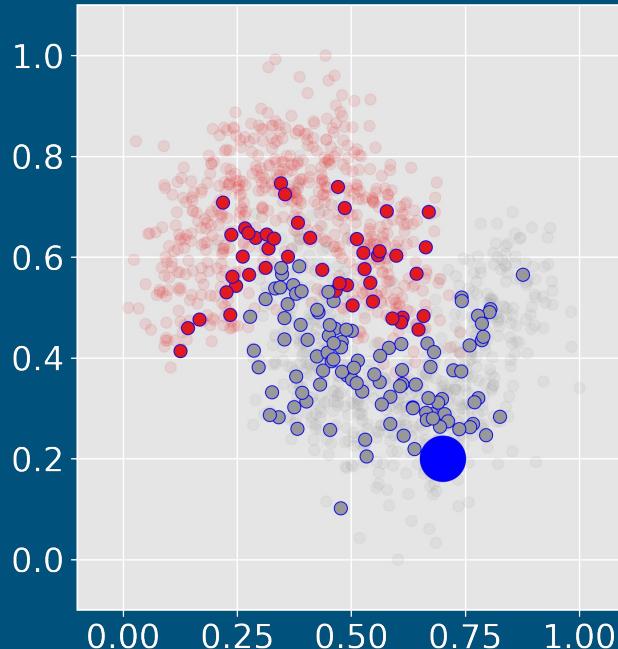


Data Sampling: Original (ctd.)

Class Discovery



Mixup

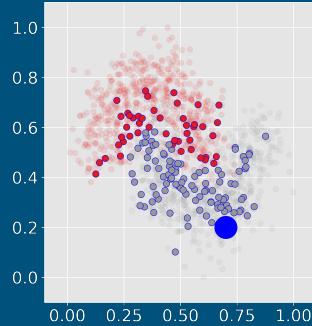
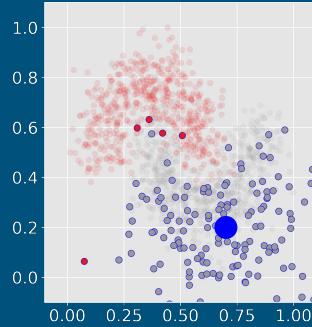


Data Sampling -- *Comparison*

Diverse sample → good chance of approximating black-box decision boundary.

(Whereas interpretable representation should be as pure as possible.)

- *Binary/discrete sampling*, in principle, discover classes as they are somewhat global. (Caveat: large number of hyper-rectangles to sample from.)
- *Original data domain sampling* must explicitly discover the neighbourhood.

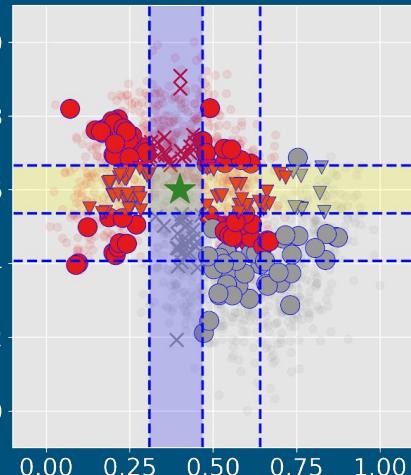


Explanation Generation -- Weighting Sample

But in which domain?

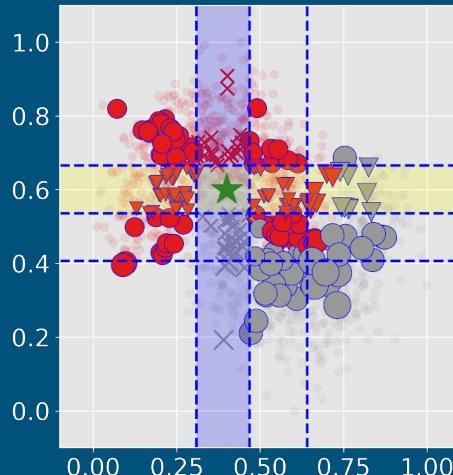
Binary

$$\mathring{x}' = [1, 1]$$



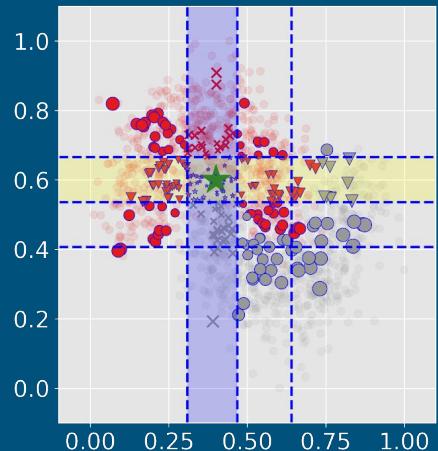
Discrete

$$\hat{\mathring{x}} = [1, 2]$$



Original

$$\mathring{x} = [0.2, 0.8]$$

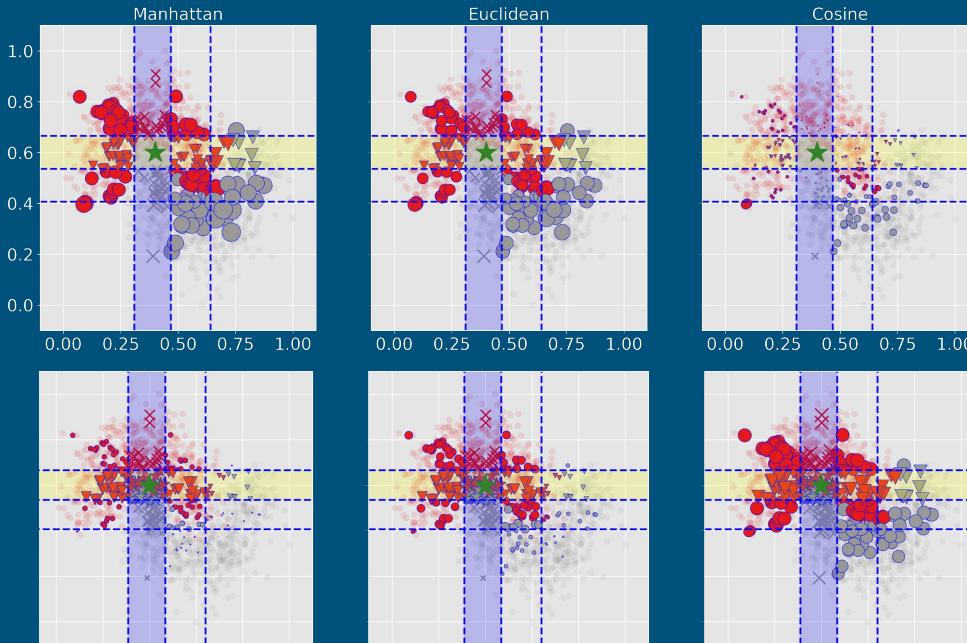


Explanation Generation -- Weighting Sample

Discrete
Distances

Kernelisation

Kernelisation... But in which domain?



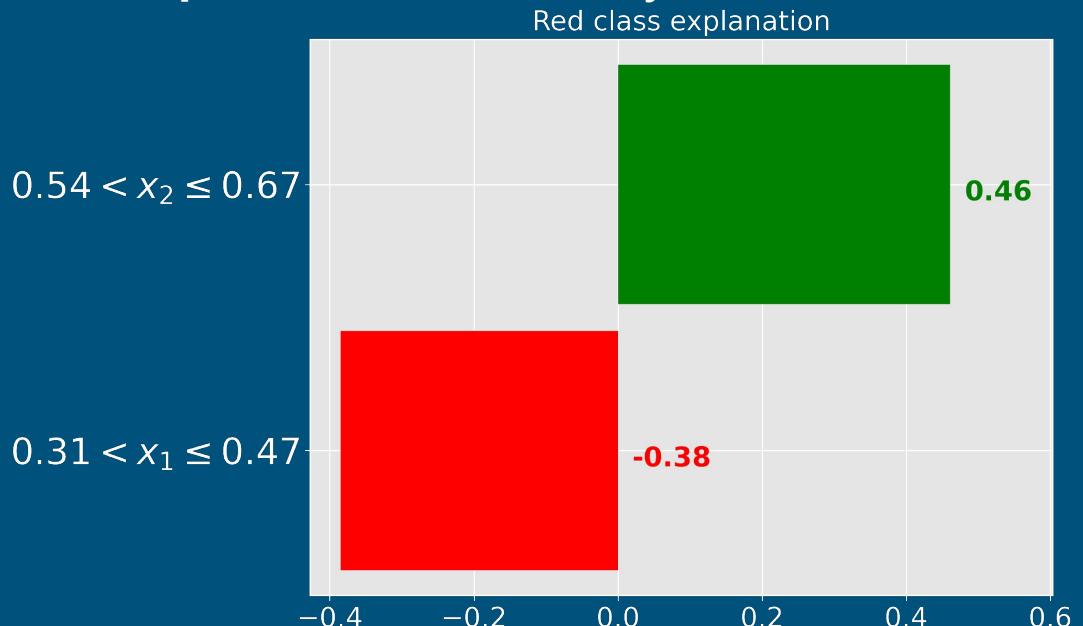
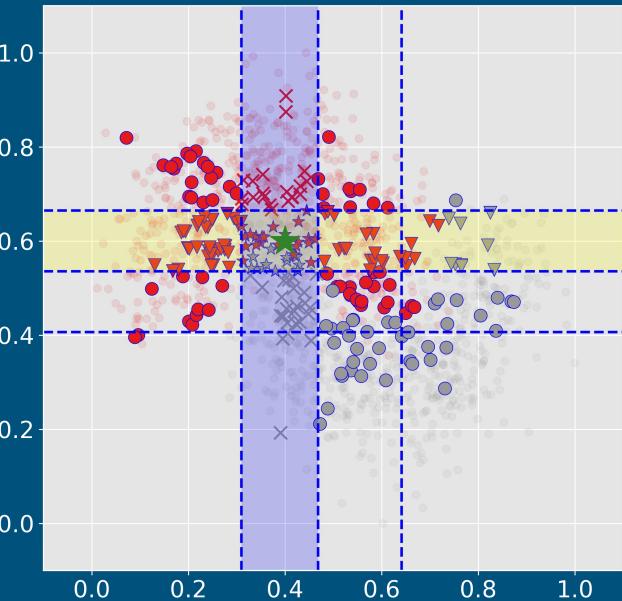
Explanation Generation -- Feature Selection

- Not required for image and text data -- the explanation presentation is as intelligible as the explained instance.
- Can be *computed* for any representation, but *applies* to the binary interpretable -- introducing sparsity to the bar plot.
 - lasso path;
 - forward selection; and
 - highest weights.
- Interpretable representations based on **tree splits** have sparsity mechanisms built in (e.g., impurity reduction and pruning).



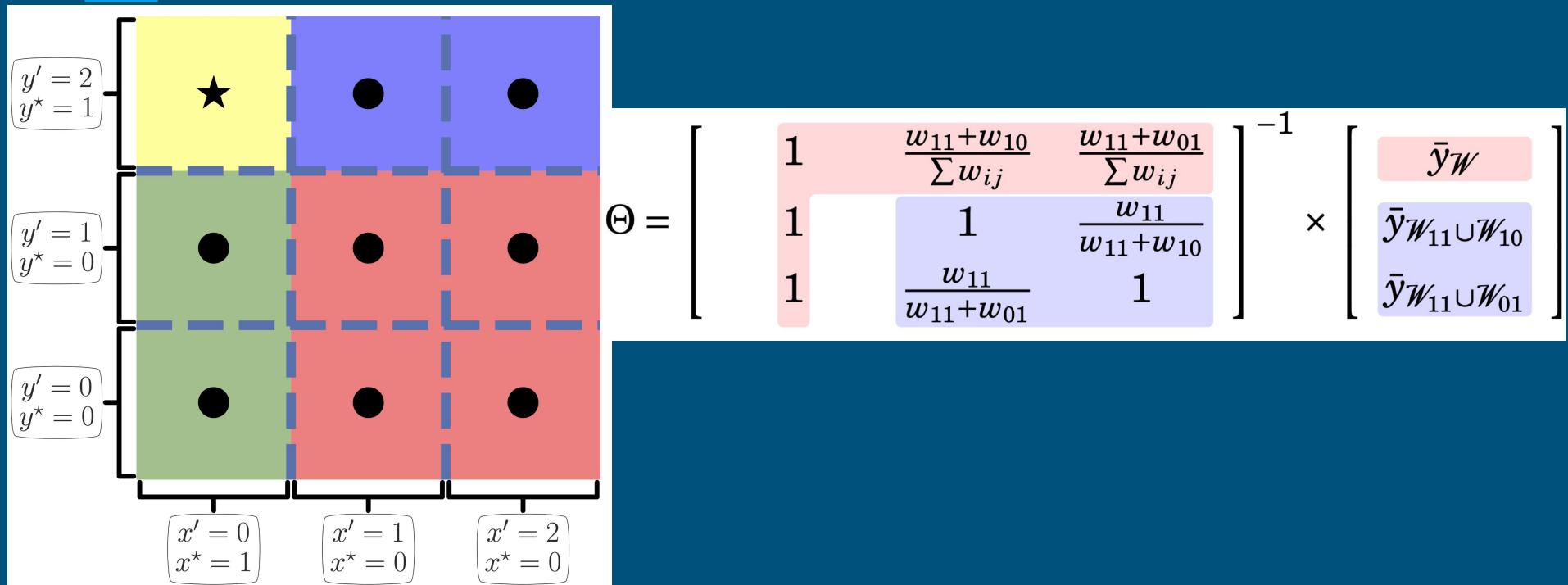
Linear Surrogate + Discretisation/Binarisation

Caveats: feature **independence** and **linearity**.



DEMO

But Why? Meaning of the Explanation



Conclusions

Summary

- For explainers to make ML system *trustworthy*, they must be **trustworthy** in the first place.
- These **diagnostic tools** only become **explainers** when their *properties* and *outputs* are well understood.
- Explainers **are not** *monolithic* entities.
- They need to be **configured** or **tailor-made** for the application at hand.

You Need to Choose Wisely

There is no magic formula -- it takes in-depth understanding and effort.



Reproducibility



- FAT Forensics
 - Fairness, Accountability and Transparency software
 - <https://fat-forensics.org/>
 - <https://joss.theoj.org/papers/10.21105/joss.01904>
- Hands-on surrogate explainability
 - https://events.fat-forensics.org/2020_ecml-pkdd
- Self-paced Online Learning (The Alan Turing Institute)
 - Interactive online training resources on *interpretability, explainability and transparency*
 - Arriving later this year
- BIAS Summer School
 - Parameterisation of surrogate explainers
 - https://events.fat-forensics.org/2021_bias

The cover features the JOSS logo at the top left. The title 'FAT Forensics: A Python Toolbox for Implementing and Deploying Fairness, Accountability and Transparency Algorithms in Predictive Systems' is centered. Below the title, the authors' names are listed: Kacper Sokol¹, Alexander Hepburn², Rafael Poyiadzi², Matthew Clifford¹, Raul Santos-Rodriguez², and Peter Flach¹. At the bottom, it says 'DOI: 10.21105/joss.01904'.



**ECML
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The header includes the title './ FAT Forensic Events' and a subtitle 'Hands-on Tutorial on Explainable ML with FAT Forensics'. Below this are links for 'Source Code' and 'Documentation'. A 'Resources' section contains buttons for 'Recordings', 'Slides', 'Jupyter Notebooks', and 'Slack'. At the bottom, a DOI link 'DOI: 10.5281/zenodo.4035128' is shown.

Break

Hands-on

HANDS-ON

https://github.com/fat-forensics/resources/blob/master/tabular_surrogate_builder/tabular_surrogate_builder.ipynb