

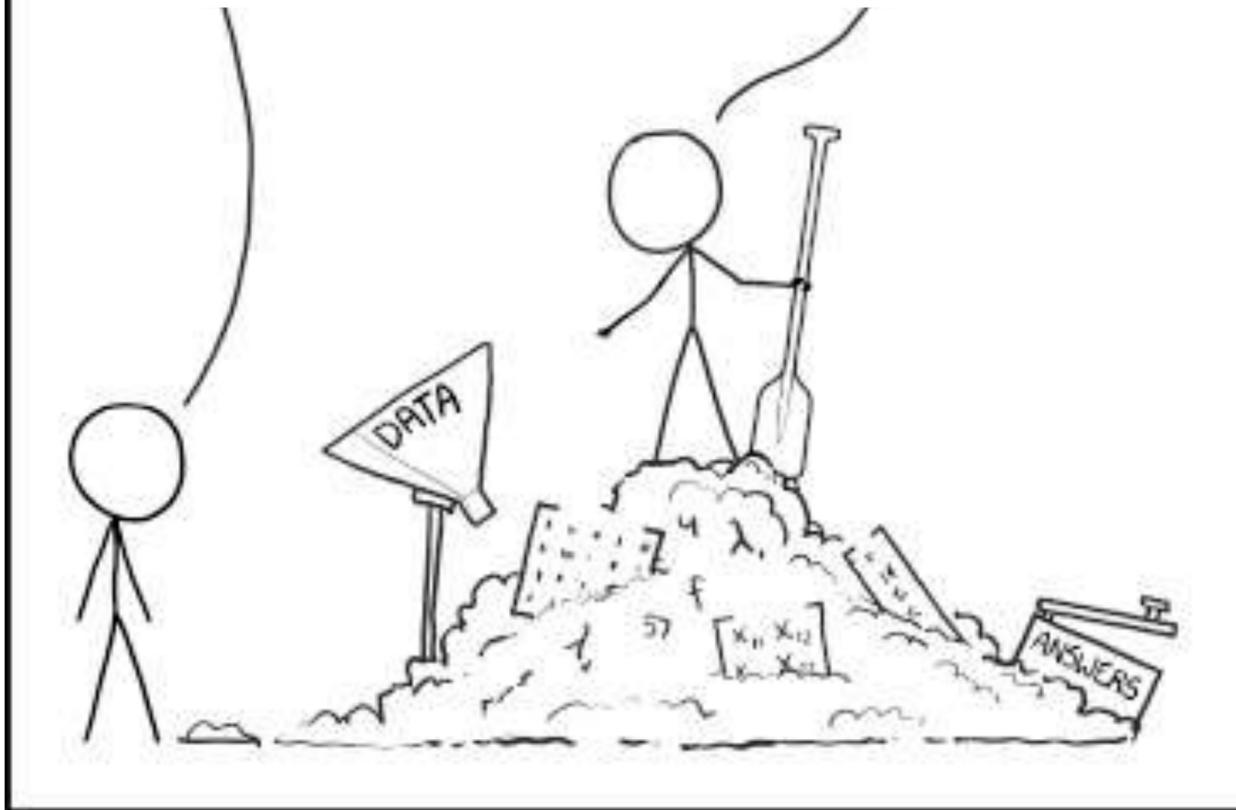
MLSS 2021

Interpretability

why, what and how to

Been Kim

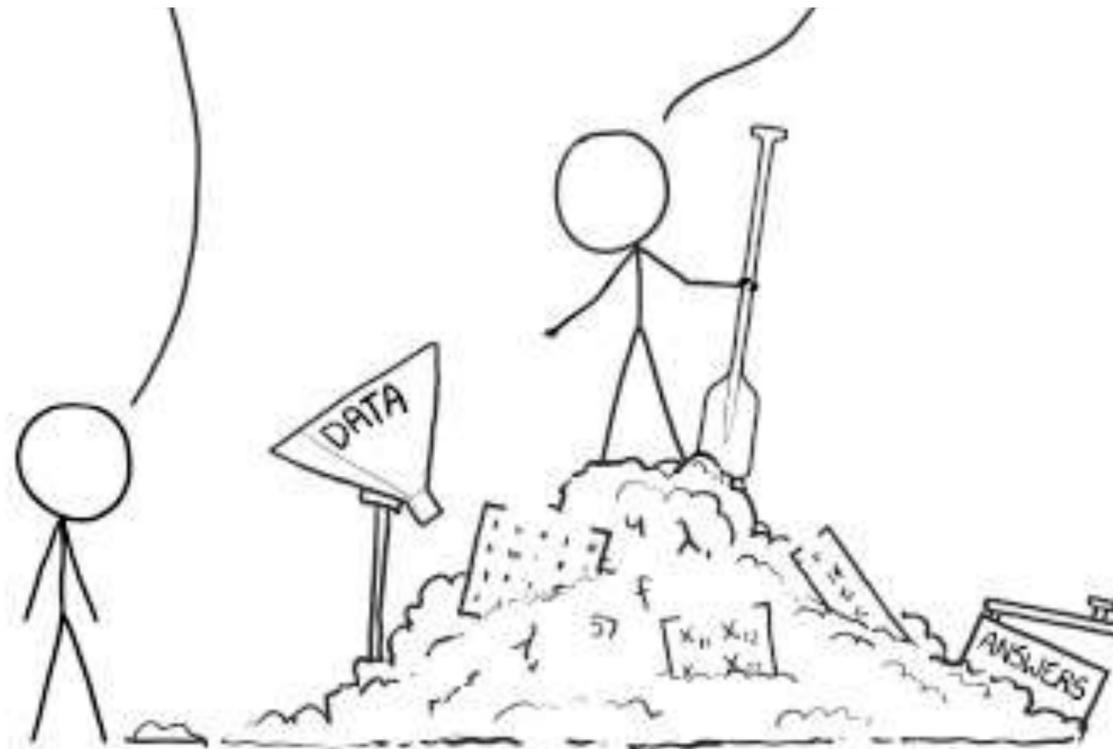
THIS IS YOUR MACHINE LEARNING SYSTEM?



<https://xkcd.com/>

THIS IS YOUR MACHINE LEARNING SYSTEM?

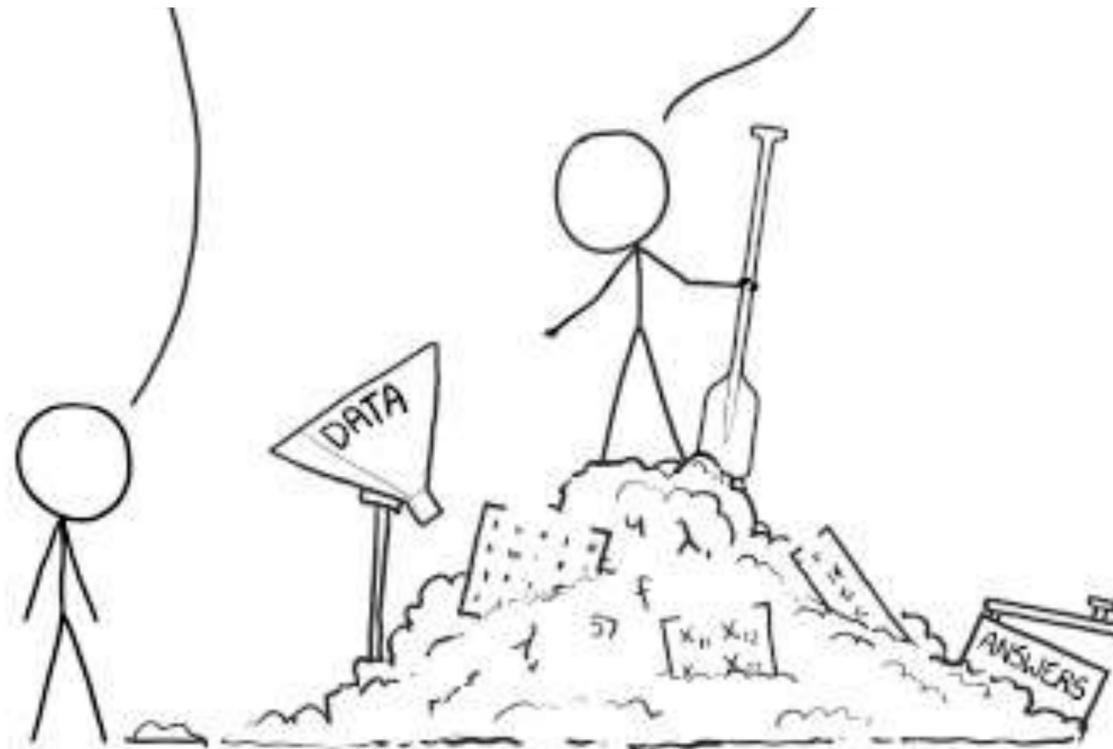
YUP! YOU POUR THE DATA INTO THIS BIG PILE OF LINEAR ALGEBRA, THEN COLLECT THE ANSWERS ON THE OTHER SIDE.



THIS IS YOUR MACHINE LEARNING SYSTEM?

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WHAT IF THE ANSWERS ARE WRONG?

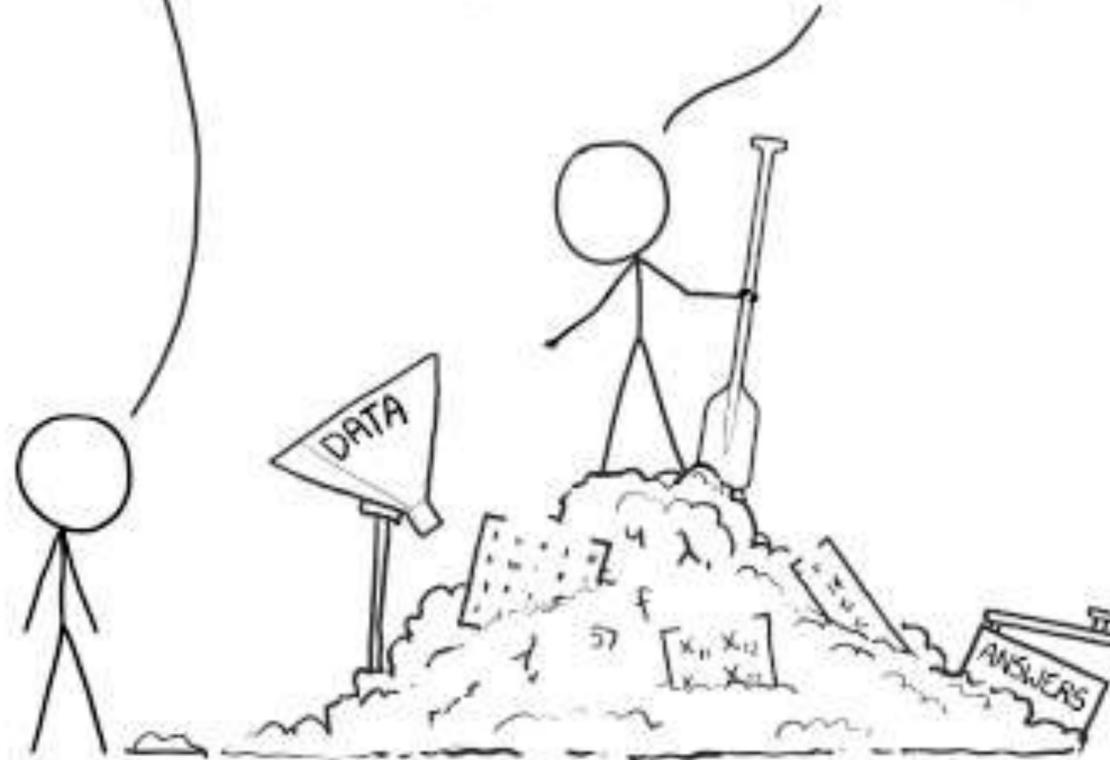


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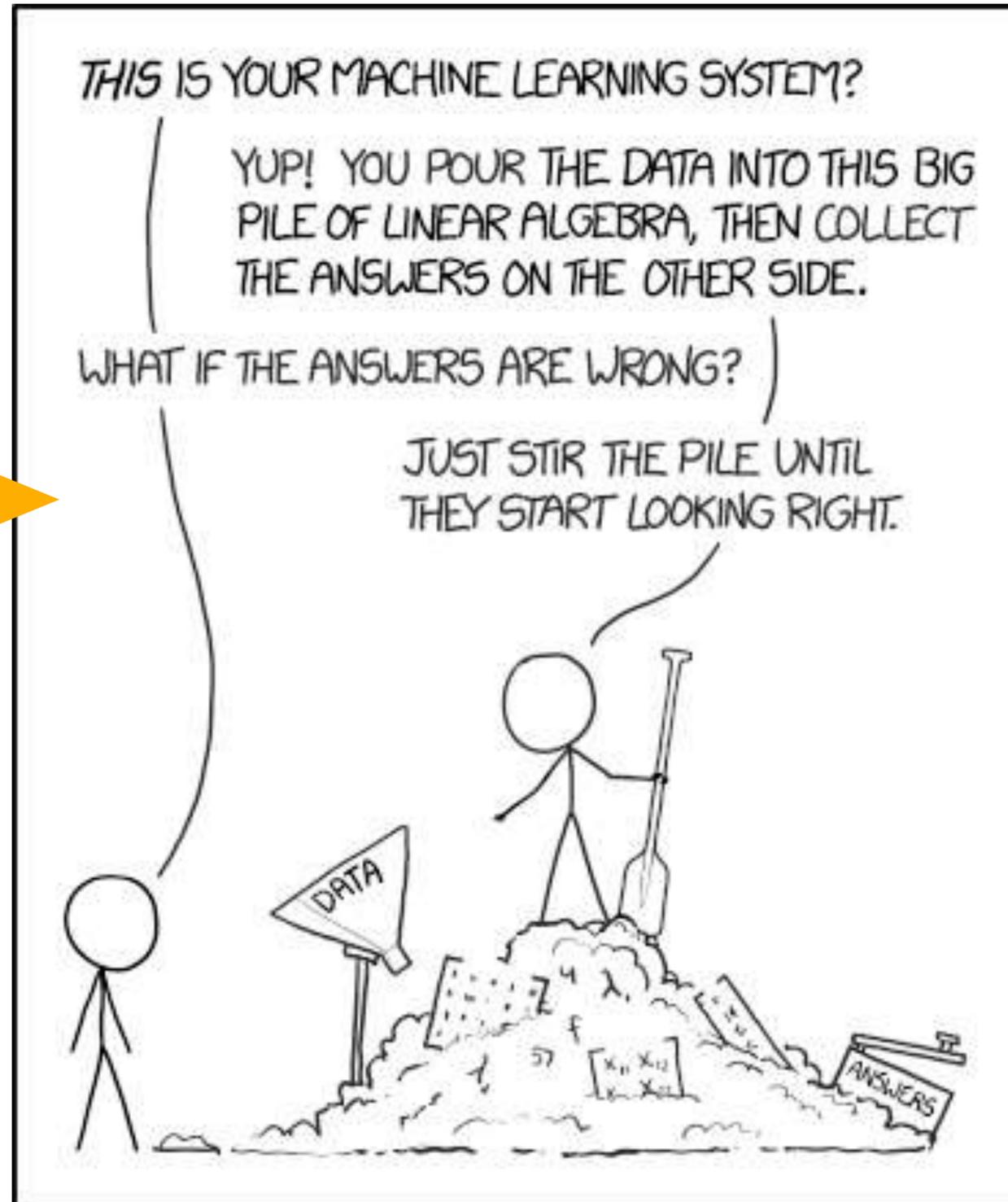
JUST STIR THE PILE UNTIL THEY START LOOKING RIGHT.



Oh no.



<https://www.youtube.com/watch?v=icqDxNab3Do>



<https://xkcd.com/>

For this reason, this tutorial won't be about list and lists of methods.

Focusing on more methods is not what we need.

Instead, it'll be about more Important things.



<https://xkcd.com/>

Agenda



- What and why



- !Caution!: Things to be careful when using and developing interpretability methods



- Evaluate: How to evaluate interpretability methods



- Methods: 3 types of methods and examples

Agenda



- What and why



- !Caution!: Things to be careful when using and developing interpretability methods



- Evaluate: How to evaluate interpretability methods



- Methods: 3 types of methods and examples

What do we mean by interpretability?

- In a dictionary (Merriam-Webster):
 - “to explain or to present in understandable terms”
- In ML (among many)
 - “ability to explain or to present in understandable terms to a human” [Doshi-Velez, K. 16]
 - “Interpretability is the degree to which a human can understand the cause of a decision.” [Miller 17]
- In cognitive science (among many)
 - “explanations are... the currency in which we exchanged beliefs” [Lombrozo 06]

Sure, but how do we make a working definition for my paper?

Operationalizing interpretability

- Define your desiderata - clearly specify what your definition is, and what you are optimizing.
- Do proper quantitative and qualitative evaluation with your end-task in mind - 'users like the explanation' says nothing (more on this later)

Real Time Image Saliency for Black Box Classifiers

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and Alan Turing Institute, London

- Smallest sufficient region (SSR) — smallest region of the image that alone allows a confident classification,
- Smallest destroying region (SDR) — smallest region of the image that when removed, prevents a confident classification.

Axiomatic Attribution for Deep Networks

Mukund Sundararajan *¹ Ankur Taly *¹ Qiqi Yan *¹

2. Two Fundamental Axioms

2.1. Axiom: Sensitivity(a)

An attribution method satisfies *Sensitivity(a)* if for every input and baseline that differ in one feature but have different predictions then the differing feature should be given a non-zero attribution. (Later in the paper, we will have a part (b) to this definition.)

2.2. Axiom: Implementation Invariance

Two networks are *functionally equivalent* if their outputs are equal for all inputs, despite having very different implementations. Attribution methods should satisfy *Implementation Invariance*, i.e., the attributions are always identical for two functionally equivalent networks. To motivate this

A Unified Approach to Interpreting Model Predictions

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3 Simple Properties Uniquely Determine Additive Feature Attributions

A surprising attribute of the class of additive feature attribution methods is the presence of a single unique solution in this class with three desirable properties (described below). While these properties are familiar to the classical Shapley value estimation methods, they were previously unknown for other additive feature attribution methods.

The first desirable property is *local accuracy*. When approximating the original model f for a specific input x , local accuracy requires the explanation model to at least match the output of f for the simplified input x' (which corresponds to the original input x).

Property 1 (Local accuracy)

$$f(x) = g(x') = \phi_0 + \sum_{i=1}^M \phi_i x'_i \quad (5)$$

The explanation model $g(x')$ matches the original model $f(x)$ when $x = h_x(x')$, where $\phi_0 = f(h_x(0))$ represents the model output with all simplified inputs toggled off (i.e. missing).

The second property is *missingness*. If the simplified inputs represent feature presence, then missingness requires features missing in the original input to have no impact. All of the methods described in Section 2 obey the missingness property.

Property 2 (Missingness)

$$x'_i = 0 \implies \phi_i = 0 \quad (6)$$

Missingness constrains features where $x'_i = 0$ to have no attributed impact.

The third property is *consistency*. Consistency states that if a model changes so that some simplified input's contribution increases or stays the same regardless of the other inputs, that input's attribution should not decrease.

Towards Automatic Concept-based Explanations

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2 Concept-based Explanation Desiderata

Our goal is to explain a machine learning model's decision making via units that are more understandable to humans than individual features, pixels, characters, and so forth. Following the literature [45, 20], throughout this work, we refer to these units as concepts. A precise definition of a concept is not easy [13]. Instead, we lay out the desired properties that a concept-based explanation of a machine learning model should satisfy to be understandable by humans.

1. **Meaningfulness** An example of a concept is semantically meaningful on its own. In the case of image data, for instance, individual pixels may not satisfy this property while a group of pixels (an image segment) containing a texture concept or an object part concept is meaningful. Meaningfulness should also correspond to different individuals associating similar meanings to the concept.
2. **Coherency** Examples of a concept should be perceptually similar to each other while being different from examples of other concepts. Examples of "black and white striped" concept are all similar in having black and white stripes.

On Completeness-aware Concept-Based Explanations in Deep Neural Networks

Chih-Kuan Yeh¹, Been Kim², Sercan Ö. Arık³, Chun-Liang Li³,
Tomas Pfister², and Pradeep Ravikumar¹

¹Machine Learning Department, Carnegie Mellon University
²Google Brain
³Google Cloud AI

ConceptSHAP: How important is each concept?

Given a set of concept vectors $C_S = \{c_1, c_2, \dots, c_m\}$ with a high completeness score, we would like to evaluate the importance of each individual concept by quantifying how much each individual concept contributes to the final completeness score. Let s_i denote the importance score for concept c_i , such that s_i quantifies how much of the completeness score $\eta(C_S)$ is contributed by c_i . Motivated by its successful applications in quantifying attributes of complex systems, we adapt Shapley values [12] to fairly assign the importance of each concept (which we call conceptSHAP):

Definition 4.1. Given a set of concepts $C_S = \{c_1, c_2, \dots, c_m\}$ and some completeness score η , we define the ConceptSHAP s_i for concept c_i as

$$s_i(\eta) = \sum_{S \subseteq C_S \setminus c_i} \frac{(m - |S| - 1)! |S|!}{m!} [\eta(S \cup \{c_i\}) - \eta(S)],$$

The main benefit of Shapley for importance scoring is that it uniquely satisfies the set of desired axioms: efficiency, symmetry, dummy, and additivity [12], which are listed in the following proposition with modification to our setting:

Proposition 4.1. Given a set of concepts $C_S = \{c_1, c_2, \dots, c_m\}$ and a completeness score η , and some importance score for each concept c_i that depends on the completeness score η , s_i defined by conceptSHAP is the unique importance assignment that satisfy the following four axioms:

- **Efficiency:** The sum of all importance value should sum up to the total completeness score, $\sum_{i=1}^m s_i(\eta) = \eta(C_S)$.
- **Symmetry:** For two concepts that are equivalent, i.e. $\eta(u \cup \{c_i\}) = \eta(u \cup \{c_j\})$ for every subset $u \subseteq C_S \setminus \{c_i, c_j\}$, $s_i(\eta) = s_j(\eta)$.
- **Dummy:** If $\eta(u \cup \{c_i\}) = \eta(u)$ for every subset $u \subseteq C_S \setminus \{c_i\}$, then $s_i(\eta) = 0$.
- **Additivity:** If η and η' have importance value $s(\eta)$ and $s(\eta')$ respectively, then the importance value of

and many more!

Is interpretability possible at all?

DAVID WEINBERGER [BACKCHANNEL](#) 04.18.17 08:22 PM

OUR MACHINES NOW HAVE KNOWLEDGE WE'LL NEVER UNDERSTAND

SHARE



The new availability of huge amounts of data, along with the statistical tools to crunch these numbers, offers a whole new way of understanding the world. Correlation supersedes causation, and science can advance even without coherent models, unified theories, or really any mechanistic explanation at all.

So wrote *Wired's* [Chris Anderson](#) in 2008. It kicked up a

Is interpretability possible at all?

DAVID WEINBERGER BACKCHANNEL 04.18.17 08:22 PM

OUR MACHINES NOW HAVE KNOWLEDGE WE'LL

Take away:

We don't need to understand every single thing about the model.

of understanding the world. Correlation supersedes causation, and science can advance even without coherent models, unified

Key Point:

Interpretability is NOT about understanding all bits and bytes of the model for all data points.

It is about knowing enough for your goals/downstream tasks.

How much is enough?

- What does it mean “the system is fair enough”?
- This hammer isn't perfect, but it's “good enough”



How much is enough?

- What does it mean “the system is fair enough”?
➔ [for what we are trying to do]
- This hammer isn’t perfect, but it’s “good enough”
➔ [for what we are trying to do]



How much is enough?

- What does it mean “the system is fair enough”?
➔ [for what we are trying to do]
- This hammer isn’t perfect, but it’s “good enough”
➔ [for what we are trying to do]

I’m better off having this tool
for [my goal].



What is the goal?

- End-task metric!
- Everyone's goals are different, but mine is generally:
 - Tools to help people use ML more effectively and responsibly such that
 1. our values are respected
 2. human knowledge is reflected when appropriate

What is the goal?

- End-task metric!
- Everyone's goals are different, but mine is generally:
 - Tools to help  everyone people use ML more effectively and responsibly such that
 1. our values are respected
 2. human knowledge is reflected when appropriate

Non-goals

Interpretability is NOT...

- about making ALL models interpretable.
- about understanding EVERY SINGLE BIT about the model
- against developing highly complex models.
- only about gaining user trust or fairness

Non-goals

Interpretability is NOT...

- about making ALL models
- about understanding EV
- against developing high
- only about gaining user



npj | Digital Medicine

Article | OPEN | Published: 30 April 2019

Deep learning predicts hip fracture using confounding patient and healthcare variables

Marcus A. Badgeley, John R. Zech, Luke Oakden-Rayner, Benjamin S. Glicksberg, Manway Liu, William Gale, Michael V. McConnell, Bethany Percha, Thomas M. Snyder & Joel T. Dudley 

npj Digital Medicine 2, Article number: 31 (2019) | [Download Citation](#) 

Take away:

Helping people to distrust the model is often more important than helping to trust it.

Interpretability is not a new problem. Why now?

- Prevalence: It's everywhere, and used to make potentially life changing decisions.
- Complexity: layers and layers of models of models



When do you need interpretability?

Fundamental *underspecification* in the problem

Humans often don't know exactly what they want.

When do you need interpretability?

example1: Safety



example 2: Science



Fundamental **underspecification** in the problem

example3: mismatched objectives



When do you need interpretability?

example1: Safety



example 2: Science



Fundamental **underspecification** in the problem

example3: mismatched objectives

Take away:

More data or more clever algorithm will not solve interpretability.

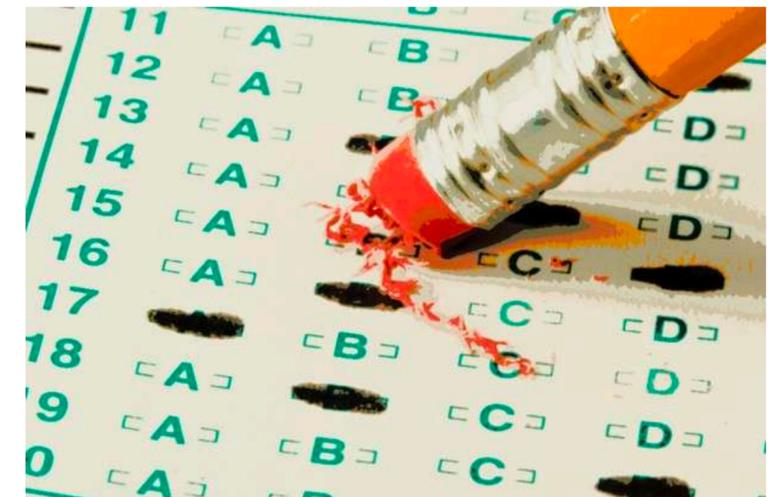
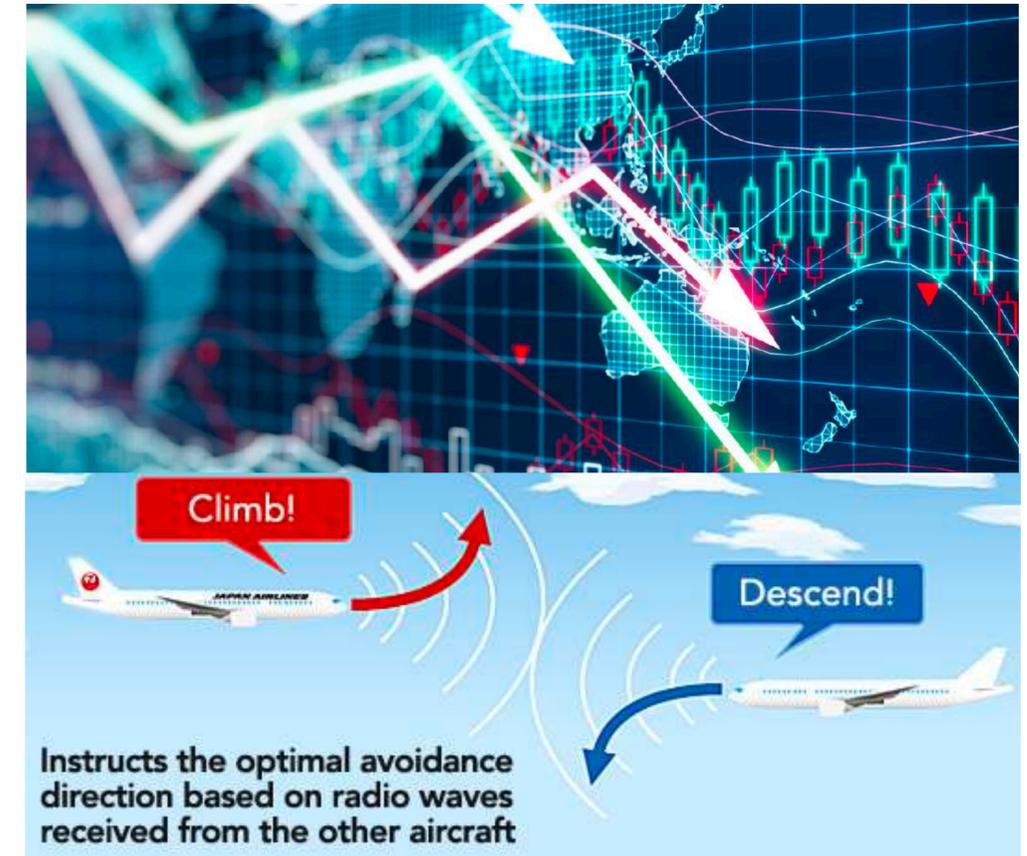
Wait, then what is NOT underspecification?



<https://www.pinterest.com/dowd3128/type-o-negative/>

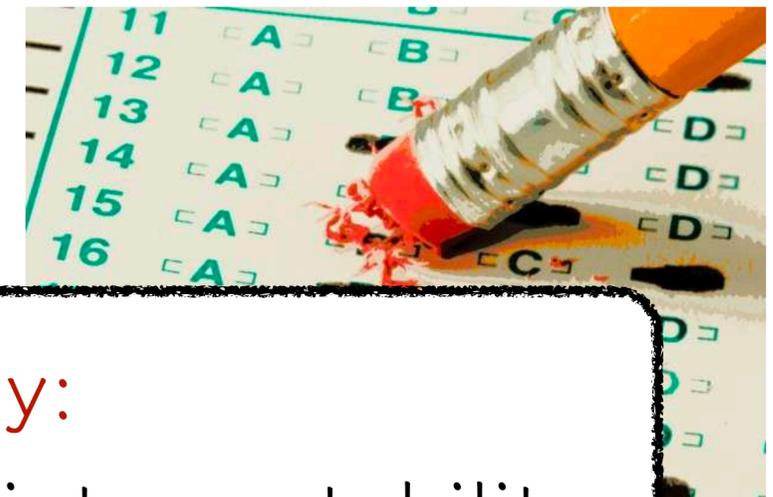
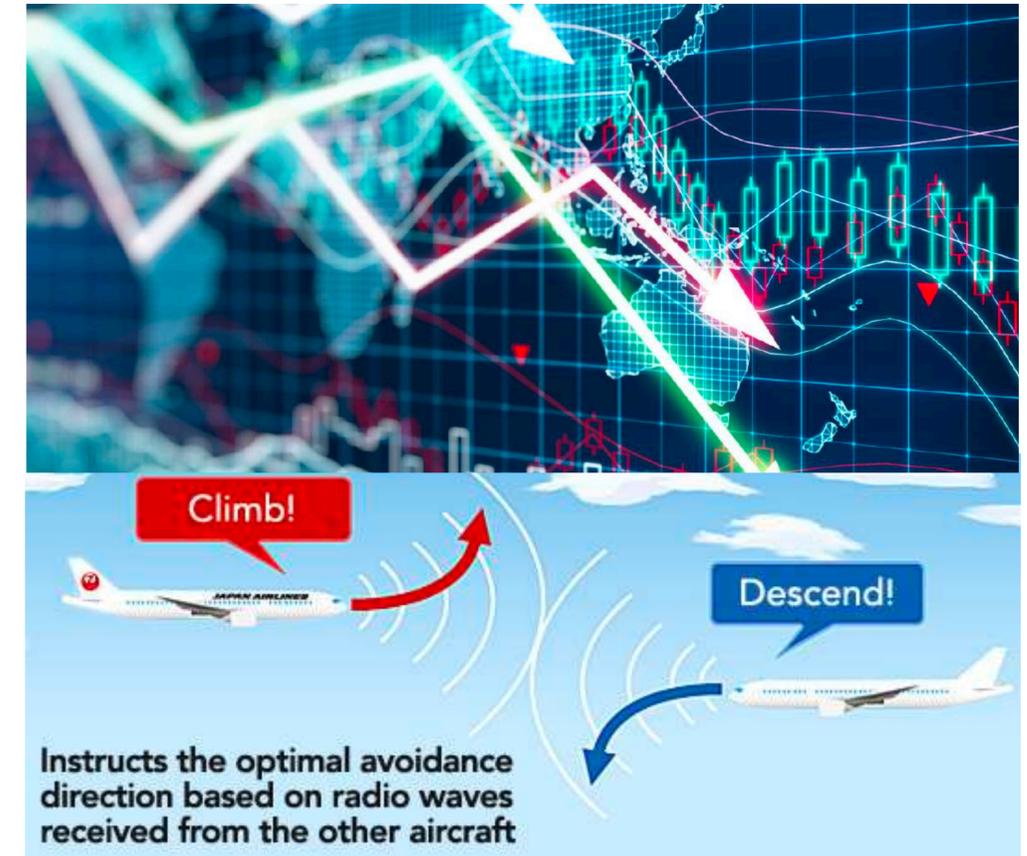
When we may not need/want interpretability

- No significant consequences. Prediction is what everyone cares.
- Sufficiently well-studied problem with abundance of empirical evidence
- People might game the system (example of mismatched objectives)



When we may not need/want interpretability

- No significant consequences. Prediction is what everyone cares.
- Sufficiently well-studied problem with abundance of empirical evidence
- People might game the system (example of mismatched objectives)



Take away:
We don't always need interpretability.

But certainly, there will be performance trade-off, right?

- “It is a myth that there is necessarily a trade-off between accuracy and interpretability.” [Rudin 19]
- Carefully building structure in the model (e.g., architecture, prior, loss function) has long been done to increase performance with or without interpretability in mind.

True that.

Here are a small subset of vast amount of evidence by many researchers.

Take away:

Interpretability and performance trade-off often don't exist.

[1] Finale Doshi-Velez, Byron Wallace, and Ryan Adams. Graph-sparse l₁: a topic model with structured sparsity. Association for the Advancement of Artificial Intelligence, 2015.

[2] Maya Gupta, Andrew Cotter, Jan Pfeifer, Konstantin Voevodski, Kevin Canini, Alexander Mangylov, Wojciech Moczydlowski, and Alexander Van Esbroeck. Monotonic calibrated interpolated look-up tables. Journal of Machine Learning Research, 2016

[3] Himabindu Lakkaraju, Stephen H Bach, and Jure Leskovec. Interpretable decision sets: A joint framework for description and prediction. In Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, pages 1675–1684. ACM, 2016

[4] Been Kim, Julie Shah, and Finale Doshi-Velez. Mind the gap: A generative approach to interpretable feature selection and extraction. In Advances in Neural Information Processing Systems, 2015b

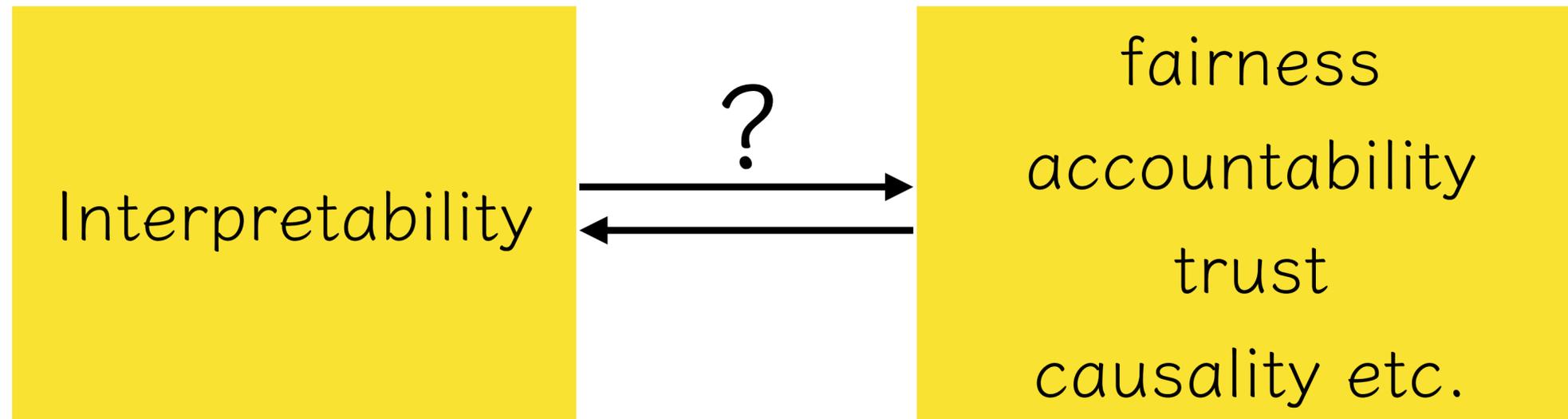
[5] Lou Y, Caruana R, Gehrke J, Hooker G. Accurate Intelligible Models with Pairwise Interactions. In: Proceedings of 19th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD). ACM; 2013.

[6] Rudin C, Passonneau R, Radeva A, Dutta H, Jerome S, Isaac D. A Process for Predicting Manhole Events In Manhattan. Machine Learning. 2010;80:1–31.

[7] Rudin C, Ustun B. Optimized Scoring Systems: Toward Trust in Machine Learning for Healthcare and Criminal Justice. Interfaces. 2018;48:399–486. Special Issue: 2017 Daniel H. Wagner Prize for Excellence in Operations Research Practice September-October 2018.

[8] Chen C, Lin K, Rudin C, Shaposhnik Y, Wang S, Wang T. An Interpretable Model with Globally Consistent Explanations for Credit Risk. In: Proceedings of NeurIPS 2018 Workshop on Challenges and Opportunities for AI in Financial Services: the Impact of Fairness, Explainability, Accuracy, and Privacy; 2018.

What about our cousins?



What about our cousins?

Interpretability

fairness
accountability
trust
causality etc.

Take away:

Trust, fairness and interpretability are not
the same thing.

What about our cousins?

Interpretability

fairness
accountability
trust
causality etc.

- Interpretability may help with them when we cannot formalize these ideas
- But once formalized, you may not need interpretability.

Agenda



- What and why



- !Caution!: Things to be careful when using and developing interpretability methods

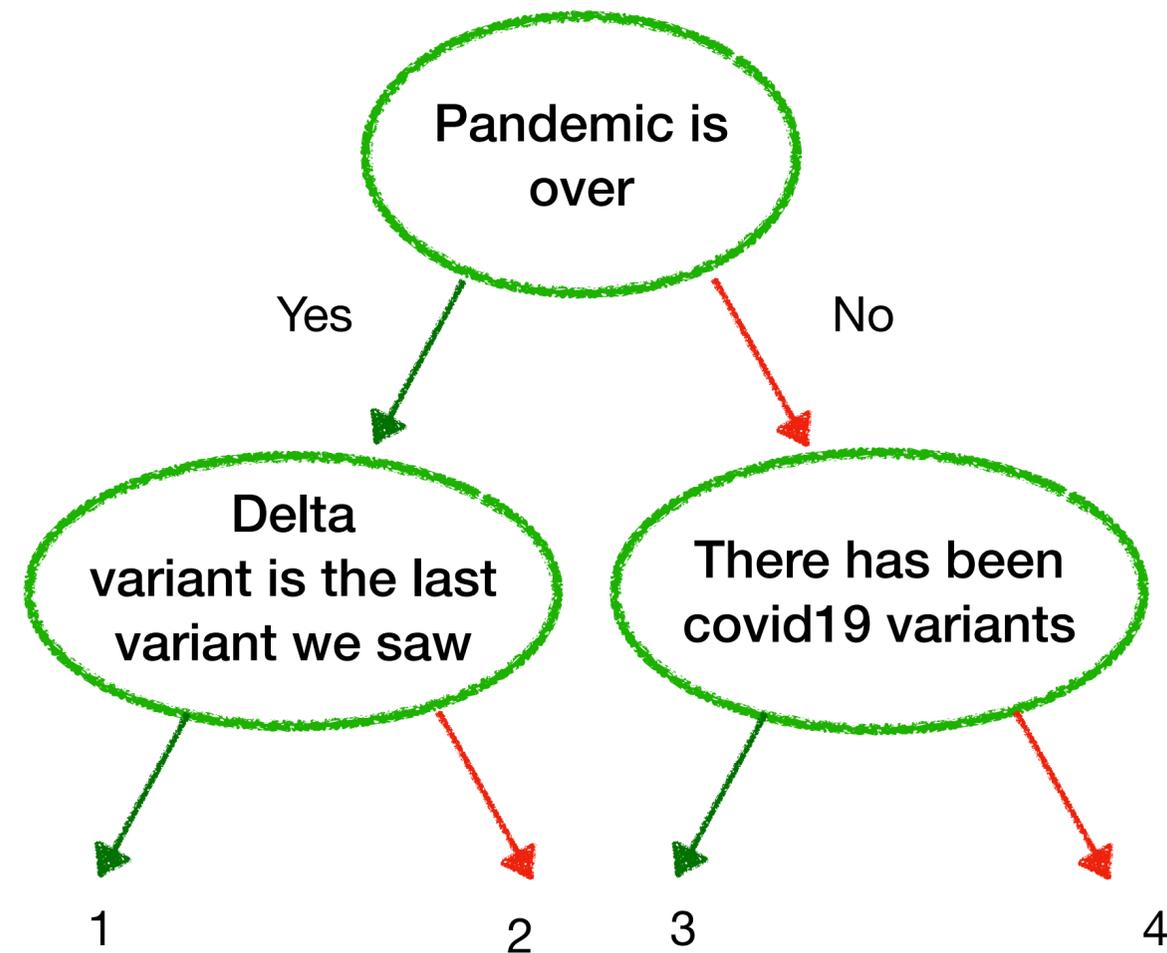


- Evaluate: How to evaluate interpretability methods

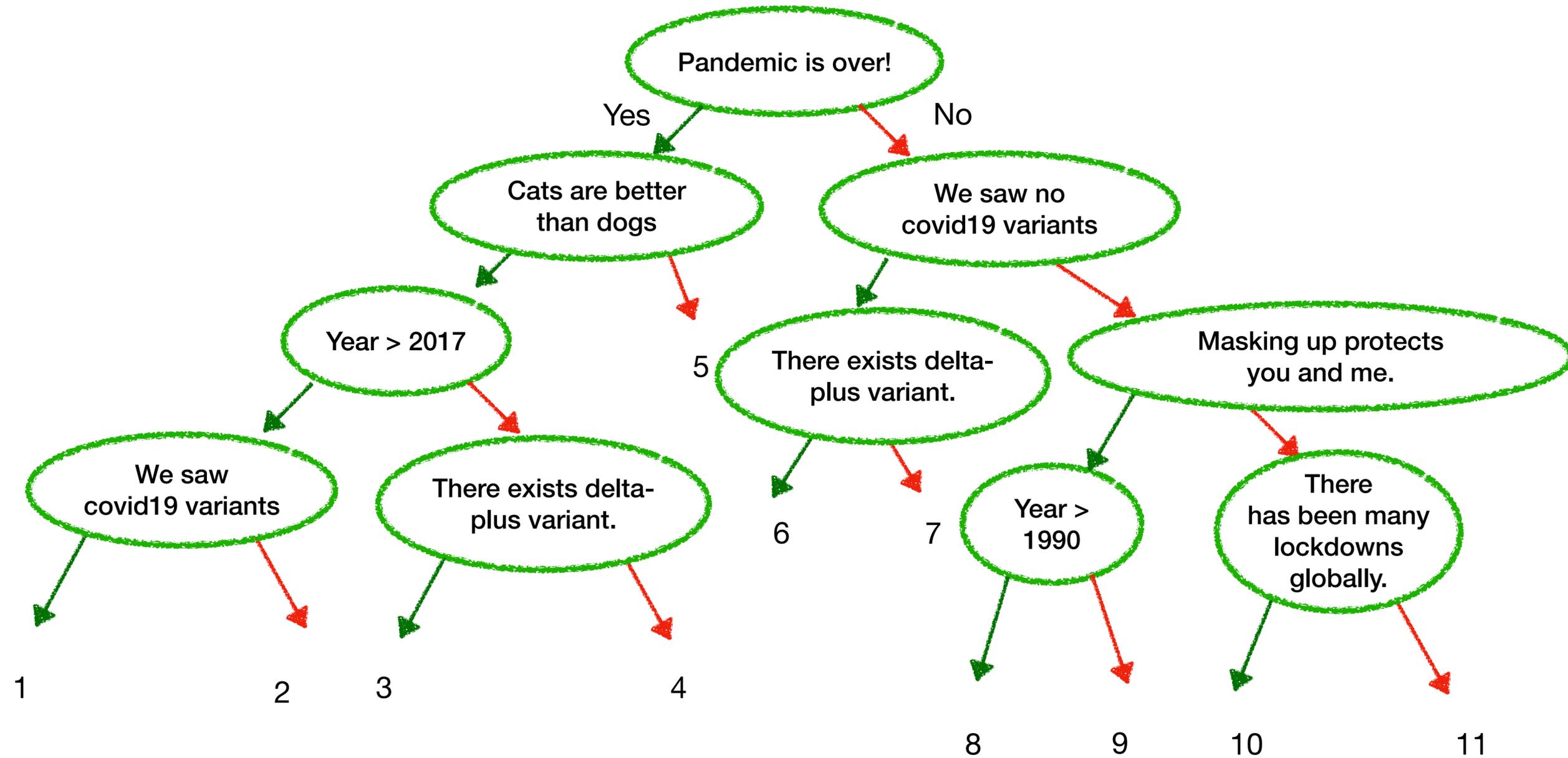


- Methods: 3 types of methods and examples

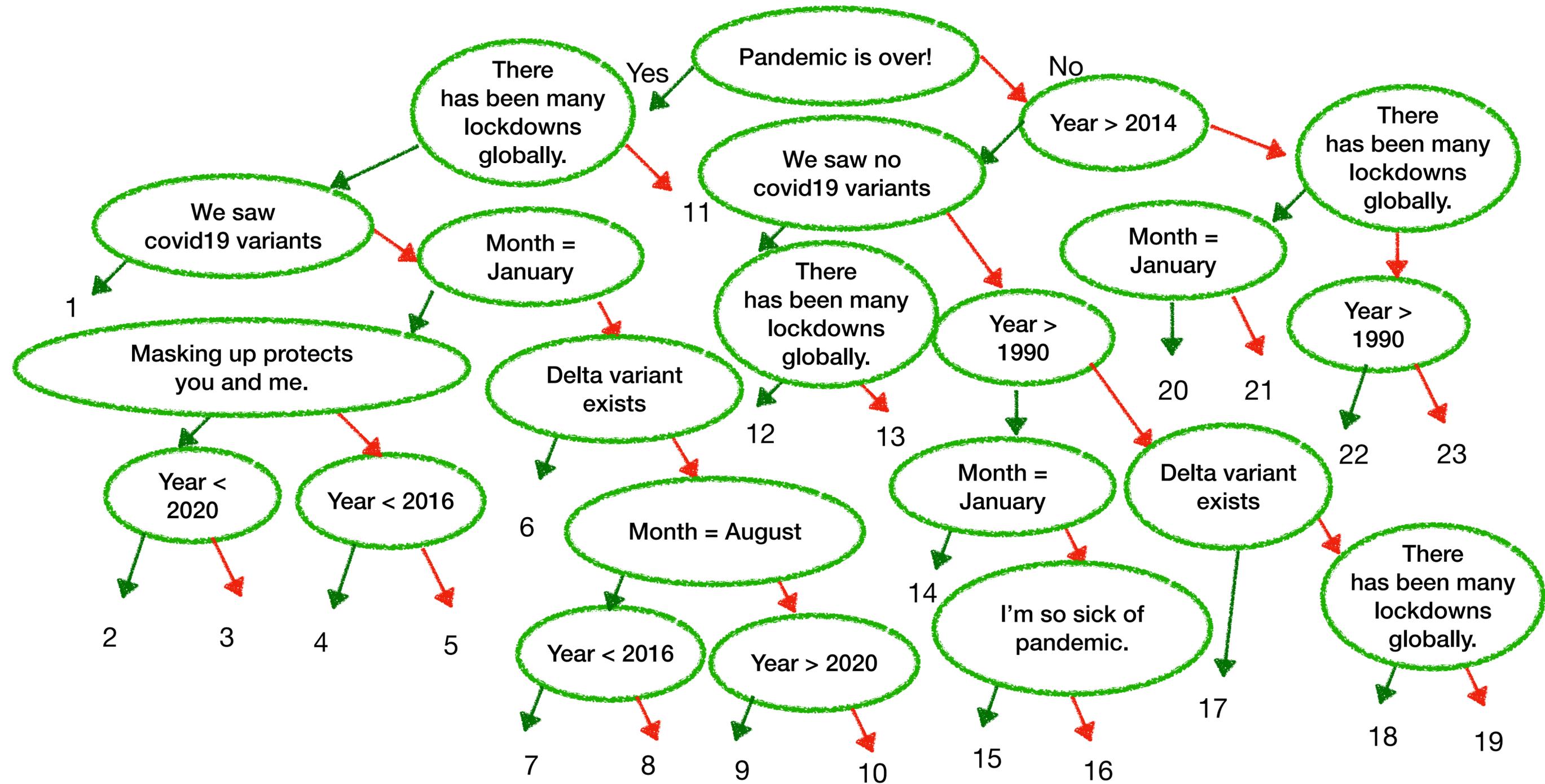
Sample decision tree #1



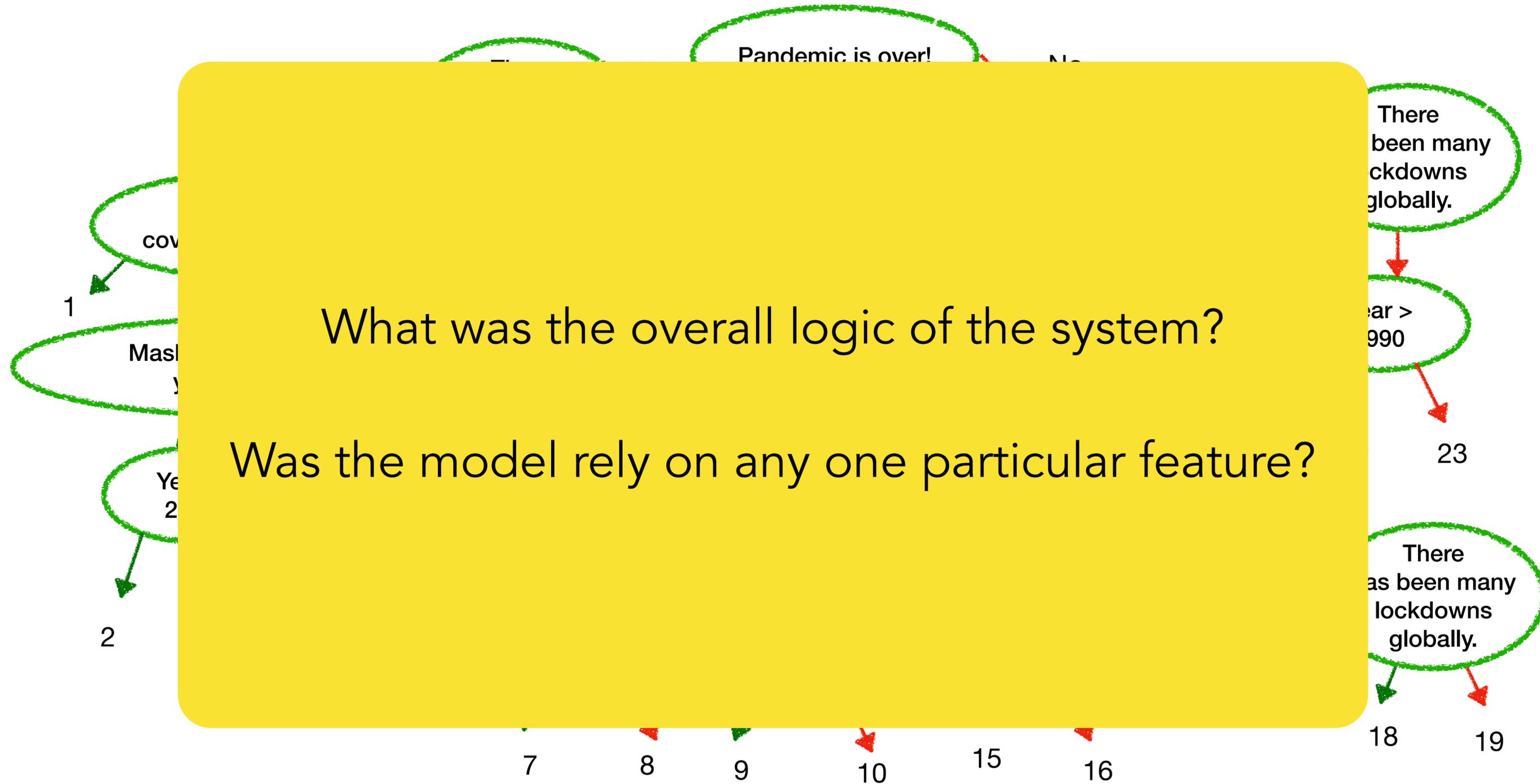
Sample decision tree #2



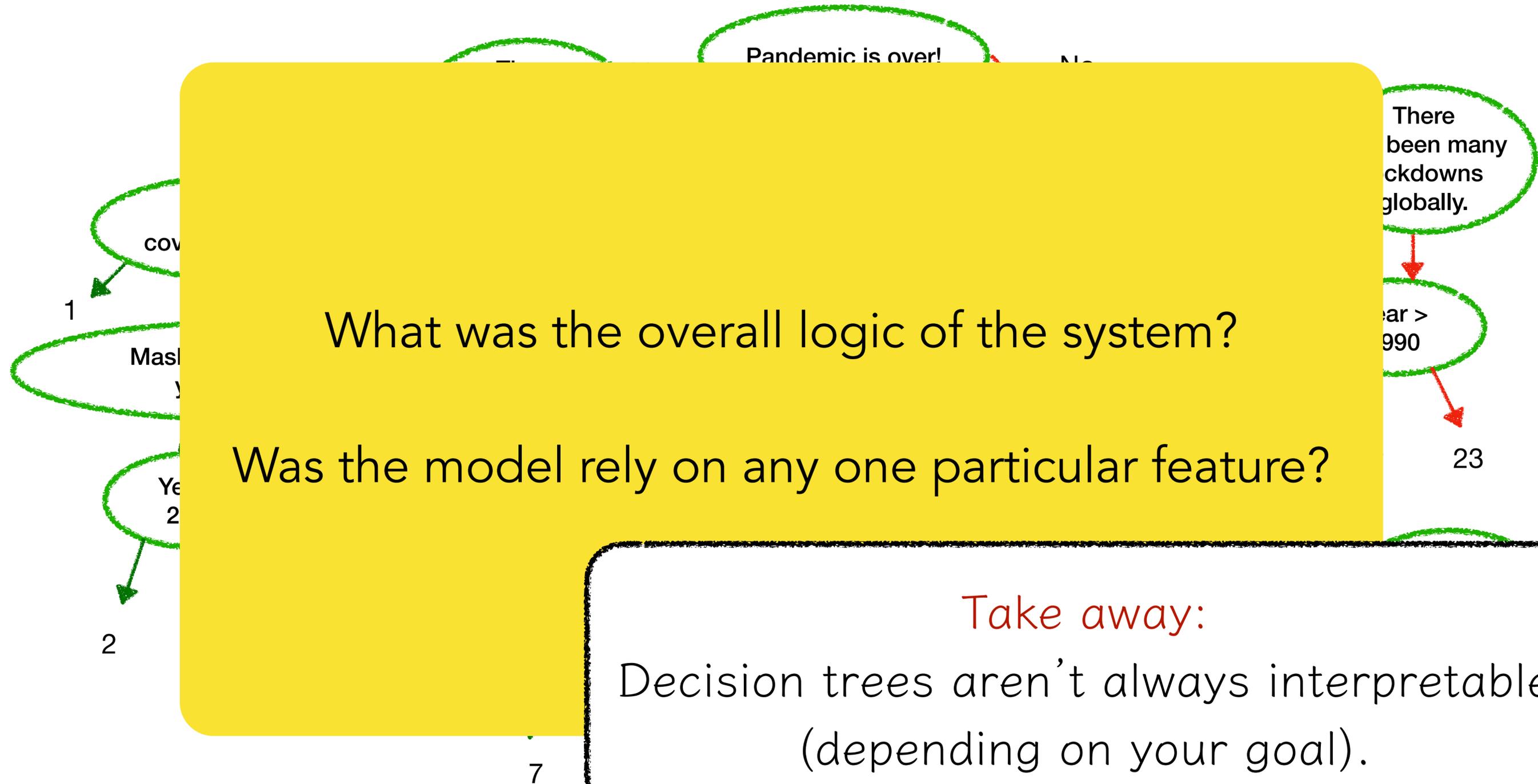
Sample decision tree #3



Sample decision tree #3



Sample decision tree #3



Do we need a different model?

How about rule lists?

If (sunny and hot)	then	go swim
Else if (sunny and cold)	then	go ski
Else	then	go work

Do we need a different model?

How about rule lists?

If (sunny and hot)	then	go swim
Else if (sunny and cold)	then	go ski
Else if (wet and weekday)	then	go work
Else if (free coffee)	then	attend tutorial
Else if (cloudy and hot)	then	go swim
Else if (snowing)	then	go ski
Else if (New Rick and Morty)	then	watch TV
Else if (paper deadline)	then	go work
Else if (hungry)	then	go eat
Else if (tired)	then	watch TV
Else if (advisor might come)	then	go work
Else if (code running)	then	watch TV
Else	then	go work

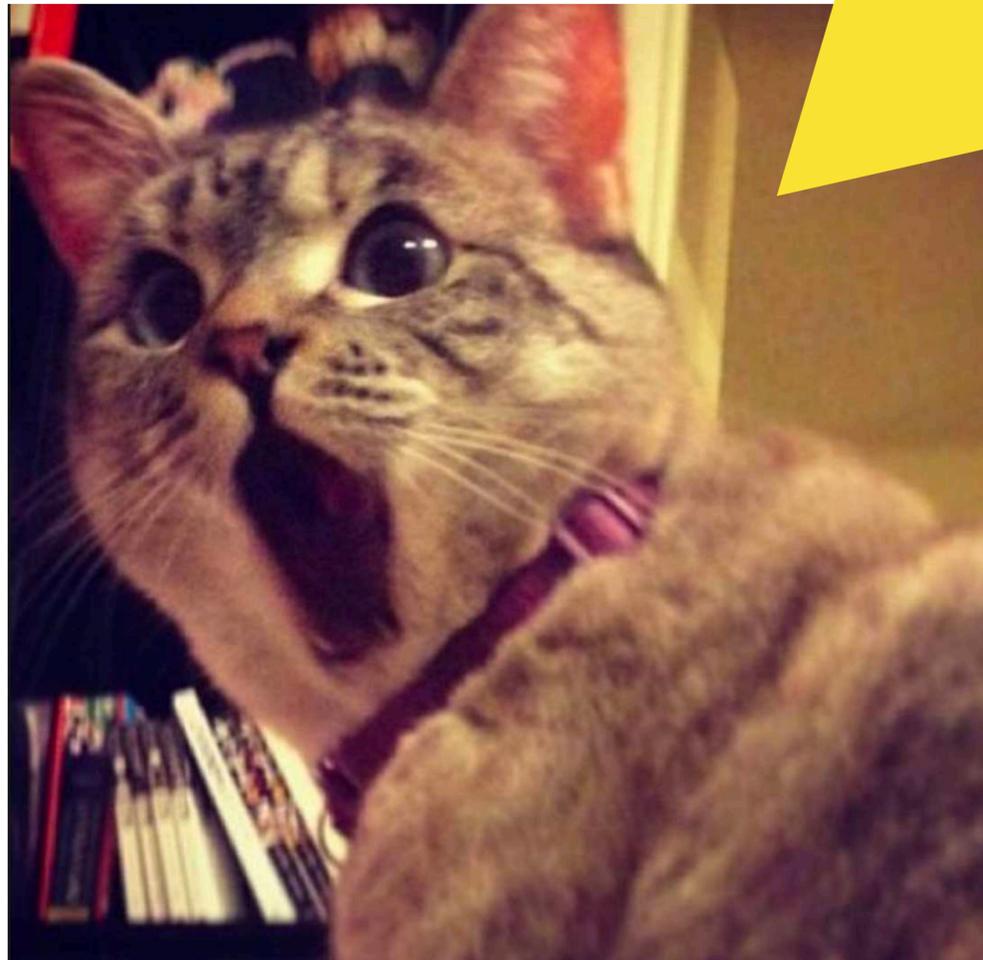
Maybe rule sets are better?

IF (sunny and hot) OR (cloudy and hot) OR
(sunny and thirsty and bored)
THEN go to beach
ELSE work

Maybe rule sets are better?

IF (sunny and hot) OR (cloudy and hot) OR
(sunny and thirsty and bored) OR (bored and
tired) OR (thirsty and tired) OR (code running)
OR (friends away and bored) OR (sunny and
want to swim) OR (sunny and friends visiting)
OR (need exercise) OR (want to build castles)
OR (sunny and bored) OR (done with deadline
and hot) OR (need vitamin D and sunny) OR
(just feel like it)
THEN go to beach
ELSE work

Are you saying decision trees, rule lists and rule sets don't work?!



Decision trees, rule lists or rule sets may work for your application!

The point here is that there is no one-size-fits-all method.

<http://blog.xfree.hu/myblog.tvn?SID=&from=20&pid=&pev=2016&pho=02&pnap=&kat=1083&searchkey=&hol=&n=sarkadykati>



Linear classifiers are interpretable, right?
So why not just fit locally linear functions everywhere?

Linear models are not always interpretable

- Can human interpret a linear model with many features, each with a floating number (normalized): e.g., feature 1 weighted 0.1, ... feature 134 weighted 0.05, feature 201 weighted 0.8..
- “Probability distortion is that people generally do not look at the value of probability uniformly between 0 and 1. Lower probability is said to be over-weighted while medium to high probability is under-weighted” - Kahneman



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Take away:
Using linear model isn't always the answer.





Causality should be the one and only methods for interpretability, right?

Pursuing causality is great, but it's not always simple

- It is one of the areas of huge importance, no doubt about that!
- But (currently) it often comes with a lot of assumptions (e.g., no hidden confounders) that starts to matter for high dimensional real-world applications.
- “Without causality, explanation is meaningless” -> I'd rather have useful, well-validated explanation than nothing at all for high stake applications.

A very intuitive (and funny) tutorial on causal inference!

<https://matheusfacure.github.io/>



Causal Inference for the Brave and True

Search this book...

Causal Inference for The Brave and True

PART I - THE YANG

01 - Introduction To Causality

02 - Randomised Experiments

03 - Stats Review: The Most Dangerous Equation

04 - Graphical Causal Models

05 - The Unreasonable Effectiveness of Linear Regression

06 - Grouped and Dummy Regression

07 - Beyond Confounders

08 - Instrumental Variables

Causal Inference for The Brave and True

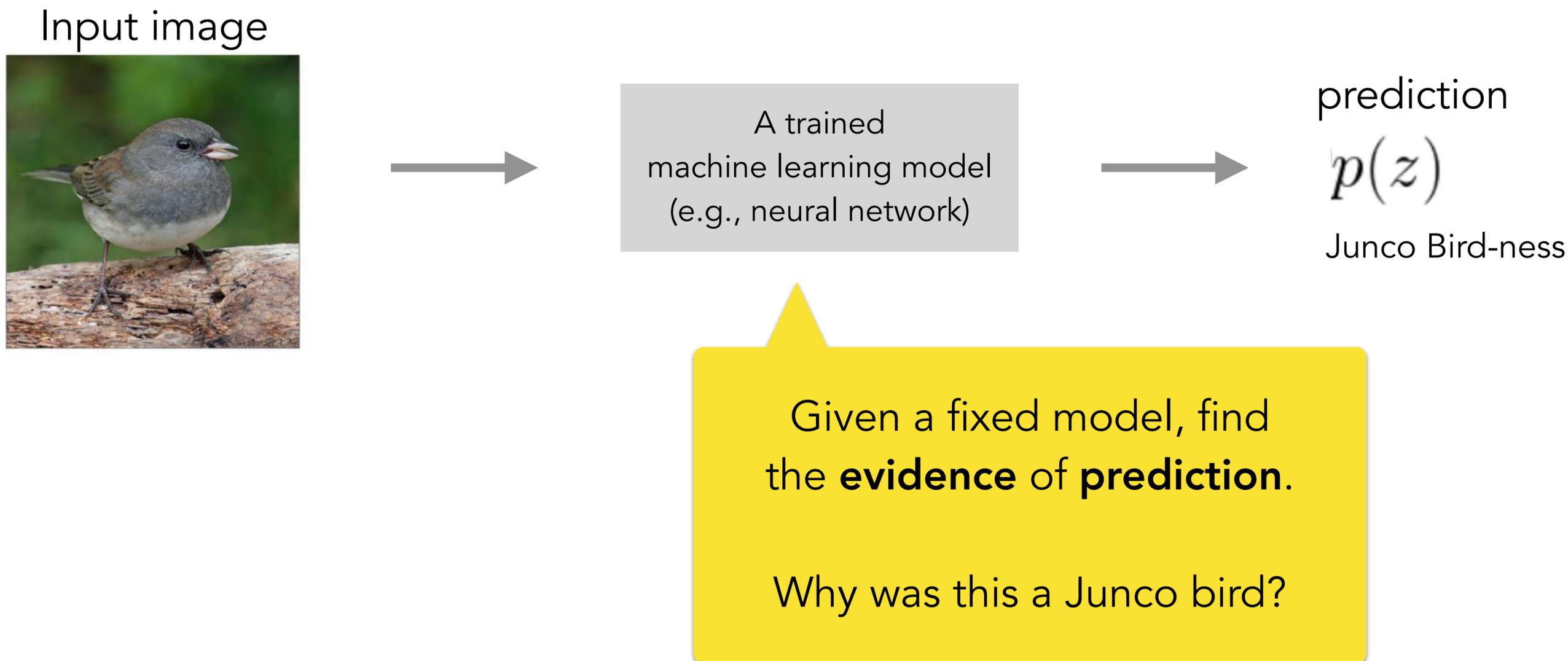


A light-hearted yet rigorous approach to learning impact estimation and sensitivity analysis. Everything in Python and with

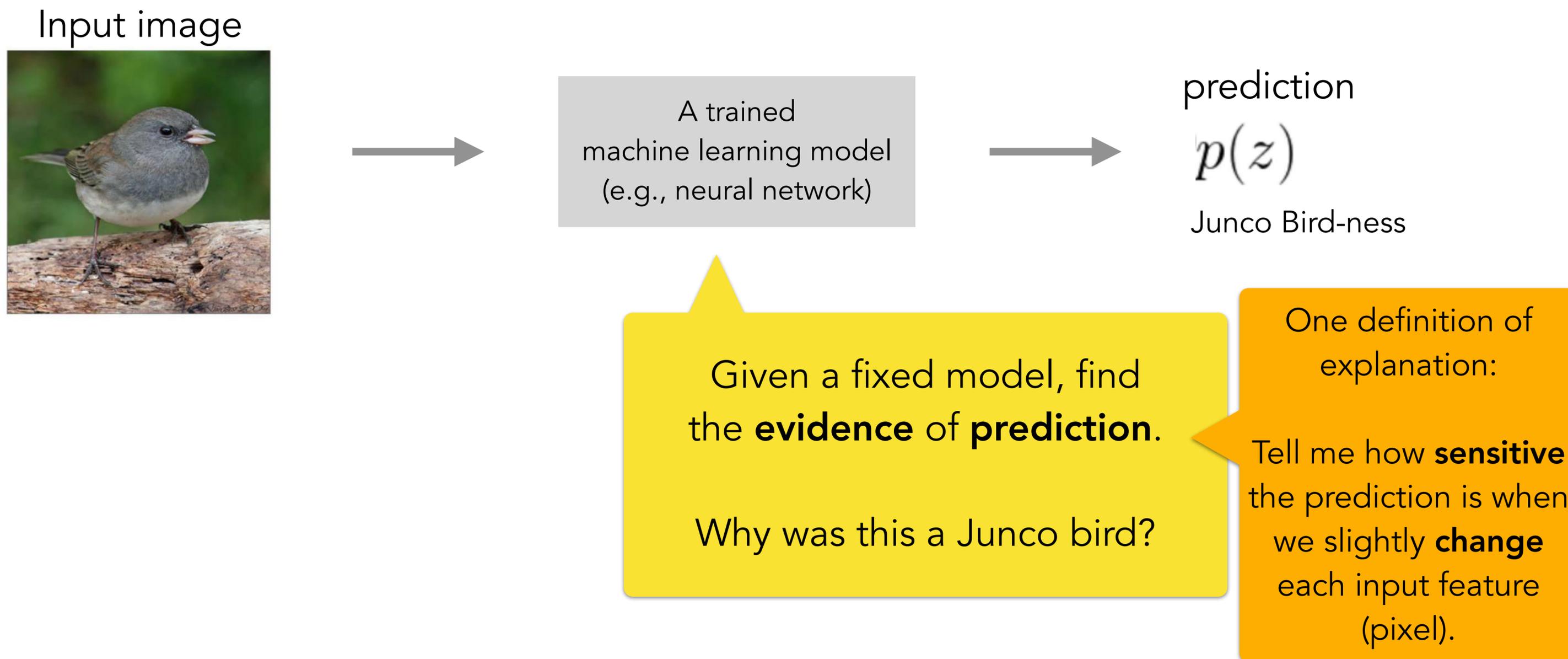


So once we have an explanation, that IS how the model thinks, right?

Some explanation methods fails a simple sanity check.



Some explanation methods fails a simple sanity check.



One of the most popular interpretability methods for images:

Saliency maps

Input image



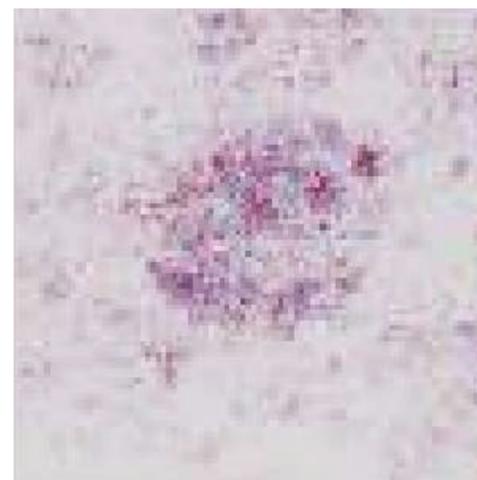
A trained
machine learning model
(e.g., neural network)



prediction

$p(z)$

Junco Bird-ness



In jargon: take derivative of the prediction wrt each pixel.

$$\begin{aligned} \text{a logit} &\rightarrow \frac{\partial p(z)}{\partial x_{i,j}} \\ \text{pixel } i,j &\rightarrow \end{aligned}$$

In English: take one pixel in the image, and imagine changing it by a little. See how much prediction changes. Do this for all pixels.

One definition of
explanation:

Tell me how **sensitive**
the prediction is when
we slightly **change**
each input feature
(pixel).

One of the most popular interpretability methods for images:

Saliency maps

Input image



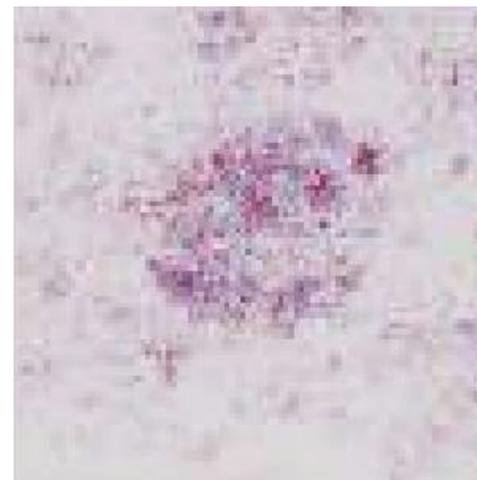
A trained
machine learning model
(e.g., neural network)



prediction

$p(z)$

Junco Bird-ness



Popular method #1



Popular method #2



My work from 2018 #1



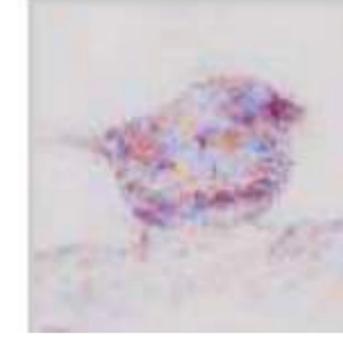
My work from 2018 #2



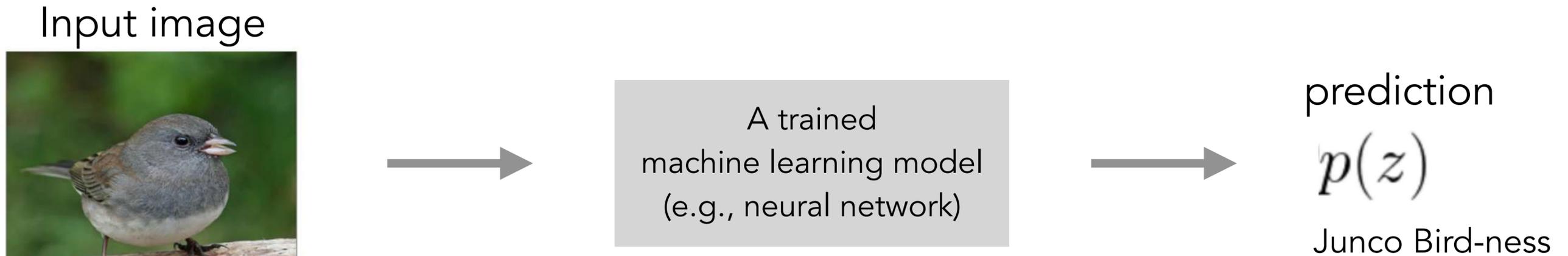
Popular method #3



Popular method #4



A sanity check question:



So these pixels are the **evidence** of **prediction**.

$g(\text{prediction}) = \text{explanation}$

When **prediction** changes, the explanations will probably change.

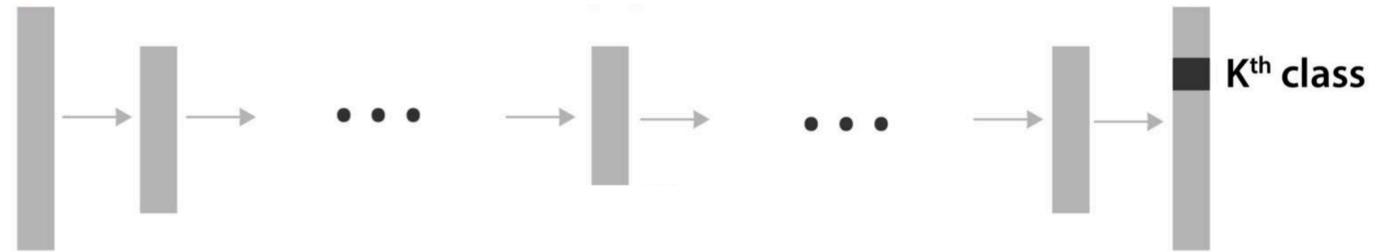
$g(\text{prediction}') = \text{explanation}'$

When **prediction** is random, the explanations really should change!

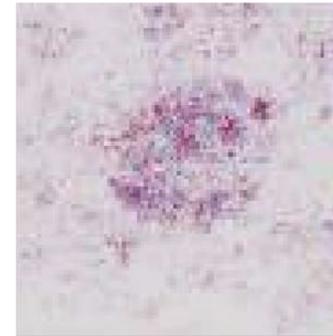
$g(\text{random}) \neq \text{explanation} ?$

A sanity check results

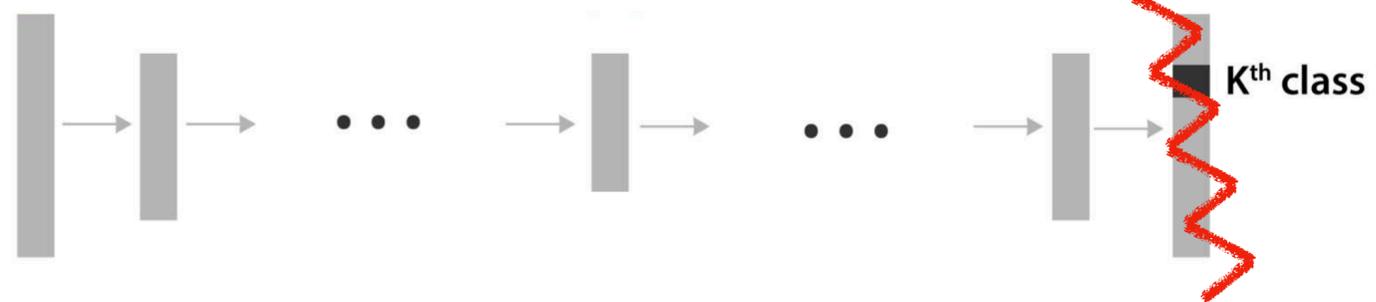
Original Image



Saliency map



Original Image



Randomized weights!
Network now makes garbage prediction.

!!!!????!?



A sanity check results

Input image



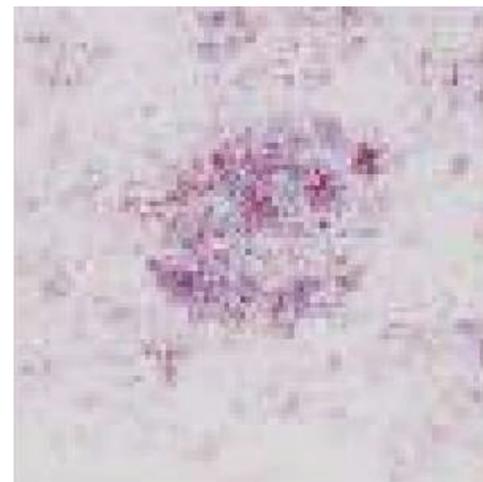
A trained
machine learning model
(e.g., neural network)



prediction

$p(z)$

Junco Bird-ness



Popular method #1



Popular method #2



My work from 2018 #1



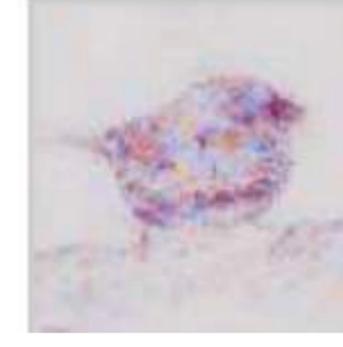
My work from 2018 #2



Popular method #3

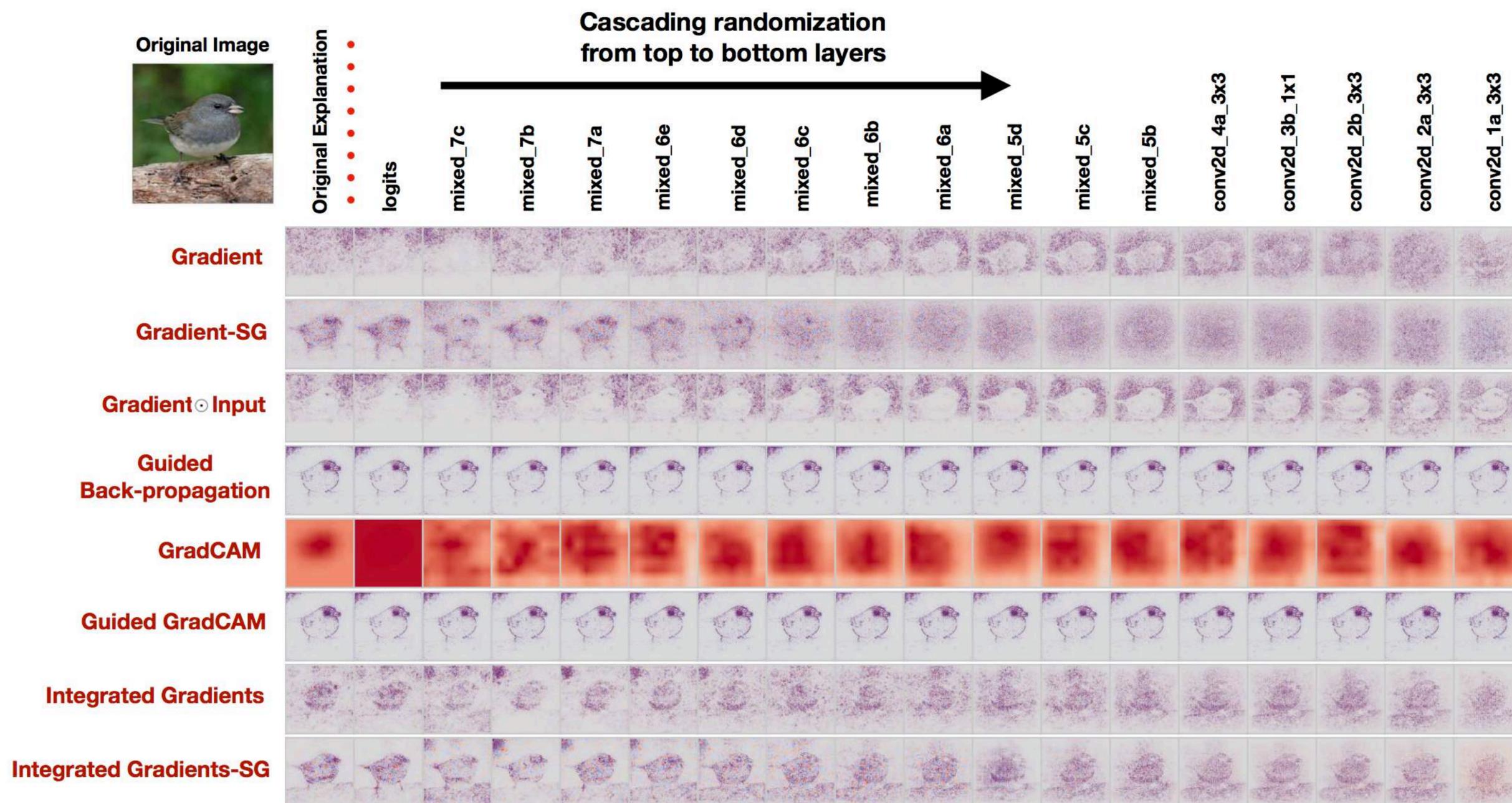


Popular method #4



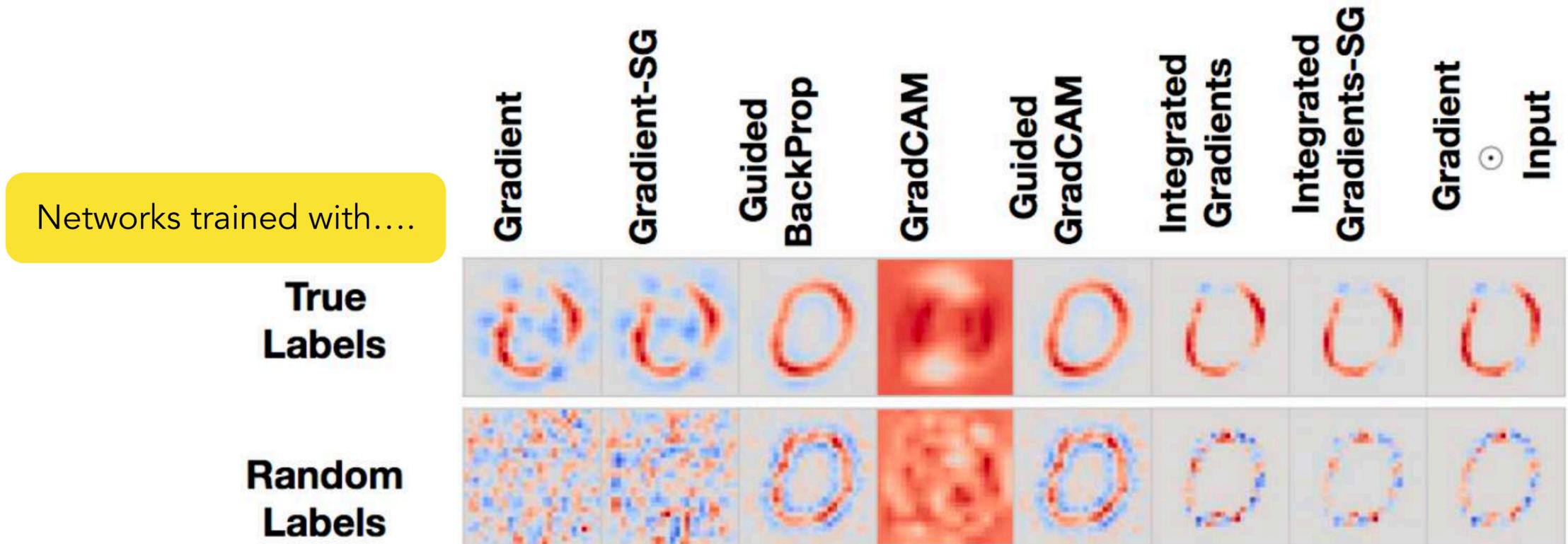
Sanity check 1: Explanations from random vs trained network

Most of methods produce quantitatively and qualitative similar results



Sanity check 2: Network trained with random vs true labels

Most of methods produce quantitatively and qualitative similar results



Explanations can be (easily) attacked!

Interpretation of Neural Networks is Fragile

Amirata Ghorbani*
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Abubakar Abid*
Dept. of Electrical Engineering
Stanford University
a12d@stanford.edu

James Zou†
Dept. of Biomedical Data Science
Stanford University
jamesz@stanford.edu

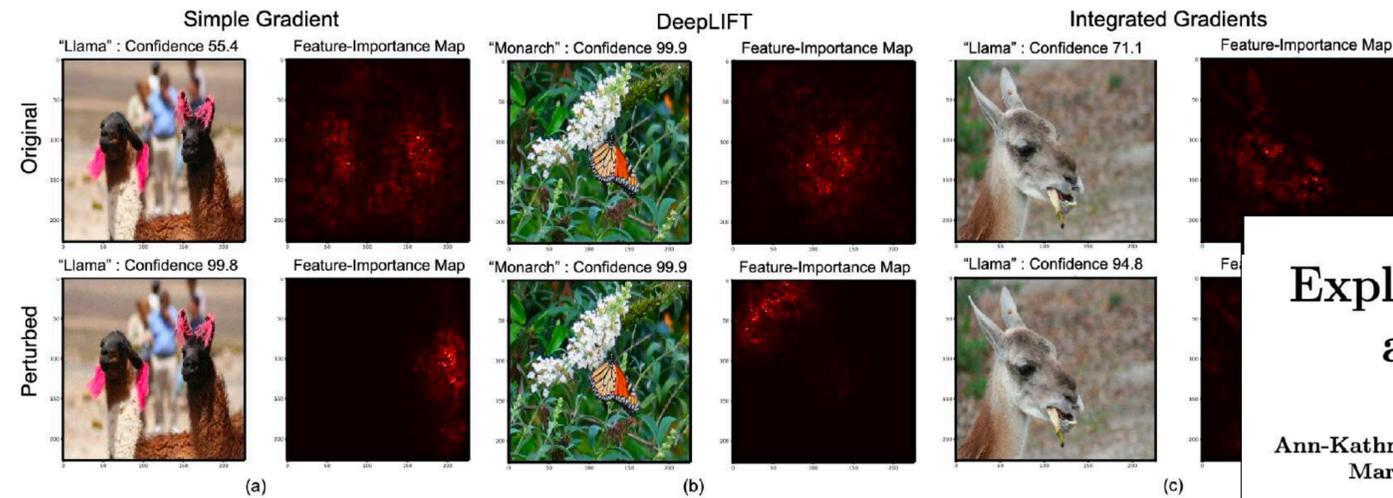


Figure 1: **Adversarial attack against feature-importance maps.** We generate feature-importance scores, also maps, using three popular interpretation methods: (a) simple gradients, (b) DeepLIFT, and (c) integrated gradients. The **top row** shows the the original images and their saliency maps and the **bottom row** shows the perturbed images (under attack with $\epsilon = 8$, as described in Section 3) and corresponding saliency maps. In all three images, the predicted change from the perturbation; however, the saliency maps of the perturbed images shifts dramatically to features that are considered salient by human perception.

Explanations can be manipulated and geometry is to blame

Ann-Kathrin Dombrowski¹, Maximilian Alber¹, Christopher J. Anders¹,
Marcel Ackermann², Klaus-Robert Müller^{1,3,4}, Pan Kessel¹

¹Machine Learning Group, EE & Computer Science Faculty, TU-Berlin

²Department of Video Coding & Analytics, Fraunhofer Heinrich-Hertz-Institute

³Max Planck Institute for Informatics

⁴Department of Brain and Cognitive Engineering, Korea University
{klaus-robert.mueller, pan.kessel}@tu-berlin.de



THE (UN)RELIABILITY OF SALIENCY METHODS

Pieter-Jan Kindermans†, Sara Hooker†, Julius Adebayo
Google Brain*
{pikinder, shooker}@google.com

Maximilian Alber, Kristof T. Schütt, Sven Dähne
TU-Berlin

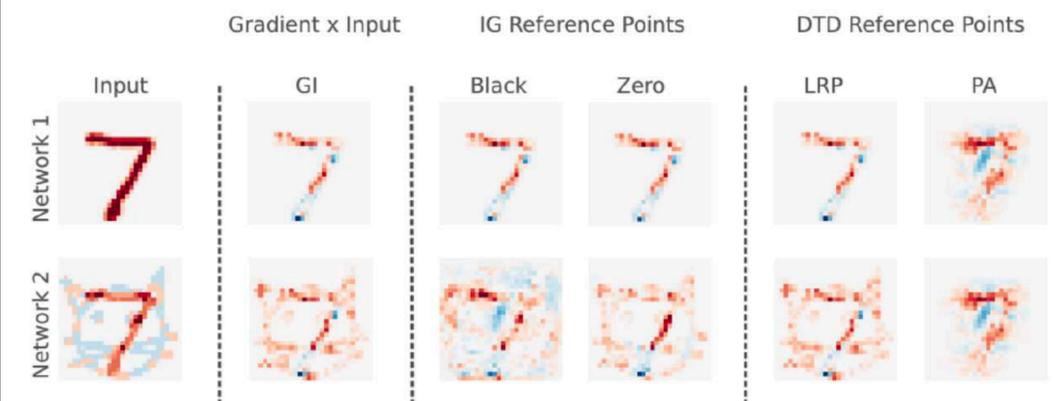
Dumitru Erhan, Been Kim
Google Brain

"Cat" astrophic Attribution Failure

MNIST + Constant Shift



Attribution Methods



Approximated explanations can be and will be wrong sometimes

- A number of methods “approximates” models behavior in some way. This means, there will be errors.
- Sometimes it’s just plain wrong (e.g., not robust to distributional shifts)

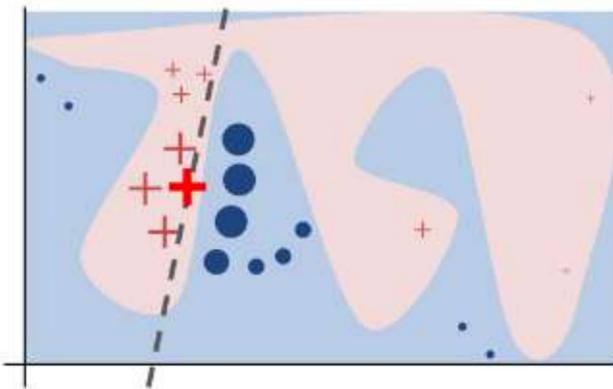
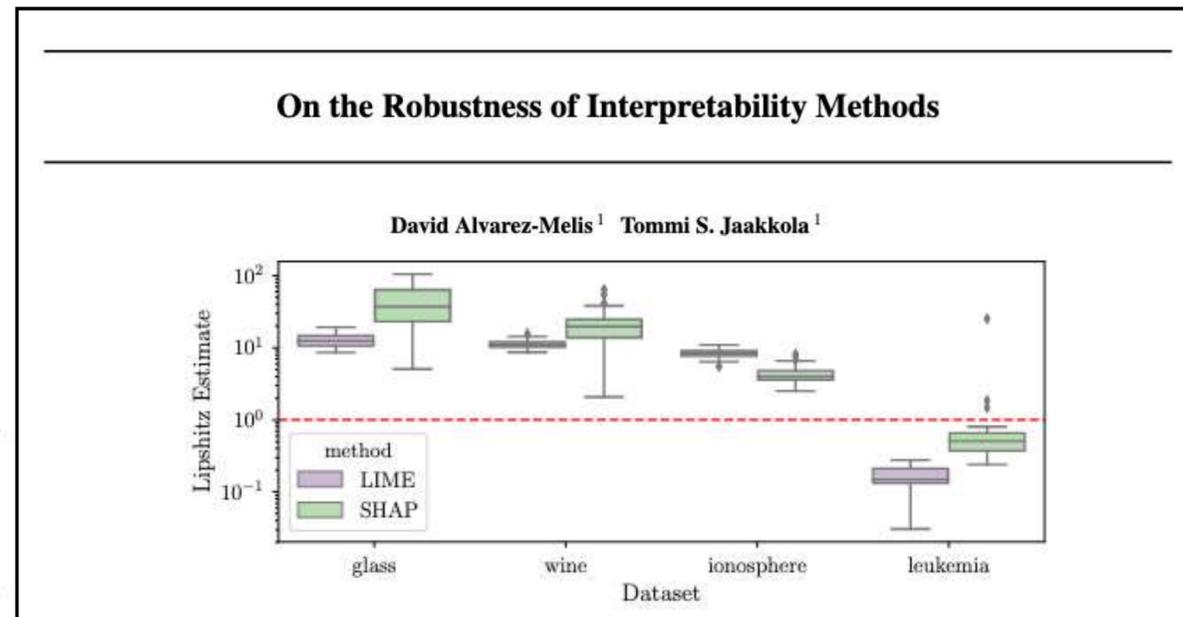


Figure 3: Toy example to present intuition for LIME. The black-box model’s complex decision function f (unknown to LIME) is represented by the blue/pink background, which cannot be approximated well by a linear model. The bold red cross is the instance being explained. LIME samples instances, gets predictions using f , and weighs them by the proximity to the instance being explained (represented here by size). The dashed line is the learned explanation that is locally (but not globally) faithful.



Published as a conference paper at ICLR 2021

INFLUENCE FUNCTIONS IN DEEP LEARNING ARE FRAGILE

Samyadeep Basu*, Phillip Pope* & Soheil Feizi
Department of Computer Science
University of Maryland, College Park
{sbasu12, pepope, sfeizi}@cs.umd.edu

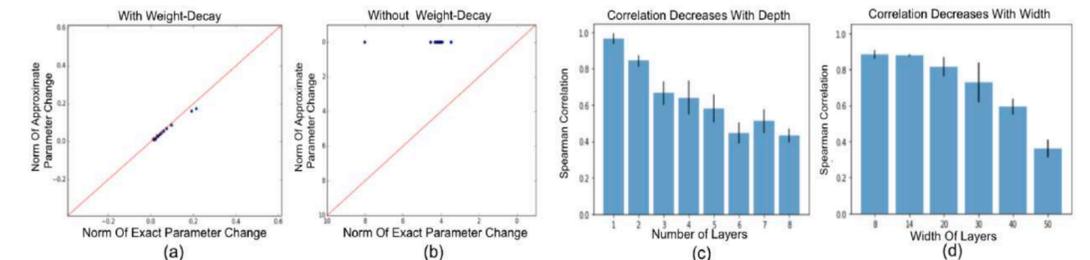


Figure 1: Iris dataset experimental results - (a,b) Comparison of norm of parameter changes computed with influence function vs re-training; (a) trained with weight-decay; (b) trained without weight-decay. (c) Spearman correlation vs. network depth. (d) Spearman correlation vs. network width.

Approximated explanations can be and will be wrong sometimes

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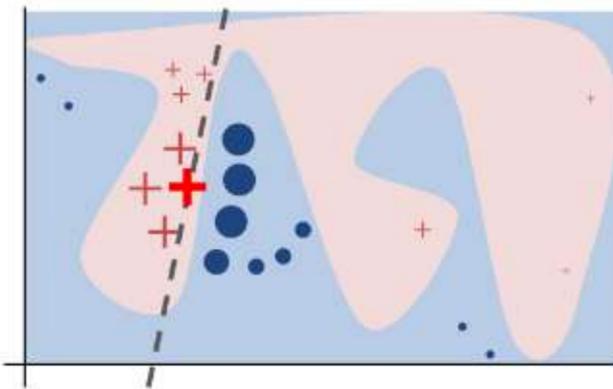
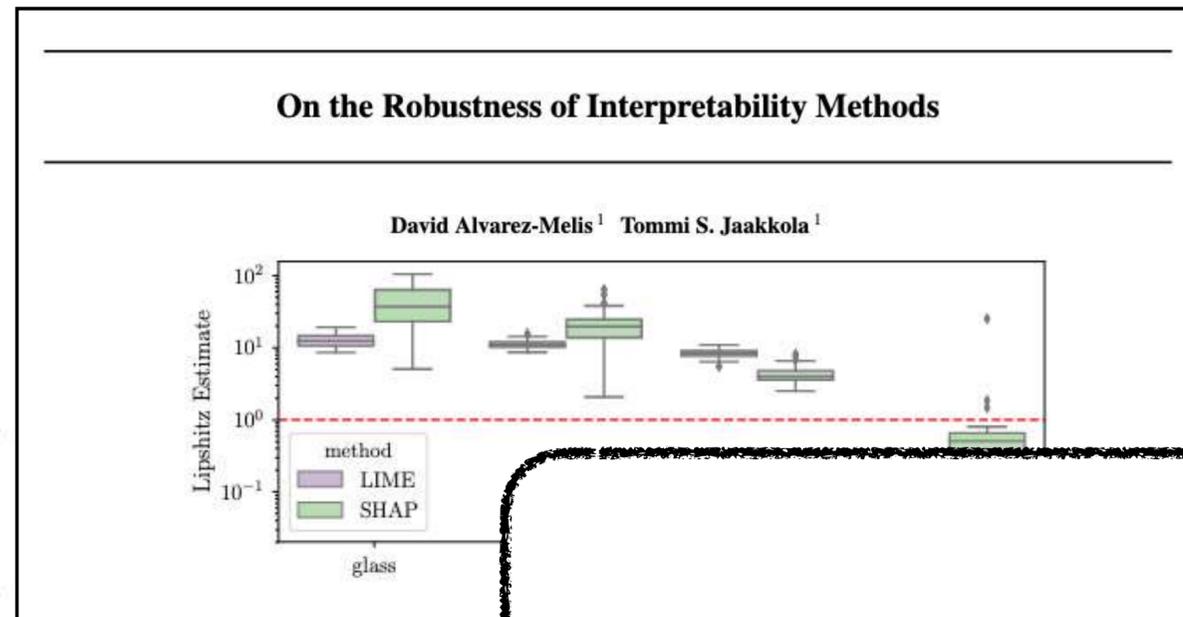


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University of Maryland, College Park
{sbasu12, pepope, sfeizi}@cs.umd.edu

Take away:
Always skeptical about the explanations you get.



We already know all the learned parameters of the function of the neural network. This is an open book and transparent system.

[This has actually been said]

Oh, *come on*.



I'm an ML person.
Human experiments are only
for HCI folks, right?

“How” explanations are presented is as important as the explanations themselves.
Knowing how that impacts users is even more important

Interpreting Interpretability: Understanding Data Scientists’ Use of Interpretability Tools for Machine Learning

Harmanpreet Kaur¹, Harsha Nori², Samuel Jenkins²,
Rich Caruana², Hanna Wallach², Jennifer Wortman Vaughan²

¹University of Michigan, ²Microsoft Research
harmank@umich.edu, {hanori,sajenkin,rcaruana,wallach,jenn}@microsoft.com

“Our results indicate that data scientists over-trust and misuse interpretability tools. Furthermore, few of our participants were able to accurately describe the visualizations output by these tools.”

Misuse and Disuse

Most participants relied too heavily on the interpretability tools. Previous work categorizes such over-use as *misuse* [17, 52]. Here, the misuse resulted from over-trusting the tools because of their visualizations; participants were excited about the visualizations and took them at face value instead of using them to dig deeper into issues with the dataset or model:

[Submitted on 22 Oct 2020]

Towards falsifiable interpretability research

Matthew L. Leavitt, Ari Morcos

“illustrative power of visualization is a double-edged sword: an evocative graphic can elicit a strong feeling of comprehension regardless of whether the graphic faithfully represents the phenomenon it is attempting to depict.”

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“illustrative power of visualization is a double-edged sword: an evocative graphic can elicit a strong feeling of comprehension regardless of whether the graphic faithfully represents the phenomenon it is attempting to depict.”

Take away:

Human factors is tricky but important.

Agenda



- What and why



- !Caution!: Things to be careful when using and developing interpretability methods



- Evaluate: How to evaluate interpretability methods



- Methods: 3 types of methods and examples

Evaluation - yes you can.

- Testing with no humans, proxy task
- Testing with humans, proxy task
- Testing with humans and real task



Using ground truth dataset and Sanity check

- Idea: Test the obvious
 1. Test hypothesis that should be true by craft a ground-truth dataset
 2. Test hypothesis that should be true using results on real dataset
 3. Do sanity check: often testing hypothesis that should NOT be true.
a.k.a. as crazy questions.

1: Test hypothesis that should be true by craft a ground-truth dataset

Forest



A thing



1: Test hypothesis that should be true by craft a ground-truth dataset

Forest



Forest



A thing



Bedroom



Kitchen



1: Test hypothesis that should be true by craft a ground-truth dataset

Forest



Forest



A thing



Bedroom



Kitchen



is NOT important for predicting scene classes.



↓
should NOT
Be part of explanation

1: Test hypothesis that should be true by craft a ground-truth dataset

Forest



Forest



A thing



Bedroom



Kitchen



is NOT important for predicting scene classes.



↓
should NOT Be part of explanation



We can also make more important to some classes by controlling when it appears.



↓
should be more important explanation in some classes than others.

1: Test hypothesis that should be true by craft a ground-truth dataset

		Model's truth	
		important	Not important
Interp. methods estimates	important	TP	FP
	not important	FN	TN

Our Focus: False positives

1: Test hypothesis that should be true by craft a ground-truth dataset

		Model's truth	
		important	Not important
Interp. methods estimates	important	TP	FP
	not important	FN	TN

Our Focus: False positives

Suggested metrics

- Model contrast score (MCS)
- Input dependence rate (IDR)
- Input independence rate (IIR)

1: Test hypothesis that should be true by craft a ground-truth dataset

		Model's truth	
		important	Not important
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Our Focus: False positives

Suggested metrics

- Model contrast score (MCS)
- Input dependence rate (IDR)
- Input independence rate (IIR)



Two models trained to classify scenes.

Model 1



Model 2



1: Test hypothesis that should be true by craft a ground-truth dataset

		Model's truth	
		important	Not important
Interp. methods estimates	important	TP	FP
	not important	FN	TN

← Our Focus

Suggested metrics

- Model contrast score (MCS)
- Input dependence rate (IDR)
- Input independence rate (IIR)

Two models trained to classify

Scene model



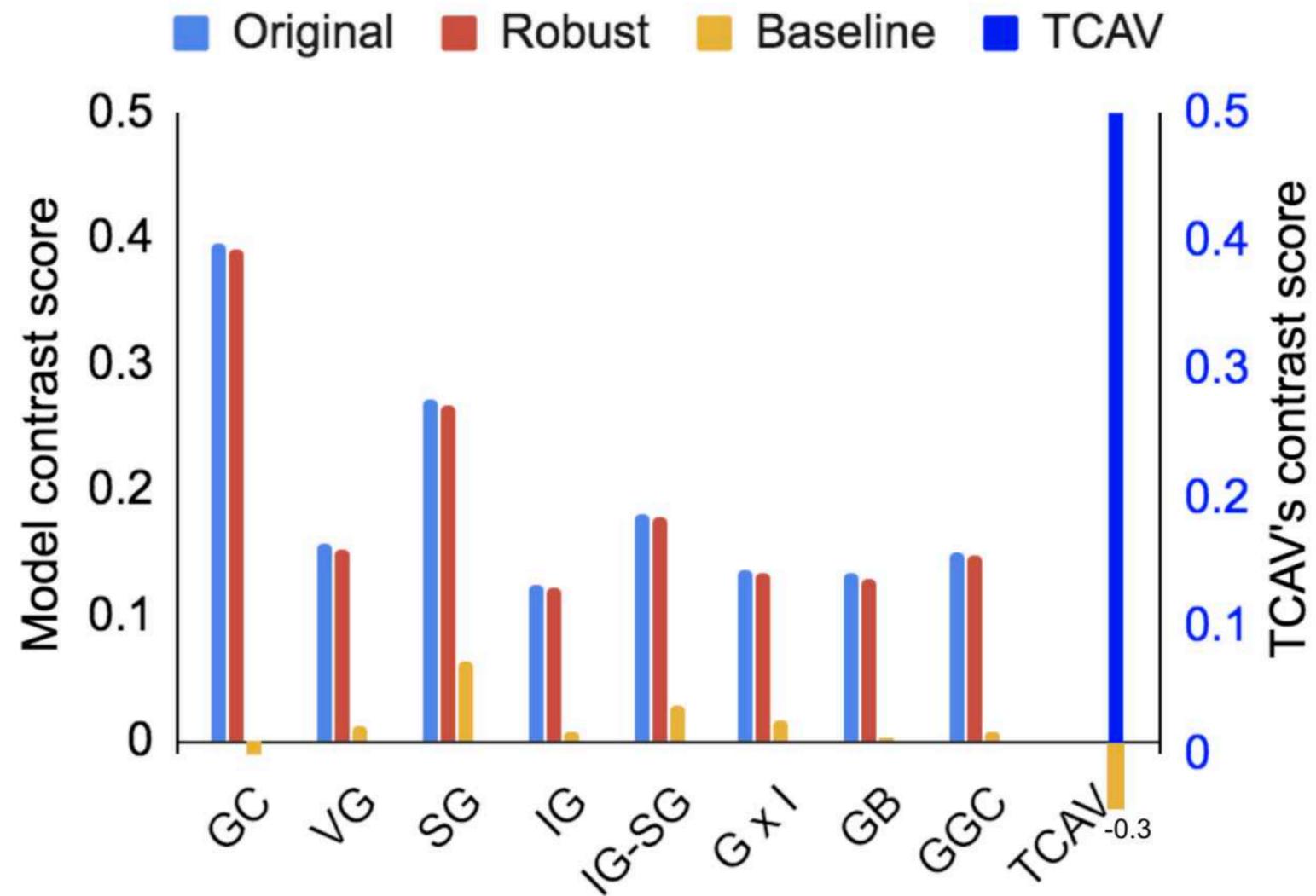
Object model



We expect big contrast on where the object is.

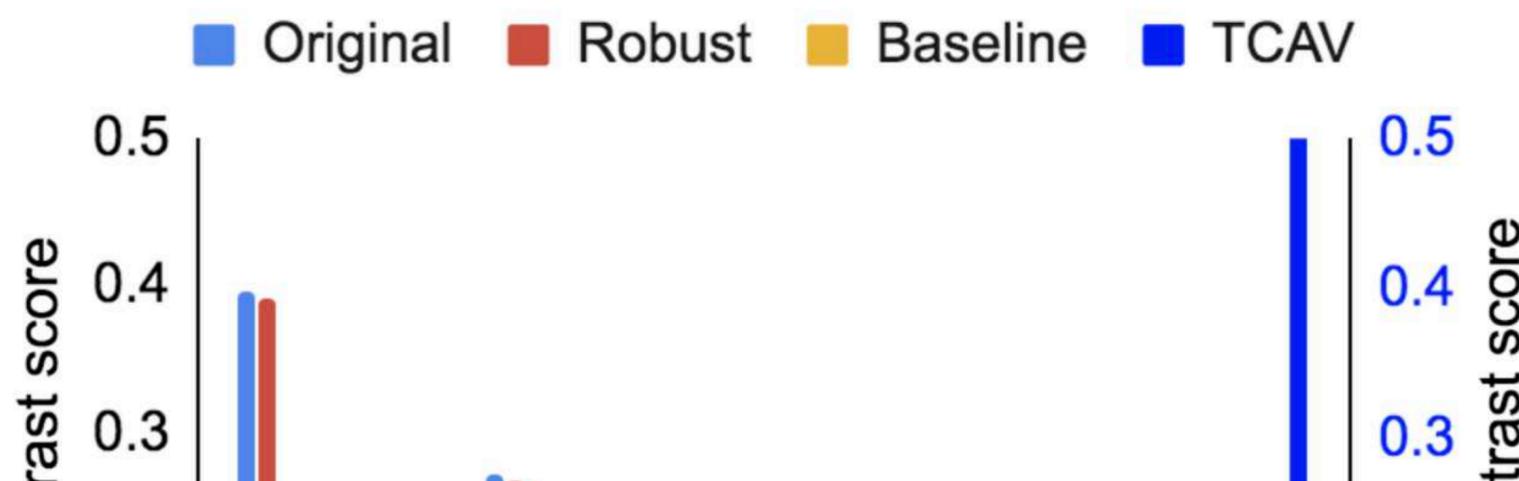
Benchmarking interpretability methods (BIM)

1: Test hypothesis that should be true by craft a ground-truth dataset



Benchmarking interpretability methods (BIM)

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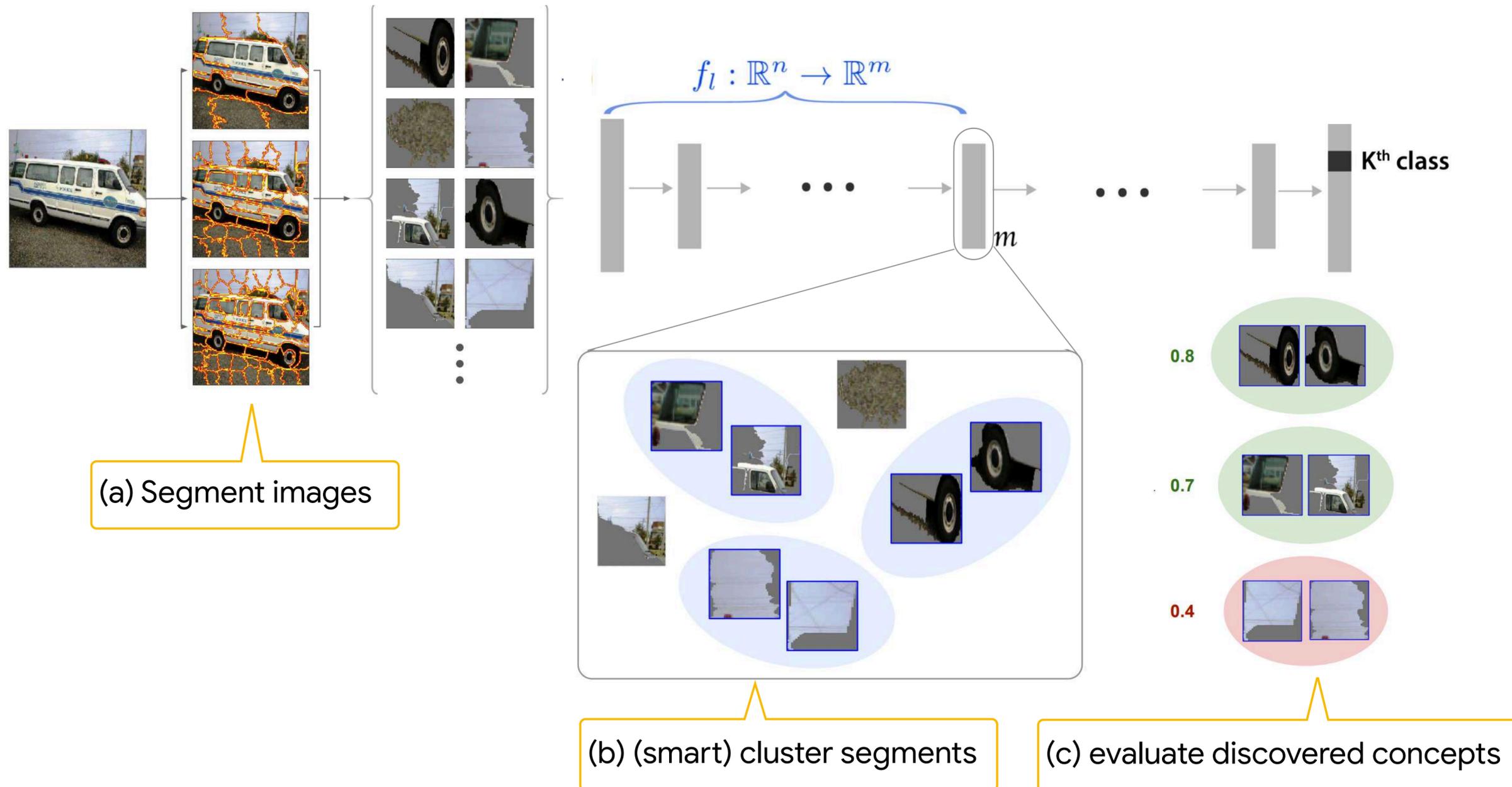
Take away:

You can craft a synthetic dataset for your domain (e.g., sequential, tabular). Add typical challenges you may encounter.

There is no point testing with humans if the method doesn't pass these tests.

2: Test hypothesis that should be true using results on real dataset

Automatic Concept-based Explanations (ACE)
[Ghorbani et al. NeurIPS 19]



no humans, proxy task

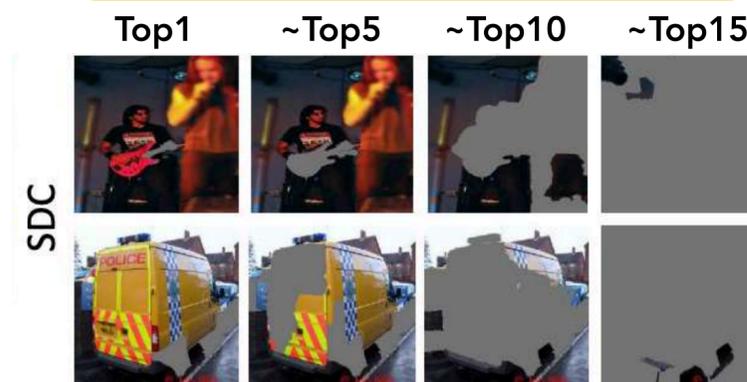
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Adding top-rated patches

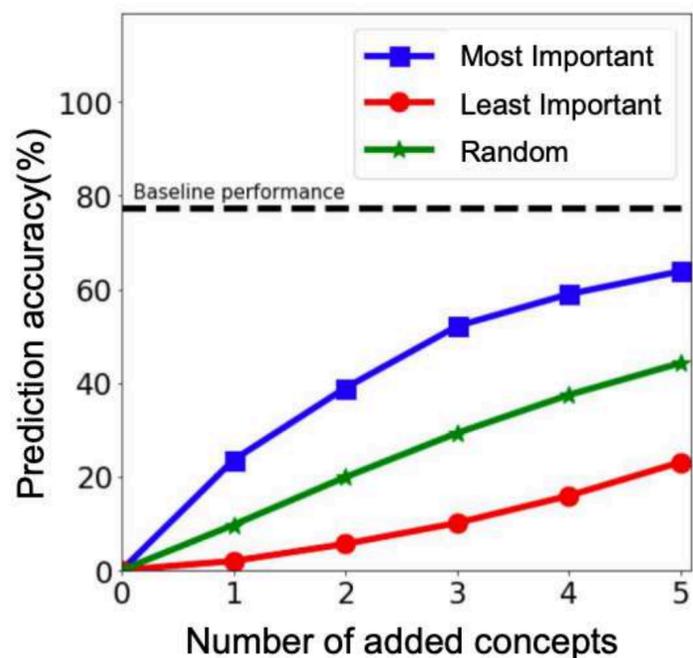


Automatic Concept-based Explanations (ACE)
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Deleting top-rated patches

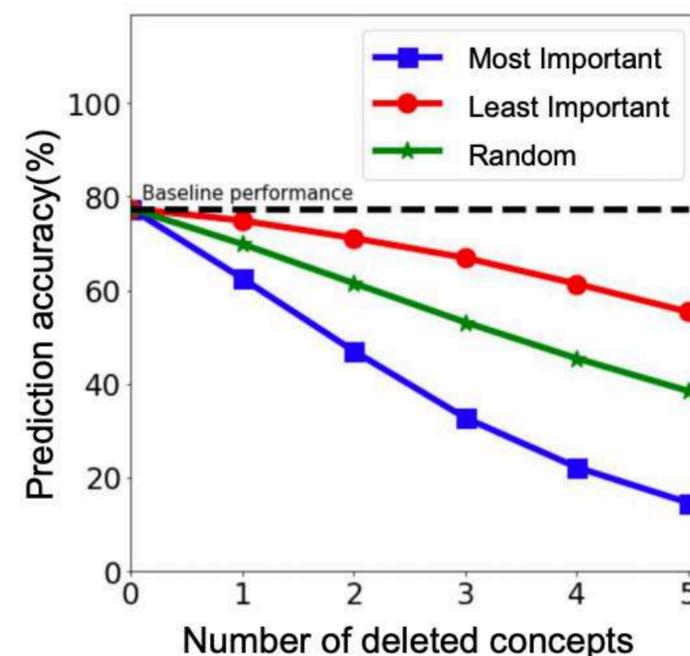


SSC



Adding the top5 discovered concepts alone achieves 70% of the original accuracy

SDC



2: Test hypothesis that should be true using results on real dataset

Real Time Image Saliency for Black Box Classifiers

Piotr Dabkowski
pd437@cam.ac.uk
University of Cambridge

Yarin Gal
yarin.gal@eng.cam.ac.uk
University of Cambridge
and Alan Turing Institute, London

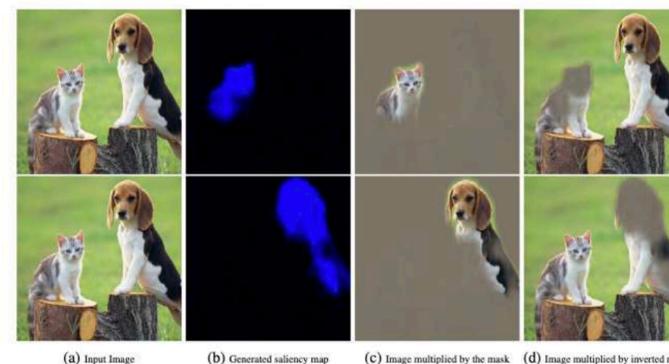


Figure 1: An example of explanations produced by our model. The top row shows the explanation for the "Egyptian cat" while the bottom row shows the explanation for the "Beagle". Note that produced explanations can precisely both highlight and remove the selected object from the image.

smallest sufficient region (SSR) - smallest region of the image that alone allows a confident classification.

We propose to find the tightest rectangular crop that *contains the entire salient region* and to feed that rectangular region to the classifier to directly verify whether it is able to recognise the requested class. We define our saliency metric simply as:

$$s(a, p) = \log(\bar{a}) - \log(p) \quad (3)$$

	Localisation Err (%)	Saliency Metric
Ground truth boxes (baseline)	0.00	0.284
Max box (baseline)	59.7	1.366
Center box (baseline)	46.3	0.645
Grad [11]	41.7	0.451
Exc [16]	39.0	0.415
Masking model (this work)	36.9	0.318

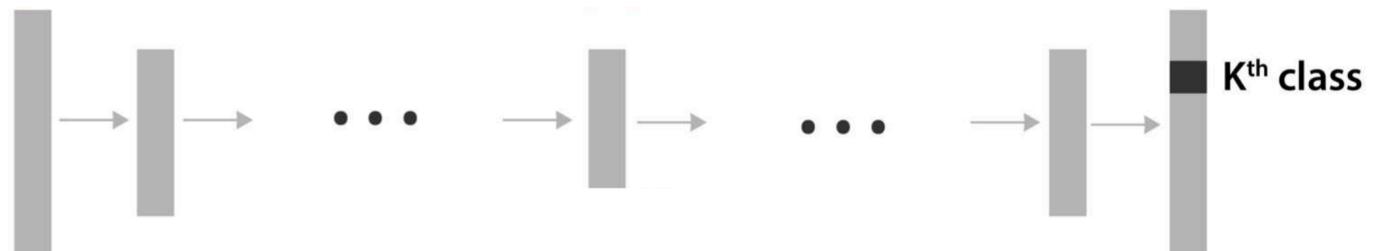
Lower is the better:

Relative amount of information between p and a (concentration of information in the cropped region)

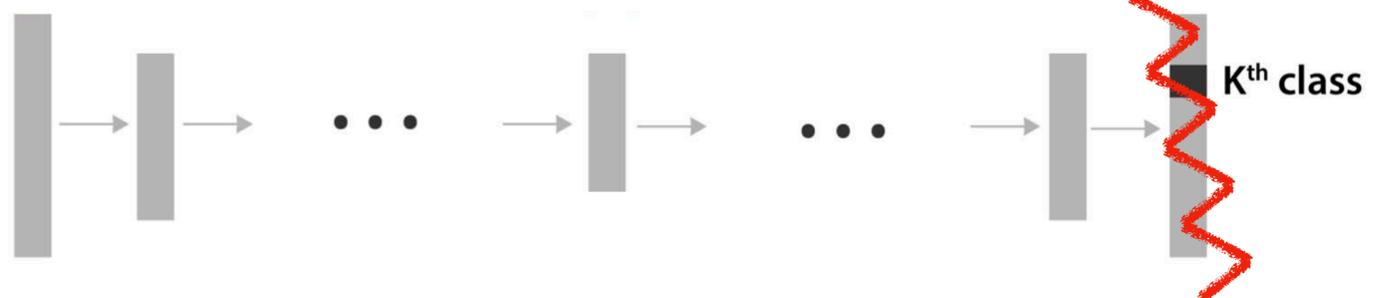
no humans, proxy task

3: Do sanity check: often testing hypothesis that should NOT be true.
a.k.a. ask crazy questions.

Original Image



Original Image



Randomized weights!
Network now makes garbage prediction.

!!!!????!



no humans, proxy task

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Sanity Checks for Saliency Metrics

Richard Tomsett,^{1*} Dan Harborne,^{2*} Supriyo Chakraborty,³ Prudhvi Gurram,⁴ Alun Preece²

¹Emerging Technology, IBM Research, Hursley, UK

²Crime and Security Research Institute, Cardiff University, Cardiff, UK

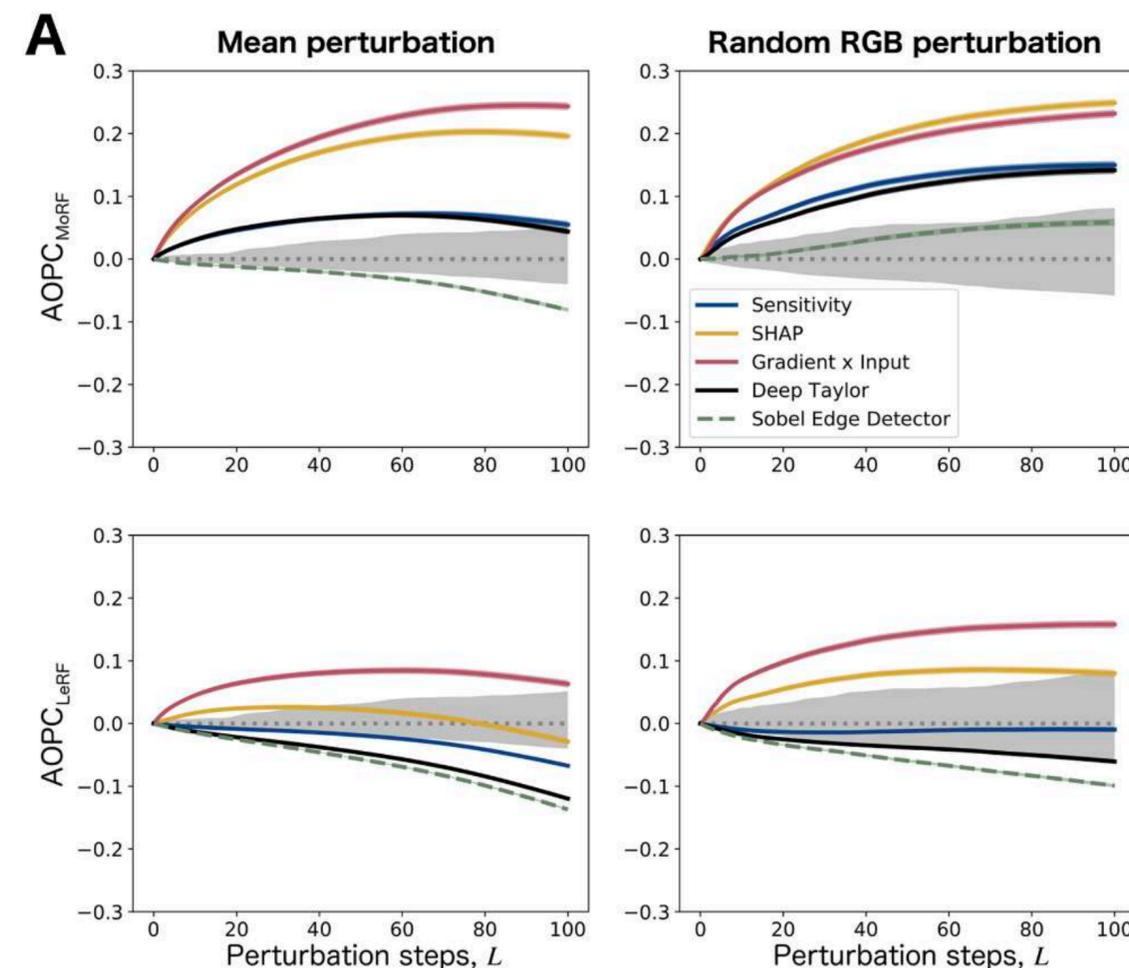
³IBM Research, Yorktown Heights, NY, USA

⁴Booz Allen Hamilton and CCDC Army Research Laboratory, Adelphi, MD, USA

rtomsett@uk.ibm.com, harbored@cardiff.ac.uk, supriyo@us.ibm.com, gurram_prudhvi@bah.com, preecead@cardiff.ac.uk

“Our results show that saliency metrics can be statistically unreliable and inconsistent, indicating that comparative rankings between saliency methods generated using such metrics can be untrustworthy.

1. Global saliency metrics had high variance
2. Saliency metrics were sensitive to the specifics of their implementation
3. Saliency maps from different saliency methods were ranked inconsistently image-by-image
4. The internal consistency of different metrics that all attempt to measure fidelity was low



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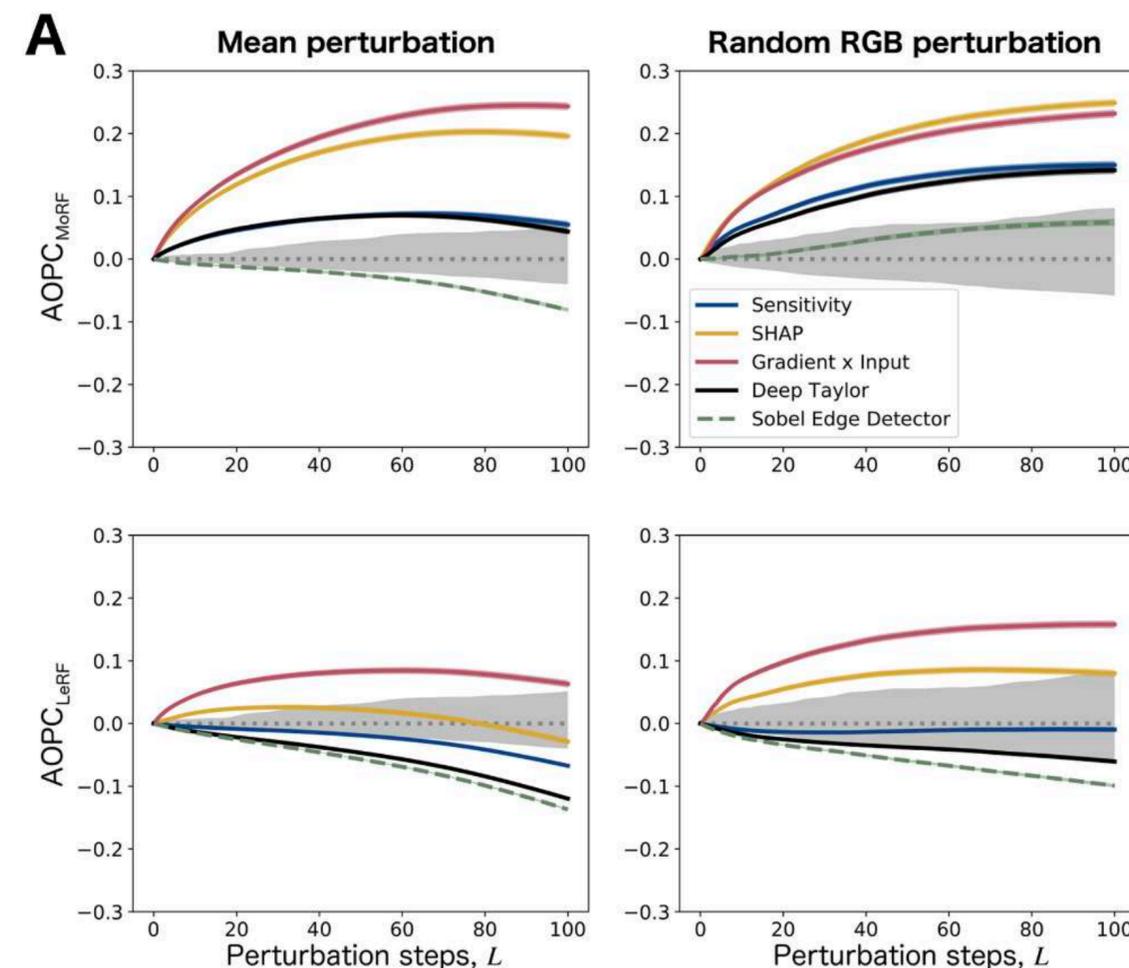
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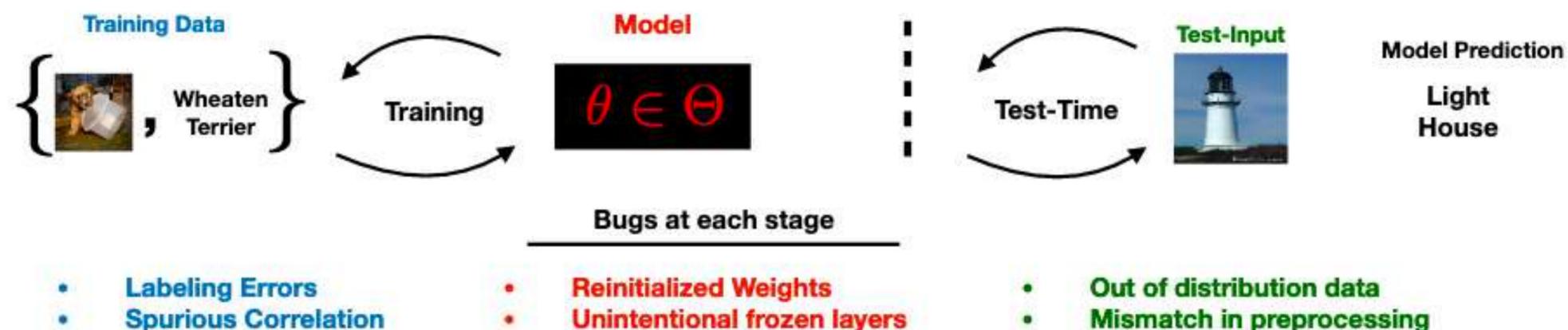
Take away:

Being skeptical can be healthy and productive.

Testing with humans, proxy task

- In a proxy task that maintains the essence of the final task (but likely ground truth is known)
- with humans who may not be your idea users (e.g., doctors) but still can help evaluating

Testing methods with users and concrete end-tasks

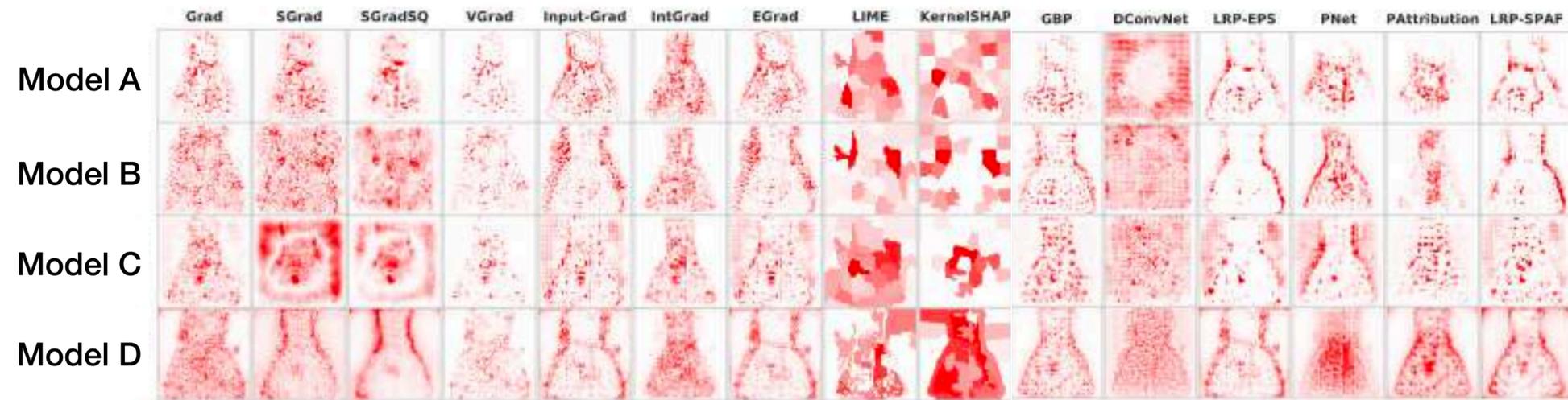
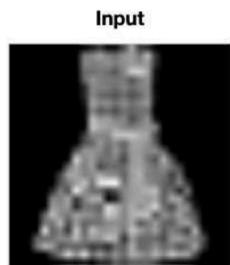


- **Task for subjects:** You work at a start-up selling animal classification ML model. Here are the images, predictions and attribution maps. (We gave users prediction labels as it is unrealistic not to).
- **Questions:** Would you recommend this model? Why? [because the wrong/correct label/explanation]? All in Likert scale.

humans, proxy task

Can these methods tell us about

Out of distribution?



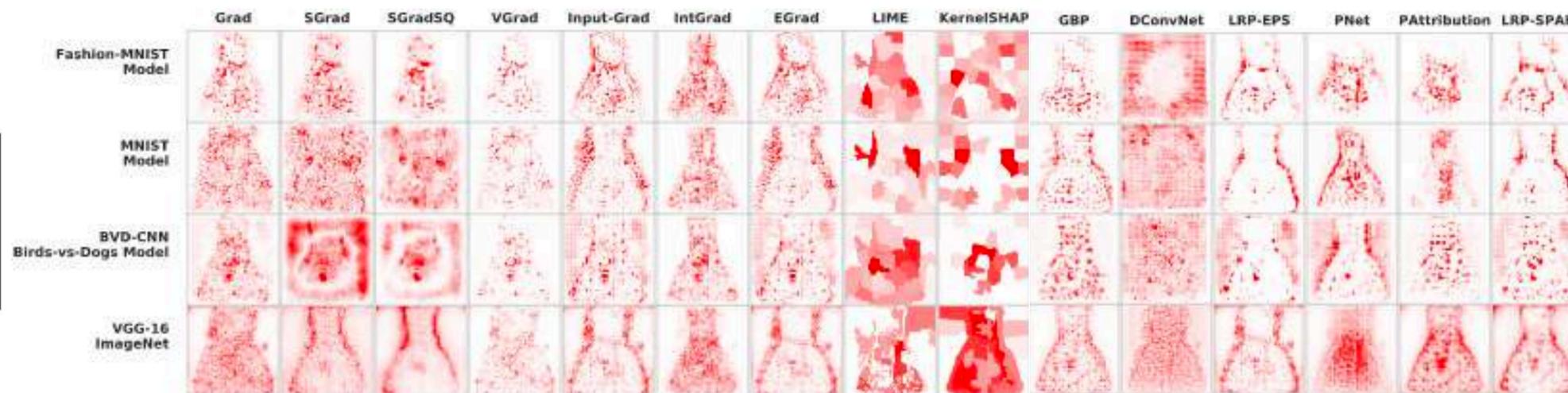
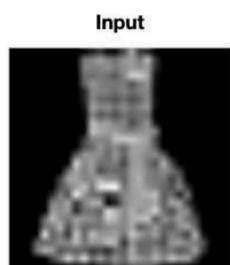
- Out of distribution data

Can these methods tell us about

Out of distribution? probably not.



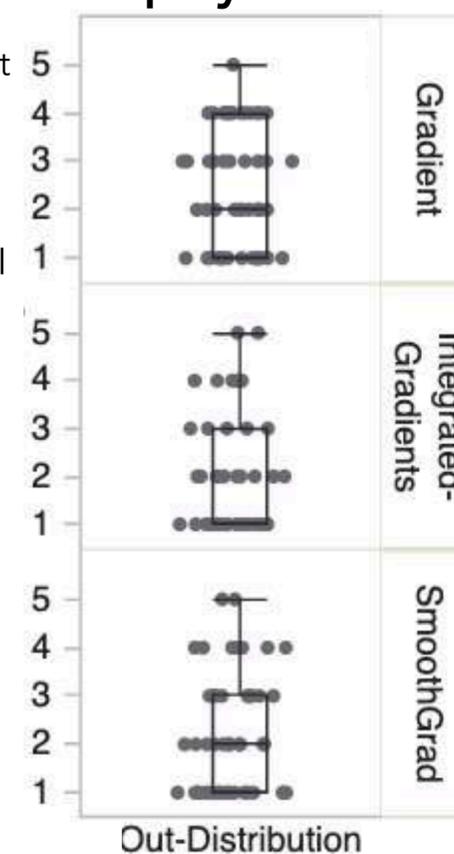
• Out of distribution data



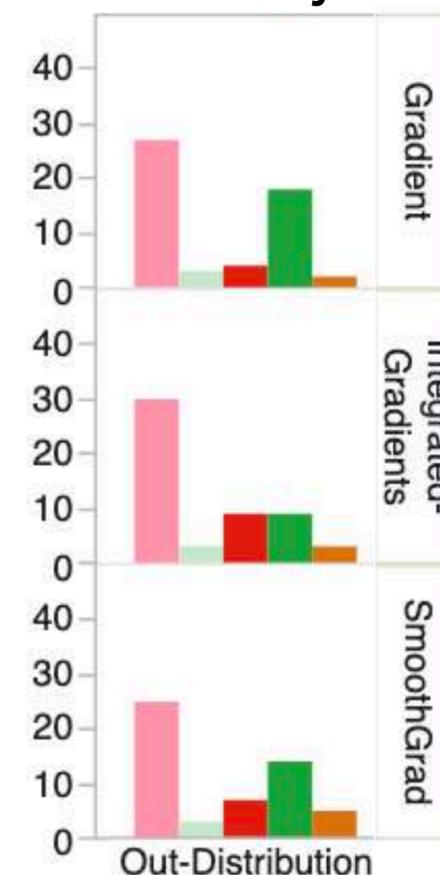
Subjects are uncertain, mostly because of wrong label, but some **expected** explanations.

How confident are you to deploy this model?

Very confident
Not confident at all



% why

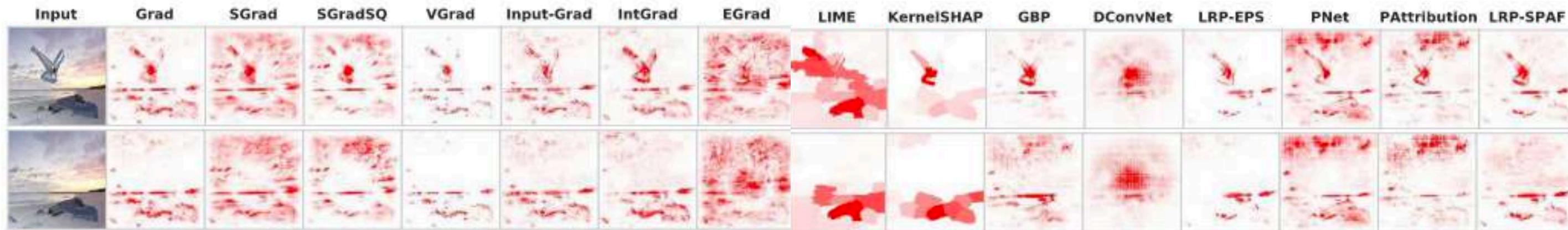


Wrong Label
Correct Label
Unexpected Explanation
Expected Explanation
Others

humans, proxy task

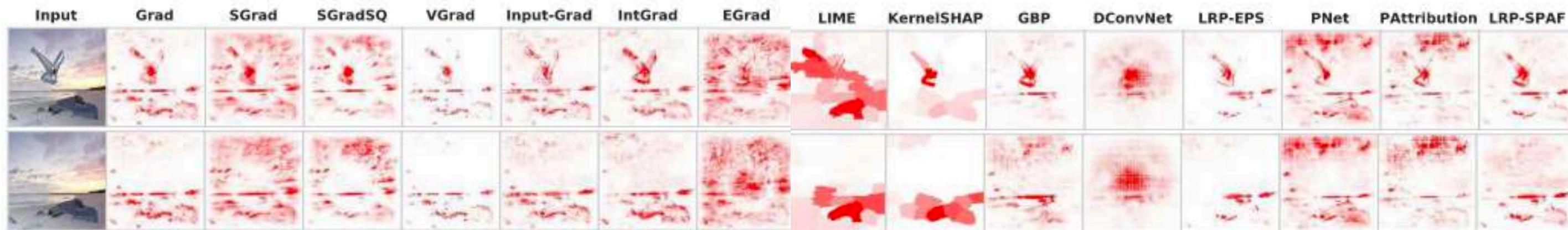
Can these methods tell us about

Spurious correlation?



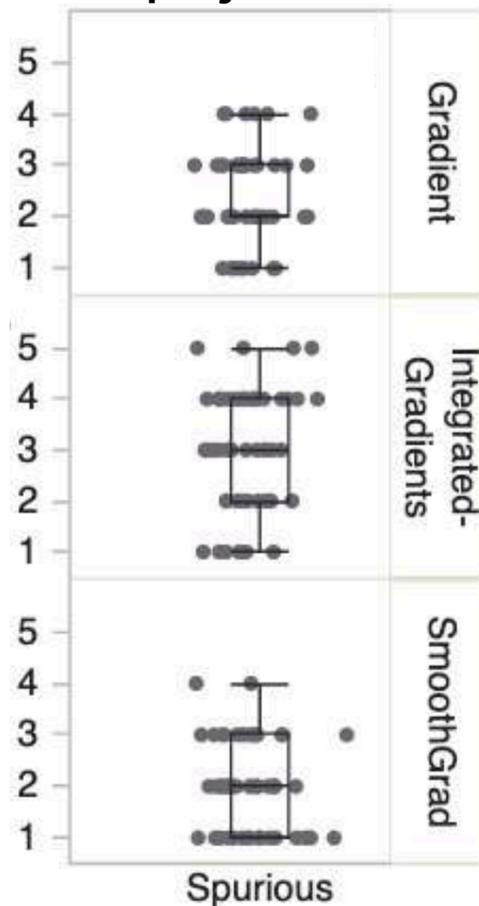
Can these methods tell us about

Spurious correlation? maybe!

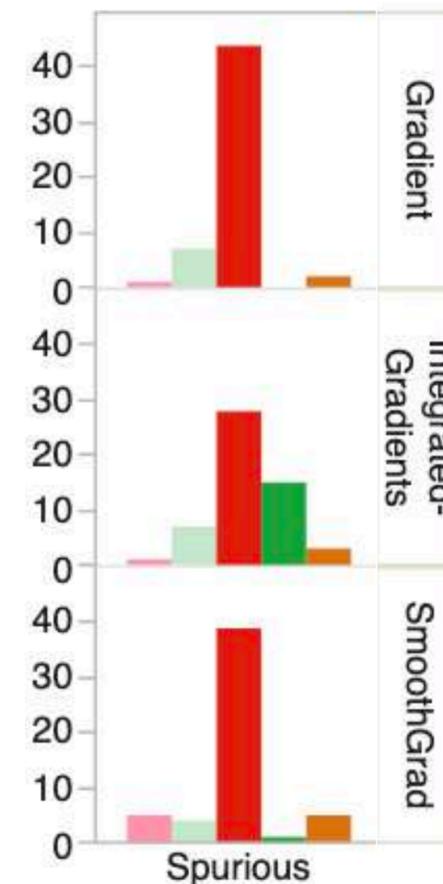


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Not confident at all



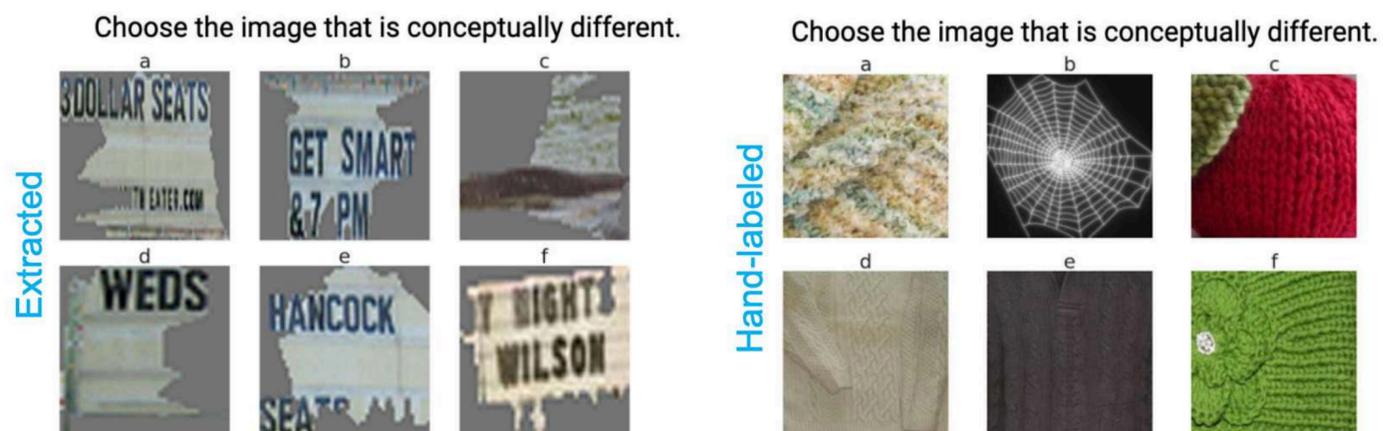
% why



Wrong Label
Correct Label
Unexpected Explanation
Expected Explanation
Others

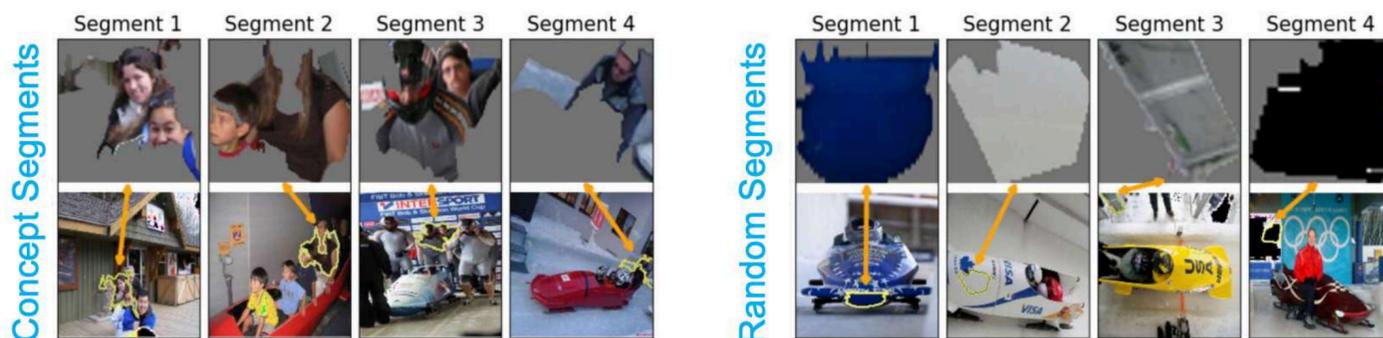
Subjects are uncertain, mostly because of **unexpected** explanations!

Example: Evaluating discovered concepts with subjects



Experiment 1: Identifying intruder concept

Look at the following two groups of segments. In each group, you should look at the top row. Each image in the top row is a zoomed-in version of another image shown on the bottom row. Now the question is that which of the groups seems more meaningful to you.

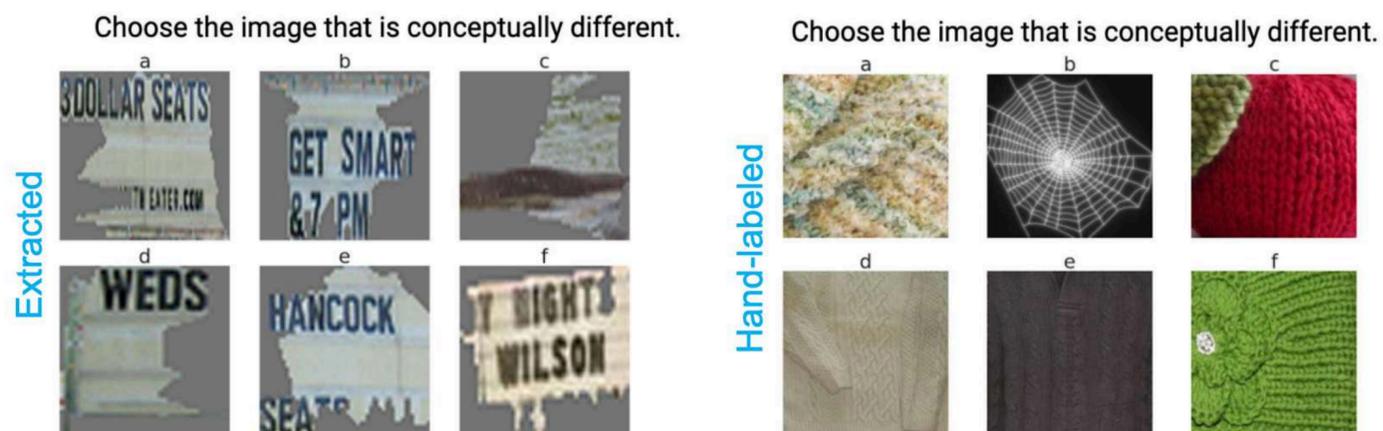


Which groups of images is more meaningful to you? right left
 If possible please describe the chosen row in one word.

Experiment 2: Identifying the meaning of concept

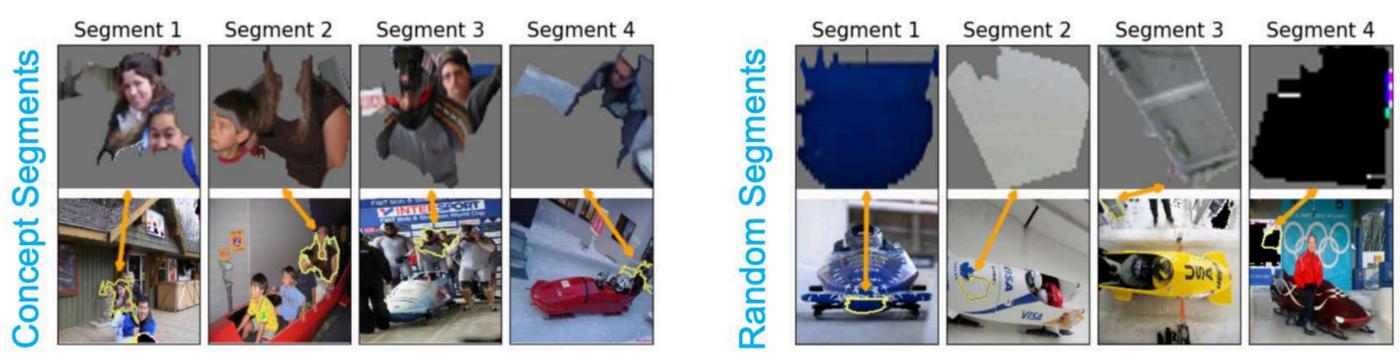
- Exp1: Intruder test
 - Task: Identify an odd one out
 - Discovered concepts: 99%, similar to hand-labeled dataset, 97%
- Exp2: Meaning test
 - Task: Select between discovered concepts vs random segments and name them.
 - Correctly chosen 95% of time
 - 56% used the same name and 77% named the same or top two terms (e.g., human, face)

Example: Evaluating discovered concepts with subjects



Experiment 1: Identifying intruder concept

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Which groups of images is more meaningful to you? right left
If possible please describe the chosen row in one word.

Experiment 2: Identifying the meaning of concepts

- Exp1: Intruder test
 - Task: Identify an odd one out
 - Discovered concepts: 99%, similar to hand-labeled dataset, 97%
- Exp2: Meaning test
 - Task: Select between discovered concepts vs random segments and name them.
 - Correctly chosen 95% of time
 - 56% used the same name and 77% named the same or top two terms

Take away:
Proxy task can be an effective way to evaluate a method (often) before running real experts on real tasks.

With humans on real tasks

“Human-Centered Tools for Coping with Imperfect Algorithms During Medical Decision-Making”

[Cai et al. 19 CHI]

“In two evaluations with pathologists, we found that these refinement tools increased the diagnostic utility of images found and increased user trust in the algorithm. The tools were preferred over a traditional interface, without a loss in diagnostic accuracy.”

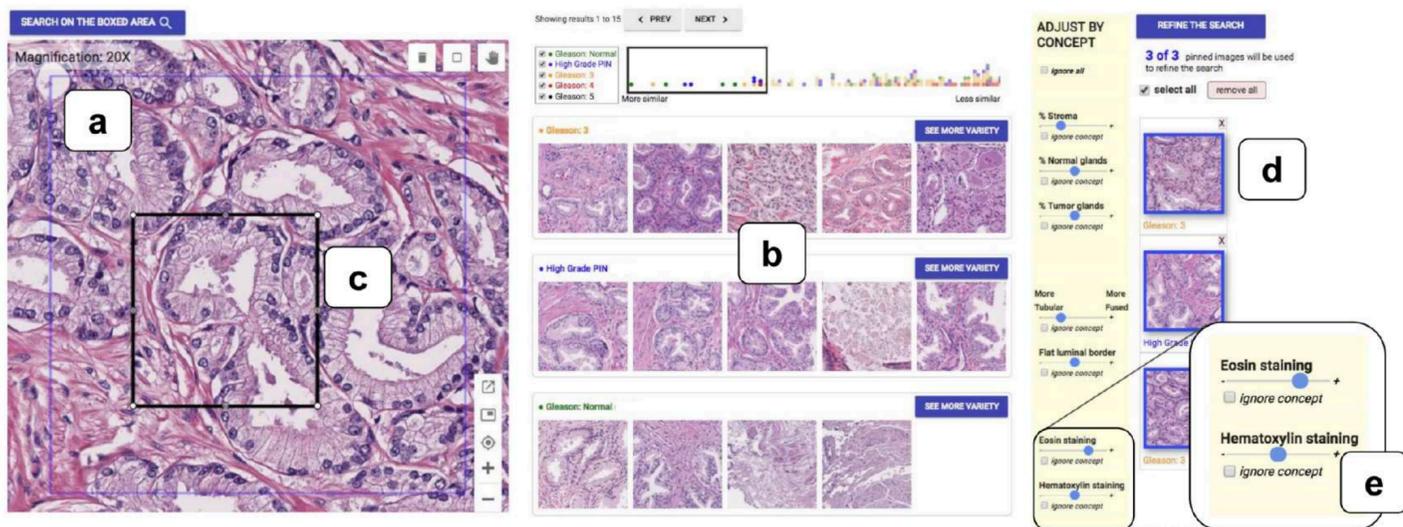


Figure 2: Key components of SMILY: a) the query image (e.g. pathology tissue possibly containing cancer), b) the search results (images from previously diagnosed cases), c) refine-by-region tool: users crop a region to emphasize its importance, d) refine-by-example tool: for clinical concepts that can't be pinpointed to a specific region (e.g. visual patterns), users can pin examples from search results to emphasize that concept, e) refine-by-concept tool: users increase or decrease the presence of clinical concepts by sliding sliders.

“Explainable machine-learning predictions for the prevention of hypoxaemia during surgery”

[Lundberg et al. 18 Nature biomedical engineering]

“The system, which was trained on minute-by-minute data from the electronic medical records of over 50,000 surgeries, improved the performance of anesthesiologists by providing interpretable hypoxaemia risks and contributing factors.”

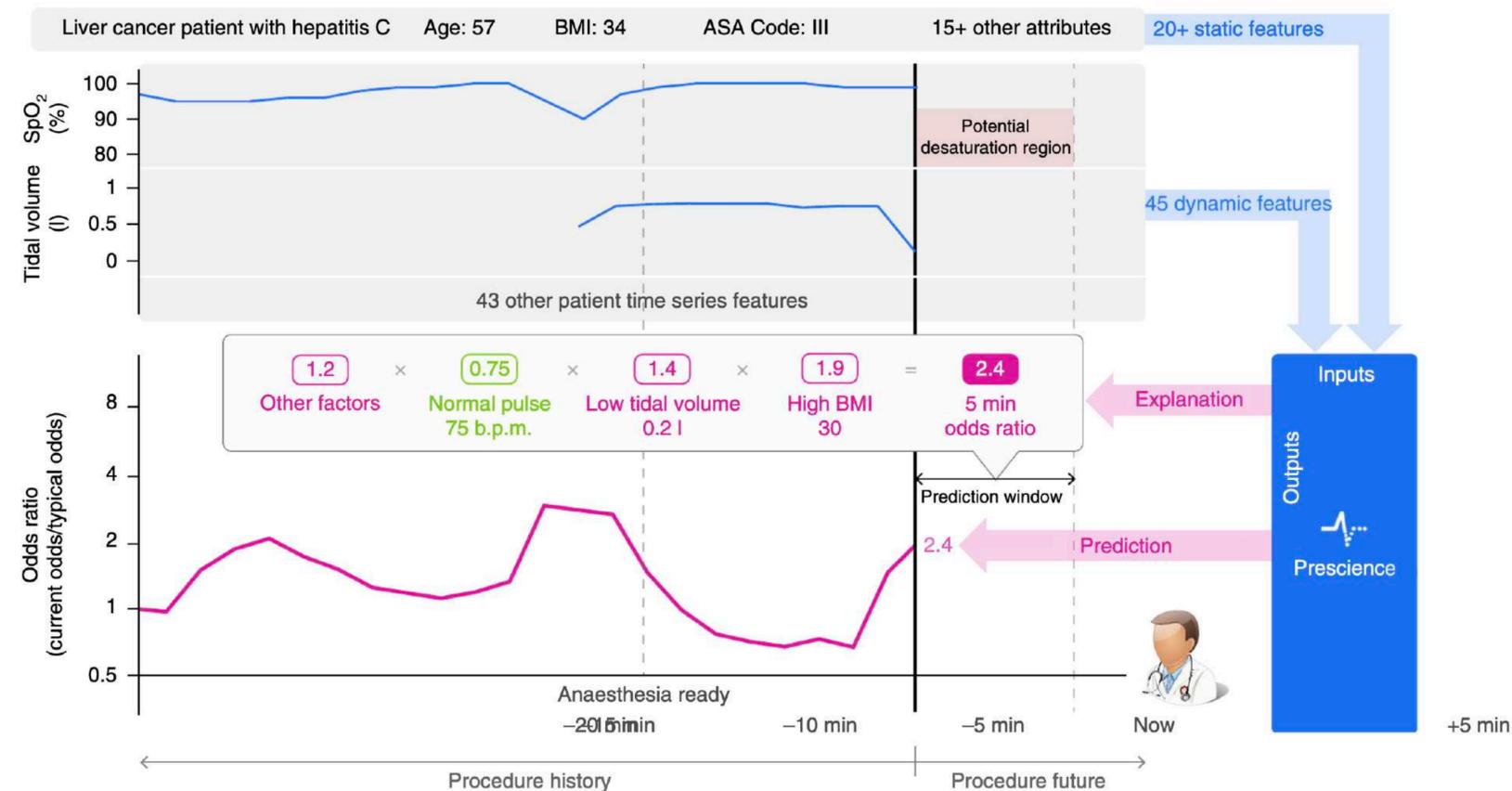


Fig. 1 | Prescience integrates many data sources into a single risk, which is explained through a succinct visual summary. A wide variety of data sources were used to build a predictive model of hypoxaemia events. An explanation (overlaid) is then built for each prediction. Pink features have values that increased risk, whereas green features decreased hypoxaemia risk. The combination of the impacts of all features is the predicted Prescience risk; in this case, the odds are 2.4 × higher than normal. Each feature impact value represents the change in risk when the value of that feature is known versus unknown. Qualitative terms such as ‘low’ or ‘high’ are based on the distribution of a feature value in our dataset.

Agenda



- What and why



- !Caution!: Things to be careful when using and developing interpretability methods



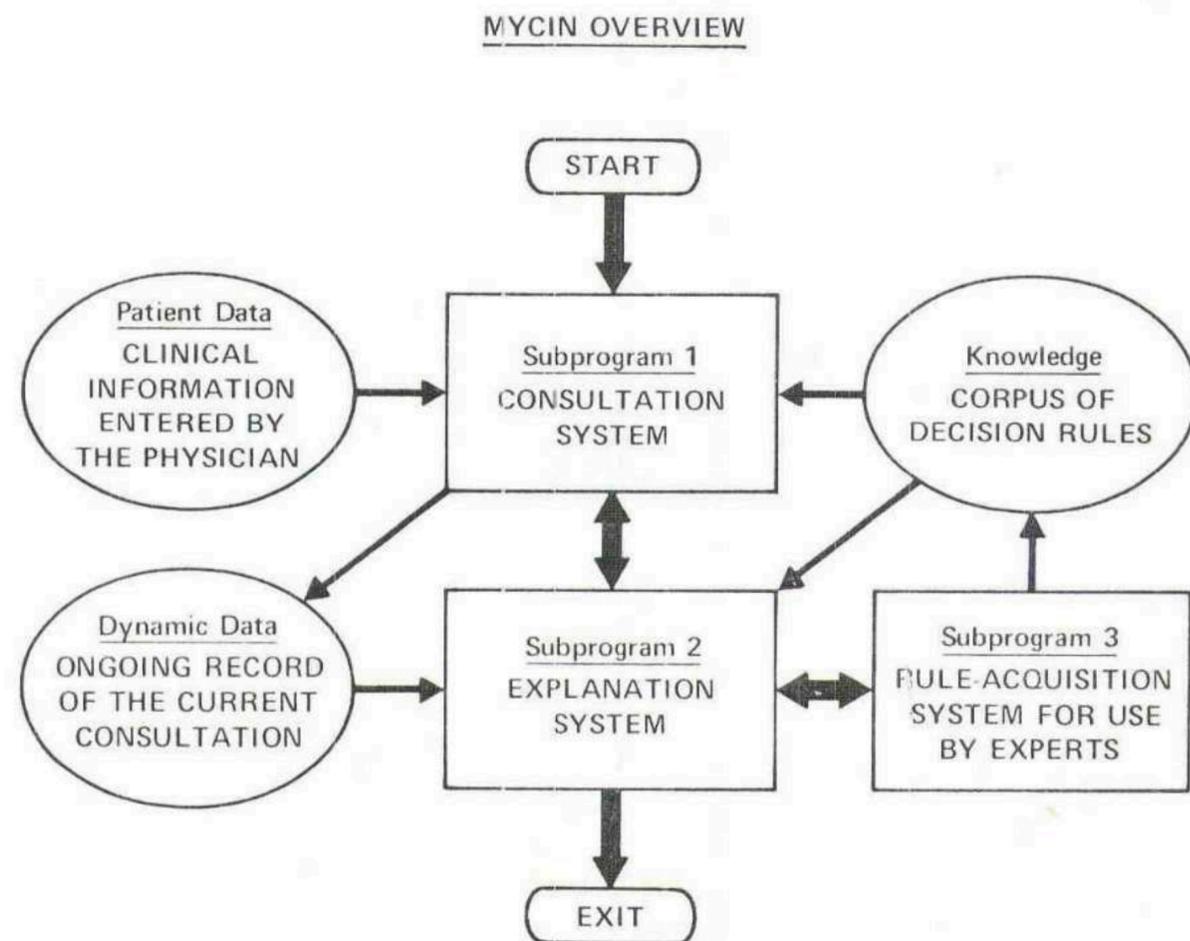
- Evaluate: How to evaluate interpretability methods



- Methods: 3 types of methods and examples

Again, it's not all about deep learning.
Interpretability isn't a new problem.

- Lots of pre-deep learning work going all the way back to 70's.



By typing WHY, the user gets a detailed explanation from the system of the type of conclusion it is trying to draw, and how the current rule is to be applied in this case to establish that conclusion.

In light of the site from which the culture was obtained, and the method of collection, do you feel that a significant number of ORGANISM-1 were obtained?

****WHY**

[1.0] It is important to find out whether there is therapeutically significant disease associated with this occurrence of ORGANISM-1

It has already been established that:

- [1.1] the site of the culture is not one of those which are normally sterile, and
- [1.2] the method of collection is sterile

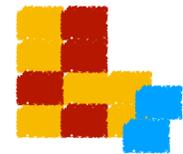
Good reference

Comprehensible Classification Models – a position paper

Alex A. Freitas
School of Computing
University of Kent
Canterbury, CT2 7NF, UK

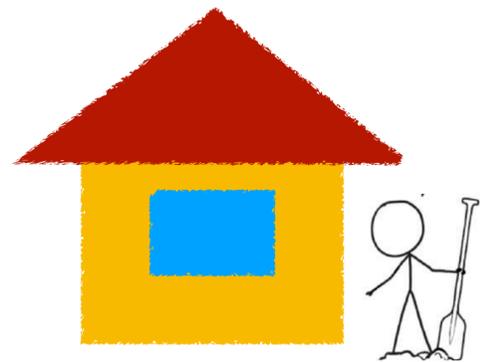
[Shortliffe et al. 1975]

Types of interpretability methods



Explaining data

$$\operatorname{argmax}_E Q(\mathbf{Explanation} | \mathbf{Human}, \mathbf{Data}, \mathbf{Task})$$



My ML



Building inherently interpretable model

$$\operatorname{argmax}_{E, M} Q(\mathbf{Explanation}, \mathbf{Model} | \mathbf{Human}, \mathbf{Data}, \mathbf{Task})$$



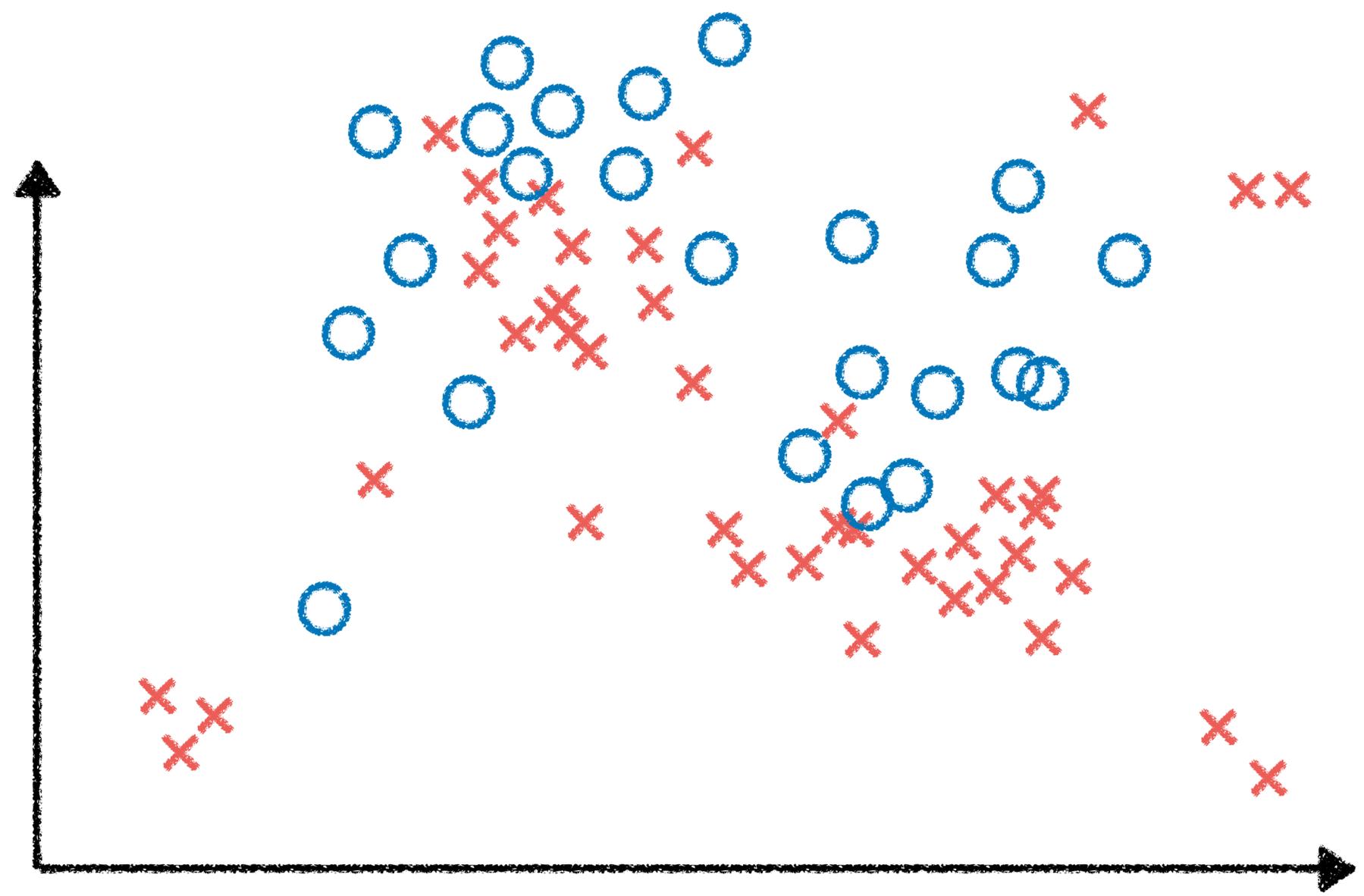
Post-training interpretability methods

$$\operatorname{argmax}_E Q(\mathbf{Explanation} | \mathbf{Model}, \mathbf{Human}, \mathbf{Data}, \mathbf{Task})$$

Interpreting data (not just the model) is important.

- Exploratory data analysis:
 - “an approach of analyzing data sets to summarize their main characteristics, often using statistical graphics and other data visualization methods. [It] is for seeing what the data can tell us beyond the formal modeling or hypothesis testing task. ”

https://en.wikipedia.org/wiki/Exploratory_data_analysis



○ Class0

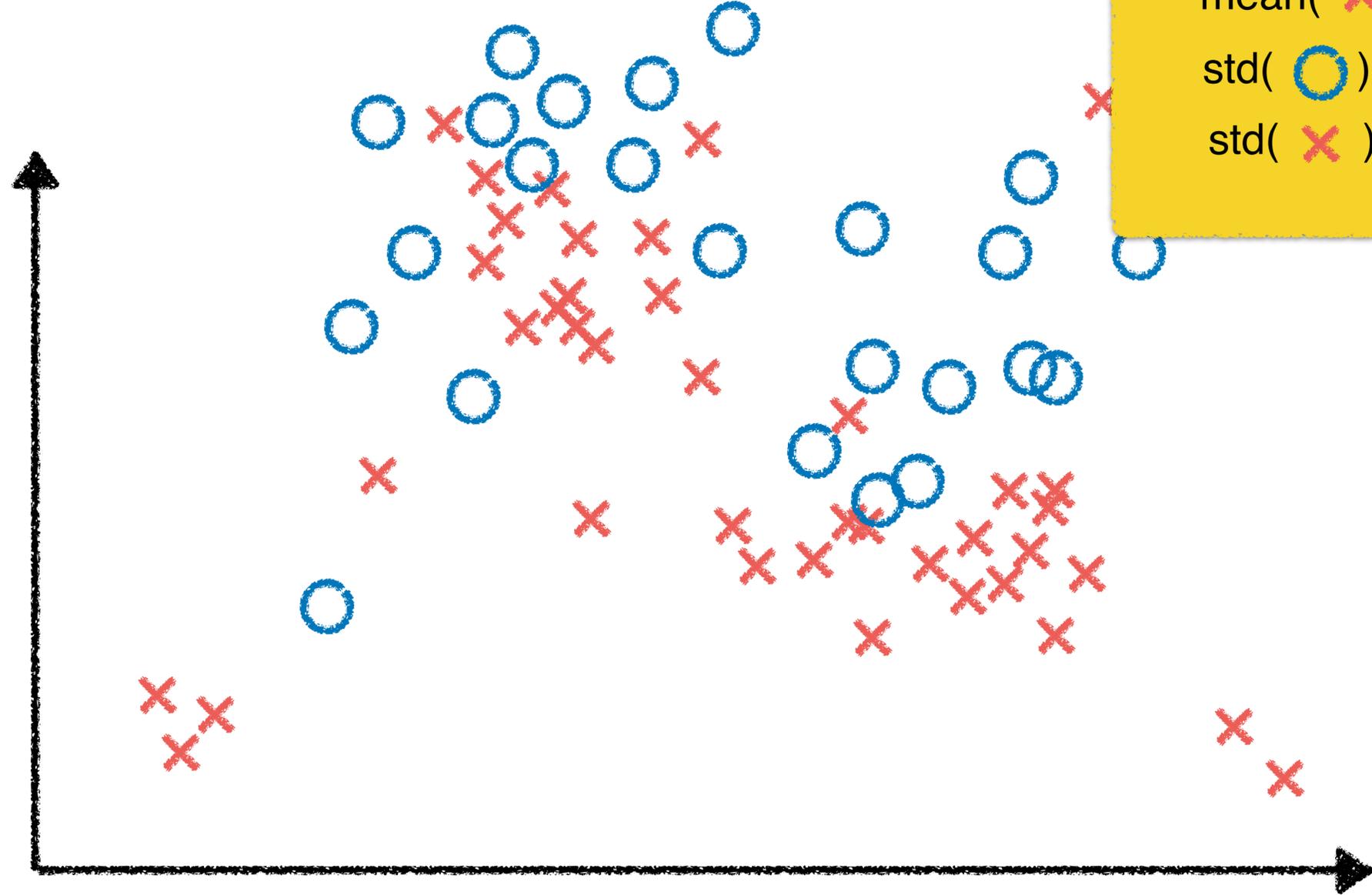
× Class1

Before building any model



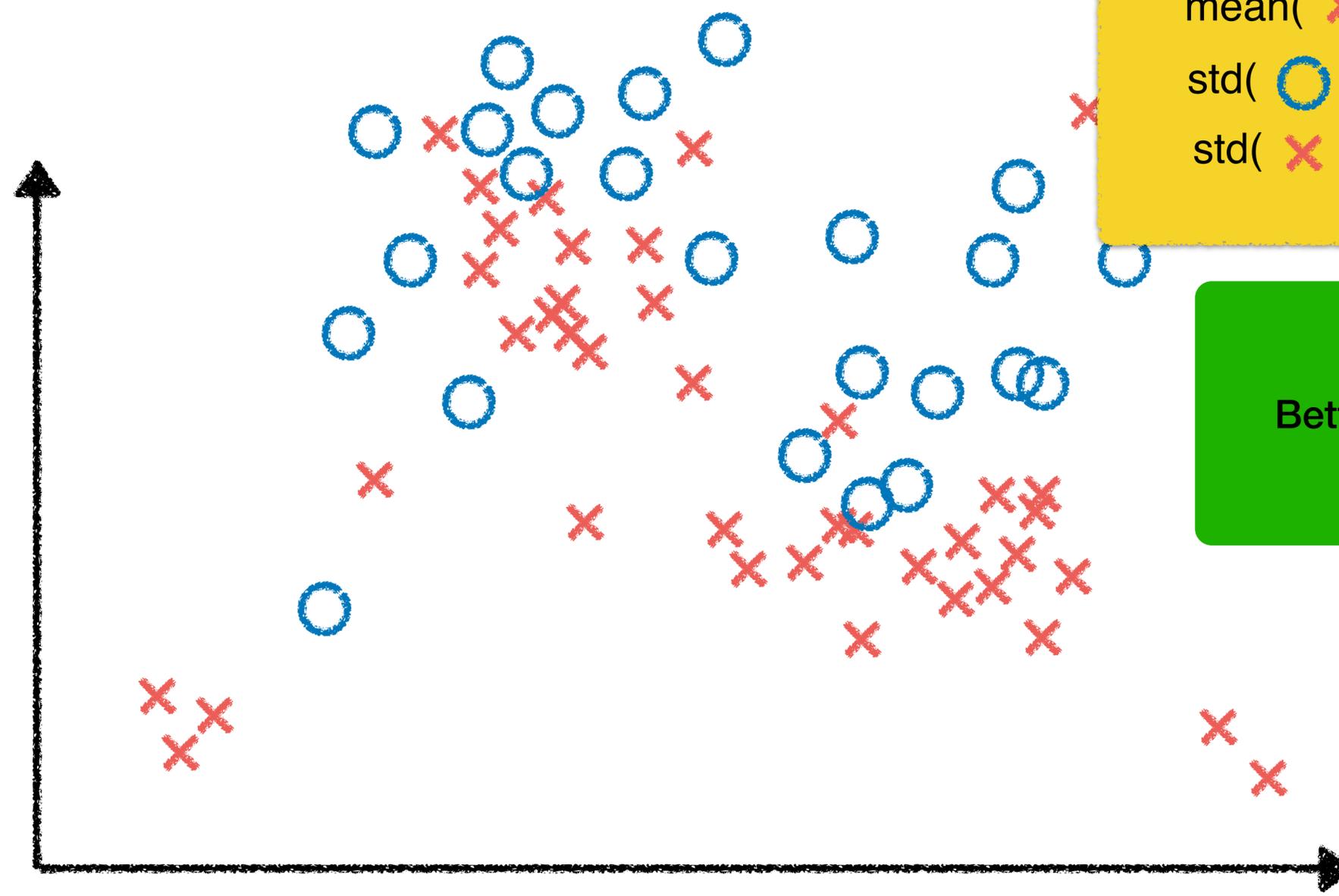
Descriptive statistics

- mean()
- mean()
- std()
- std()



 Class0
 Class1

Before building any model

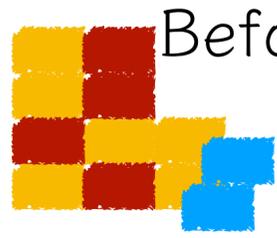


Descriptive statistics

- mean()
- mean()
- std()
- std()

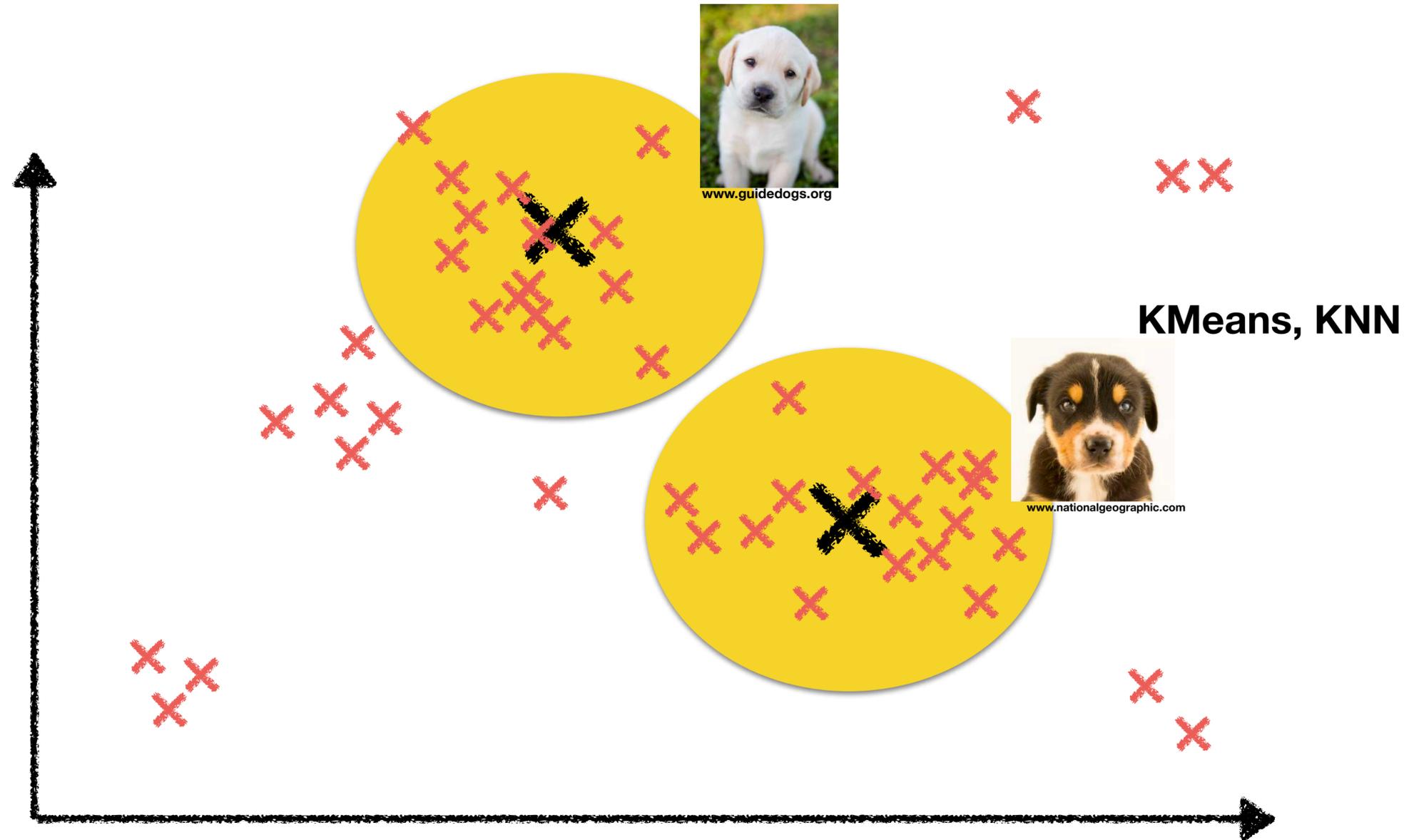
Better way?

 Class0
 Class1



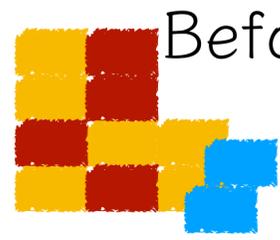
Before building any model

Exploratory data analysis



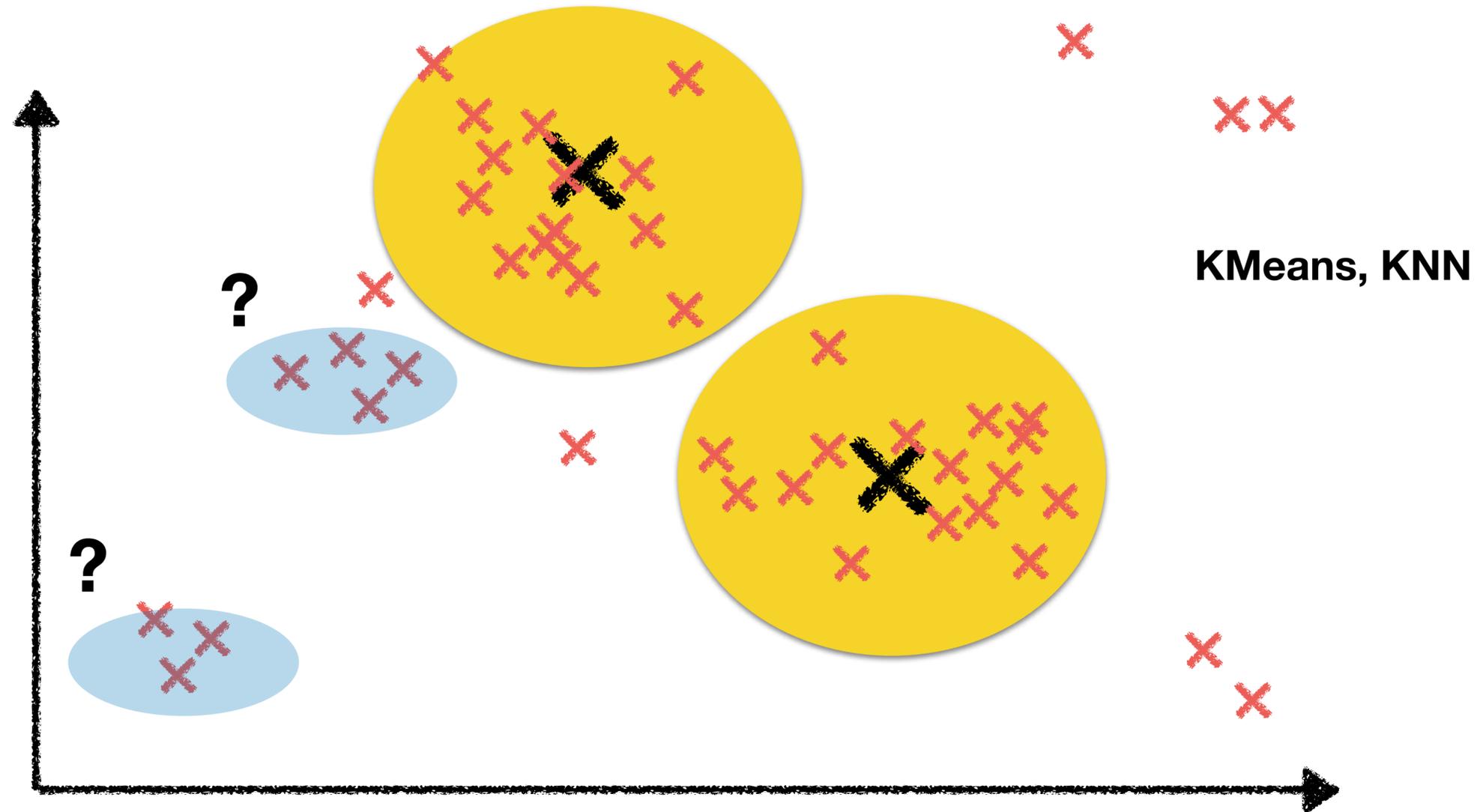
× Observed data

[Simon et al., '07]
[Lin and Bilmes, '11]



Before building any model

Exploratory data analysis



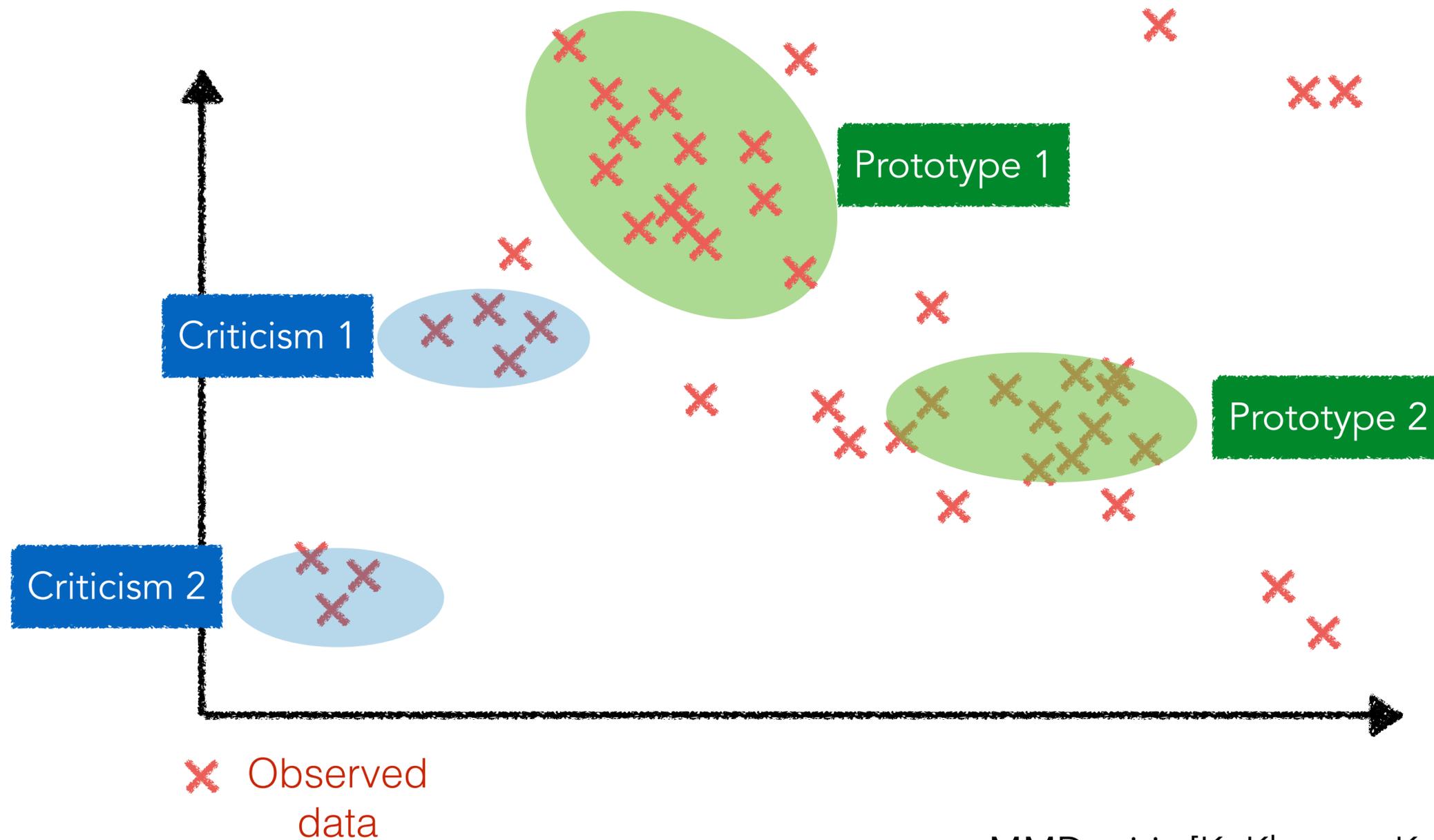
x Observed data

[Simon et al., '07]
[Lin and Bilmes, '11]

Before building any model



Exploratory data analysis

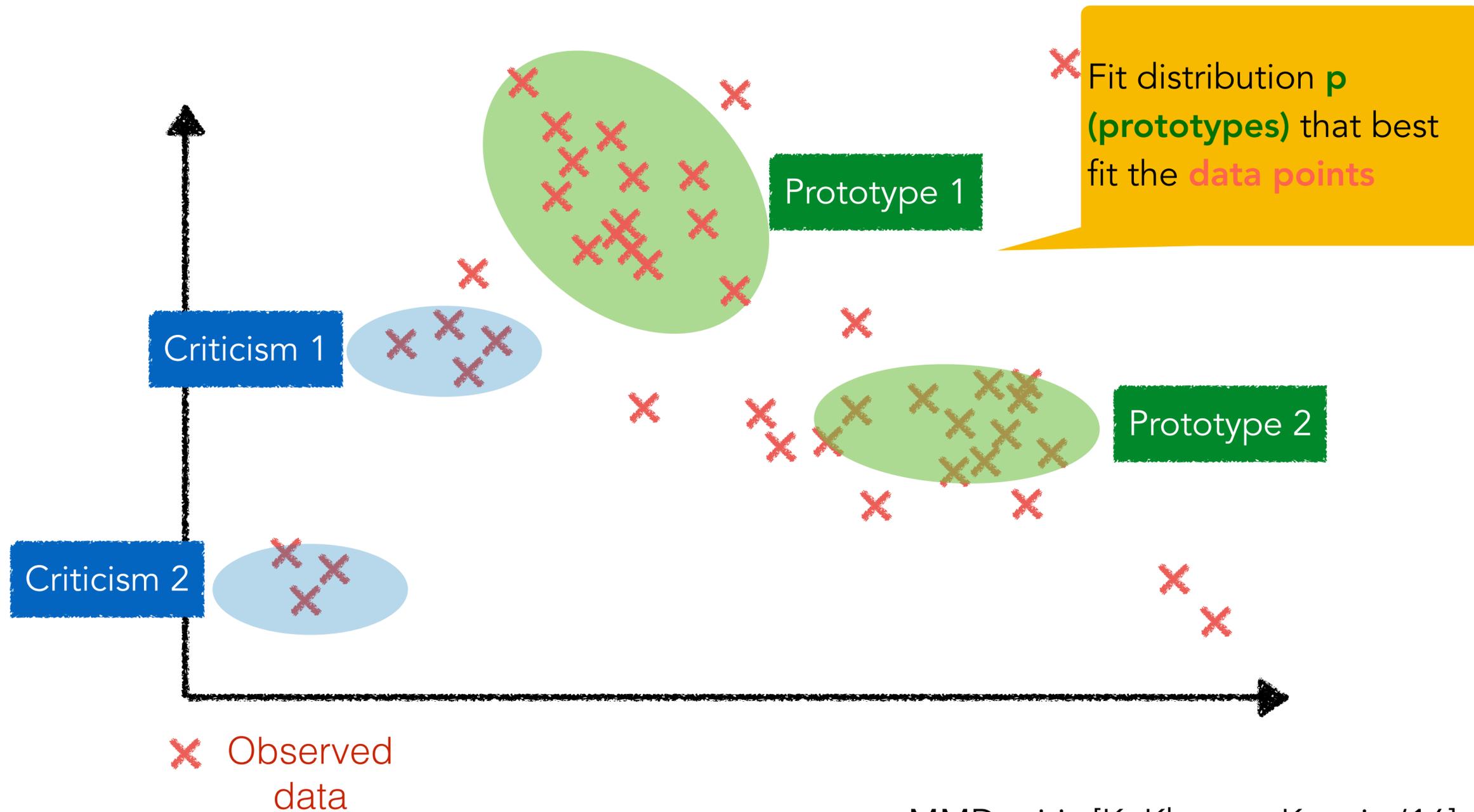


MMD-critic [K. Khanna, Koyejo '16]

Before building any model



Exploratory data analysis

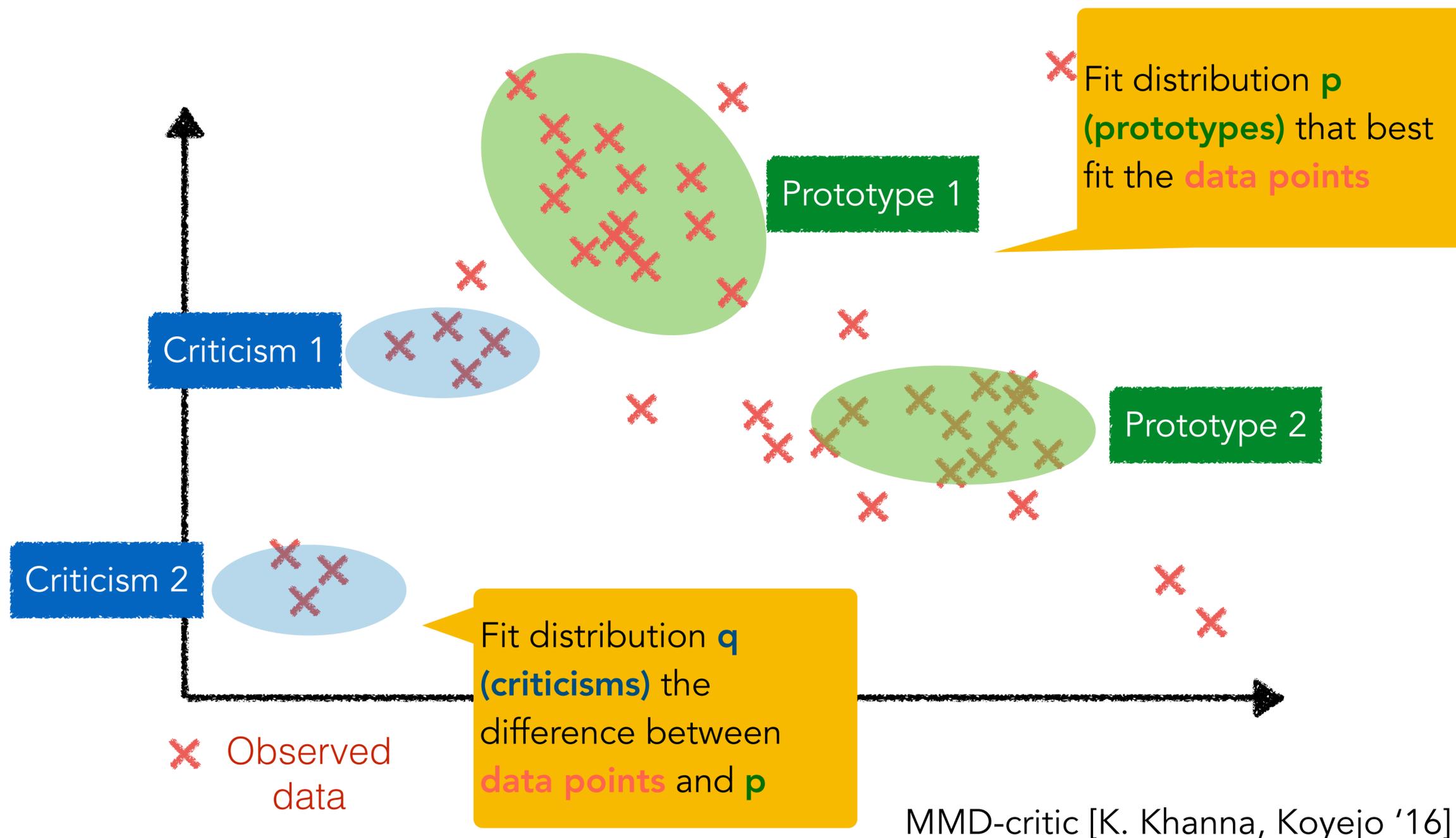


MMD-critic [K. Khanna, Koyejo '16]

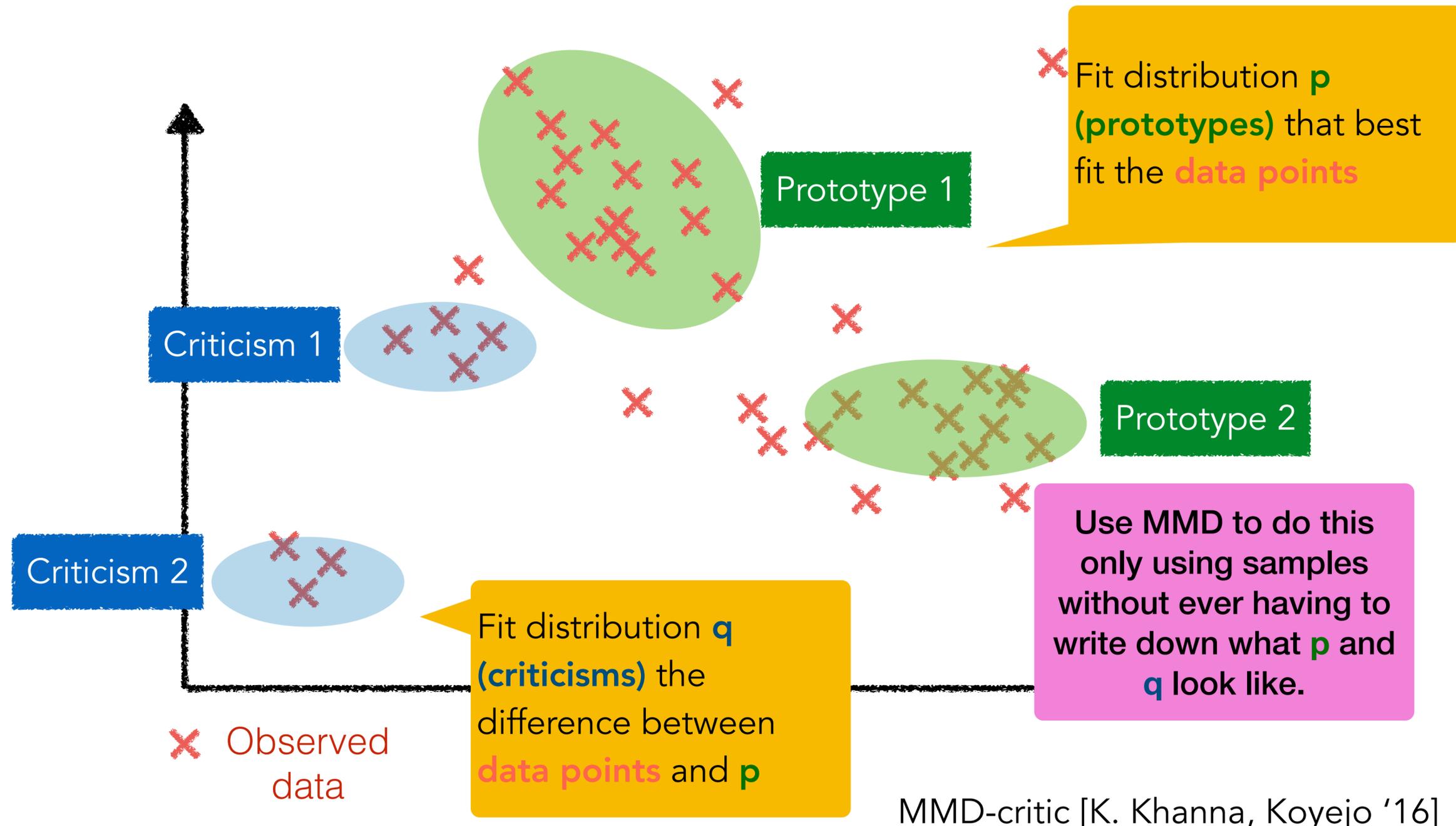


Before building any model

Exploratory data analysis



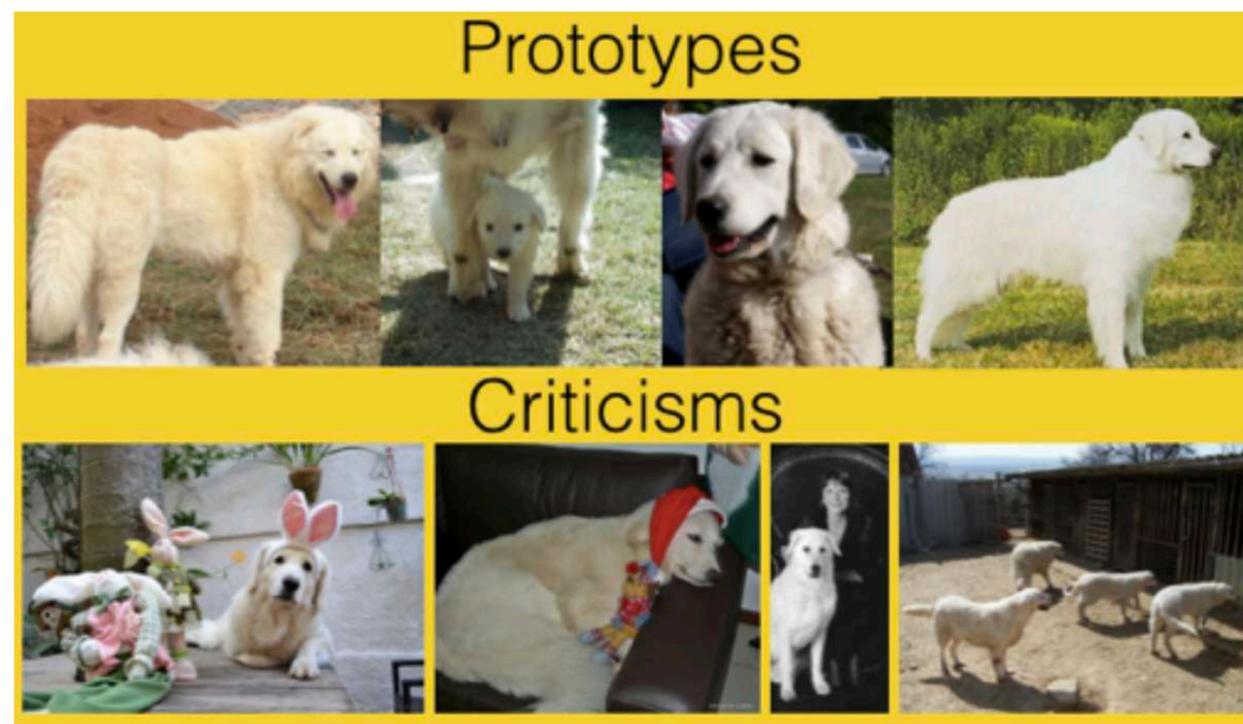
Exploratory data analysis



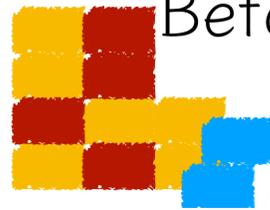


Before building any model

Exploratory data analysis



Before building any model



Exploratory data analysis

Communicating with Interactive Articles

Examining the design of interactive articles by synthesizing theory from disciplines such as education, journalism, and visualization.

Great overview of many exploratory data analysis, highly recommend.

<https://distill.pub/2020/communicating-with-interactive-articles/>

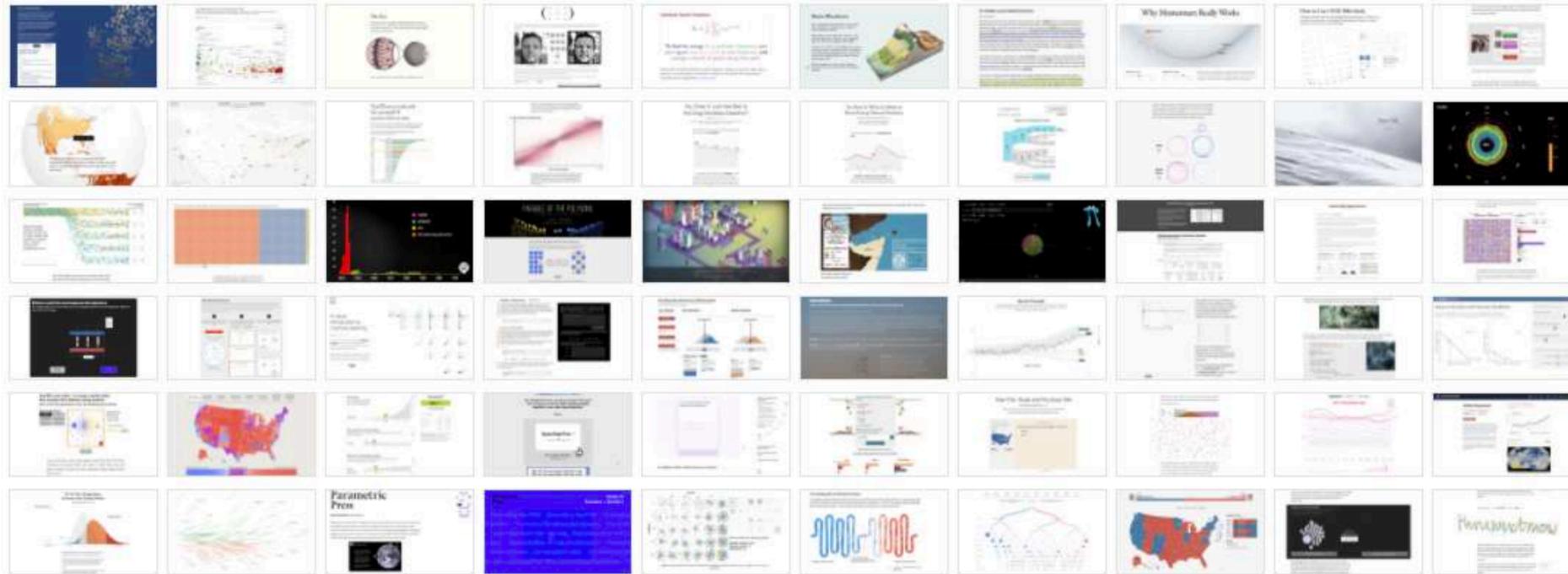
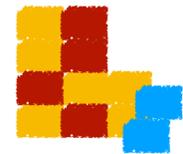


FIGURE 1: Exemplary Interactive Articles From Around The Web. Select an article for more information.

Research Dissemination	Journalism	Education	Policy and Decision Making
	<p>Journalism</p> <p>An informed public strengthens society. While many newsworthy and current events are reported daily, unfortunately the complexity and nuance of such topics are lost in the wildfire sharing of short headlines. This is effective dissemination without context. Yet many of the most impactful stories require a deep understanding of the various locations, personale, and perspectives involved. Interactive articles can be used to break down these complex topics into more approachable pieces, show their connections in relation to the main message, highlight the impact of investigative reporting, and inform a wide readership of current events and impactful stories.</p>	<p>OPPORTUNITIES</p> <ul style="list-style-type: none"> Tell stories from multiple dynamic perspectives and levels of detail Highlight importance of a story or report Improve reader comprehension of stories <p>CHALLENGES</p> <ul style="list-style-type: none"> Require active reading in a reader that may be expecting bite-sized news Many readers viewing on mobile devices requires responsive design Difficult to produce at the fast pace of news cycles 	
	<p>What's Really Warming the World? [16]</p> <p>A segmented-story that layers different natural and industrial factors recorded since 1880 on the same axis to compare and contrast which factors are correlated with the increase of the global temperature rise.</p>	<p>You Draw It: How Family Income Predicts Children's College Chances [17]</p> <p>An article with a partially complete visualization that prompts the reader to draw the trendline that completes the relationship between family income and the percentage of children who attend college, challenging one's prior belief about the data.</p>	<p>The Uber Game [18]</p> <p>A choose-your-own-adventure narrative news game that puts the reader behind the wheel and explores the economics and life of being an Uber driver.</p>

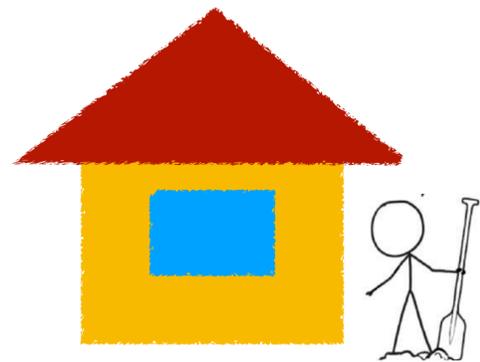
AUTHORS	AFFILIATIONS	PUBLISHED	DOI
Fred Hohman	Georgia Tech	Sept. 11, 2020	10.23915/distill.00028
Matthew Conlen	University of Washington		
Jeffrey Heer	University of Washington		
Duen Horng (Polo) Chau	Georgia Tech		

Types of interpretability methods



Explaining data

$$\operatorname{argmax}_E Q(\mathbf{Explanation} | \mathbf{Human}, \mathbf{Data}, \mathbf{Task})$$



My ML



Building inherently interpretable model

$$\operatorname{argmax}_{E, M} Q(\mathbf{Explanation}, \mathbf{Model} | \mathbf{Human}, \mathbf{Data}, \mathbf{Task})$$

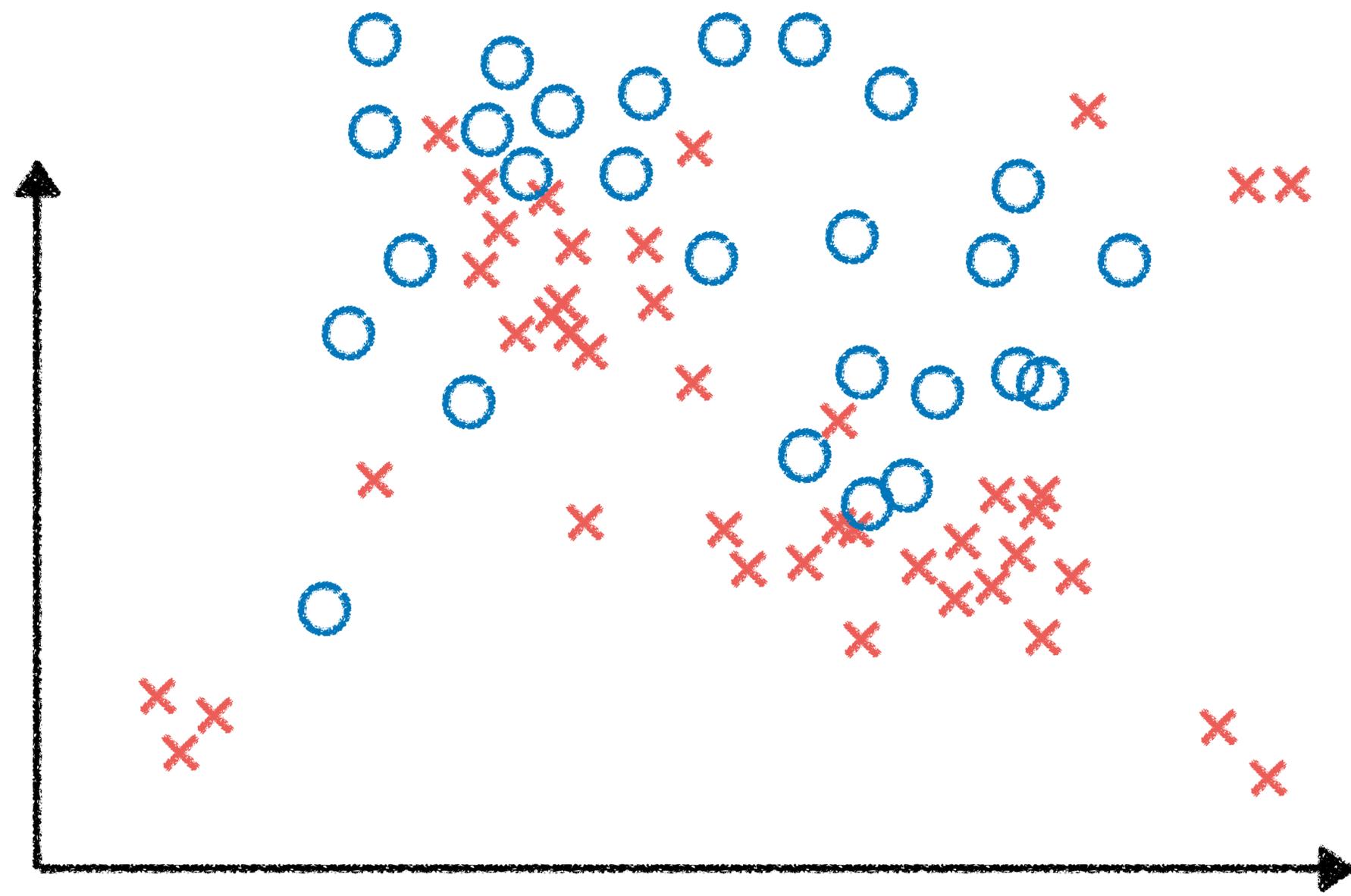
Model == explanation

No approximation needed



Post-training interpretability methods

$$\operatorname{argmax}_E Q(\mathbf{Explanation} | \mathbf{Model}, \mathbf{Human}, \mathbf{Data}, \mathbf{Task})$$

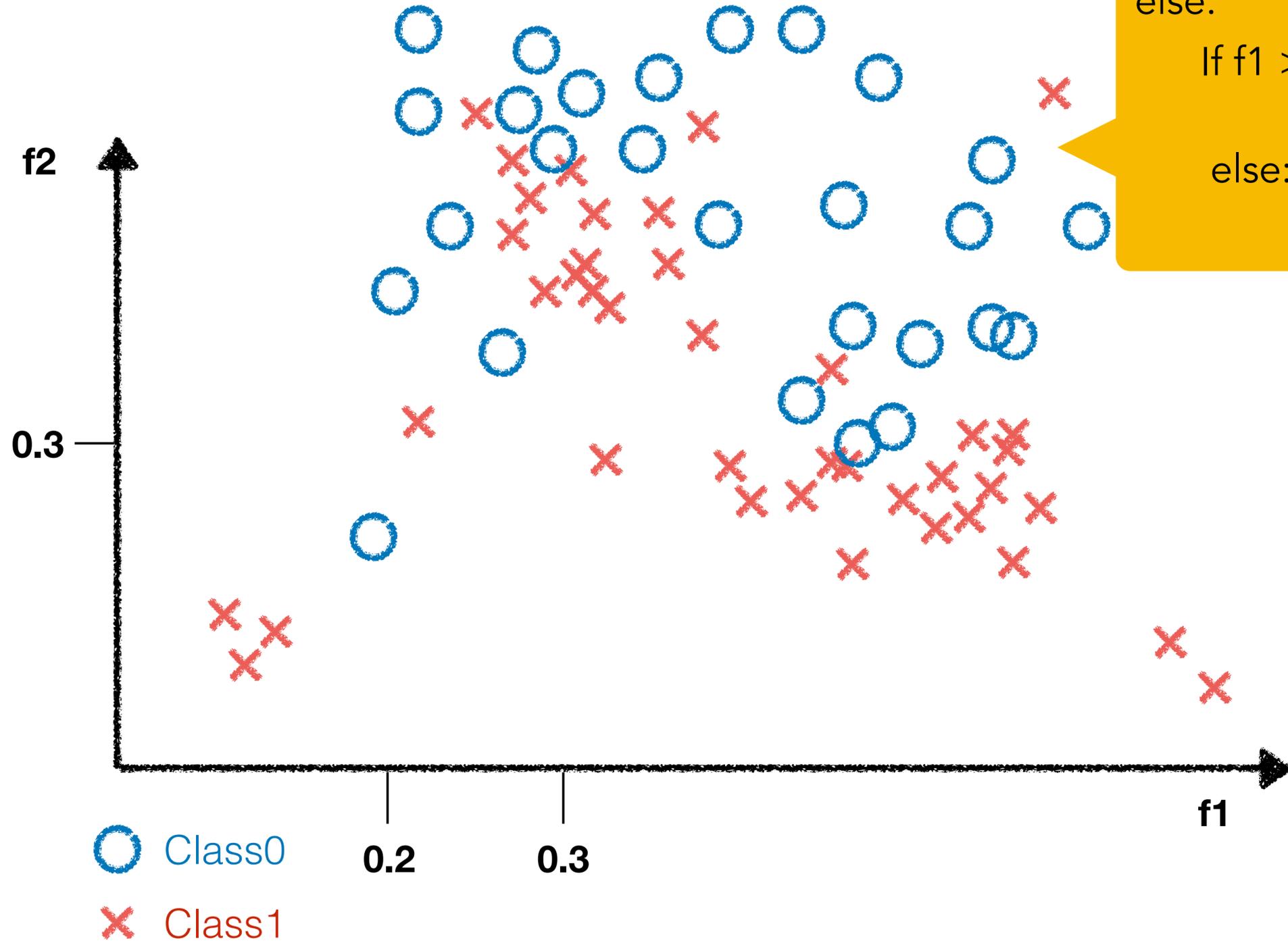


○ Class0

× Class1



Building a new model

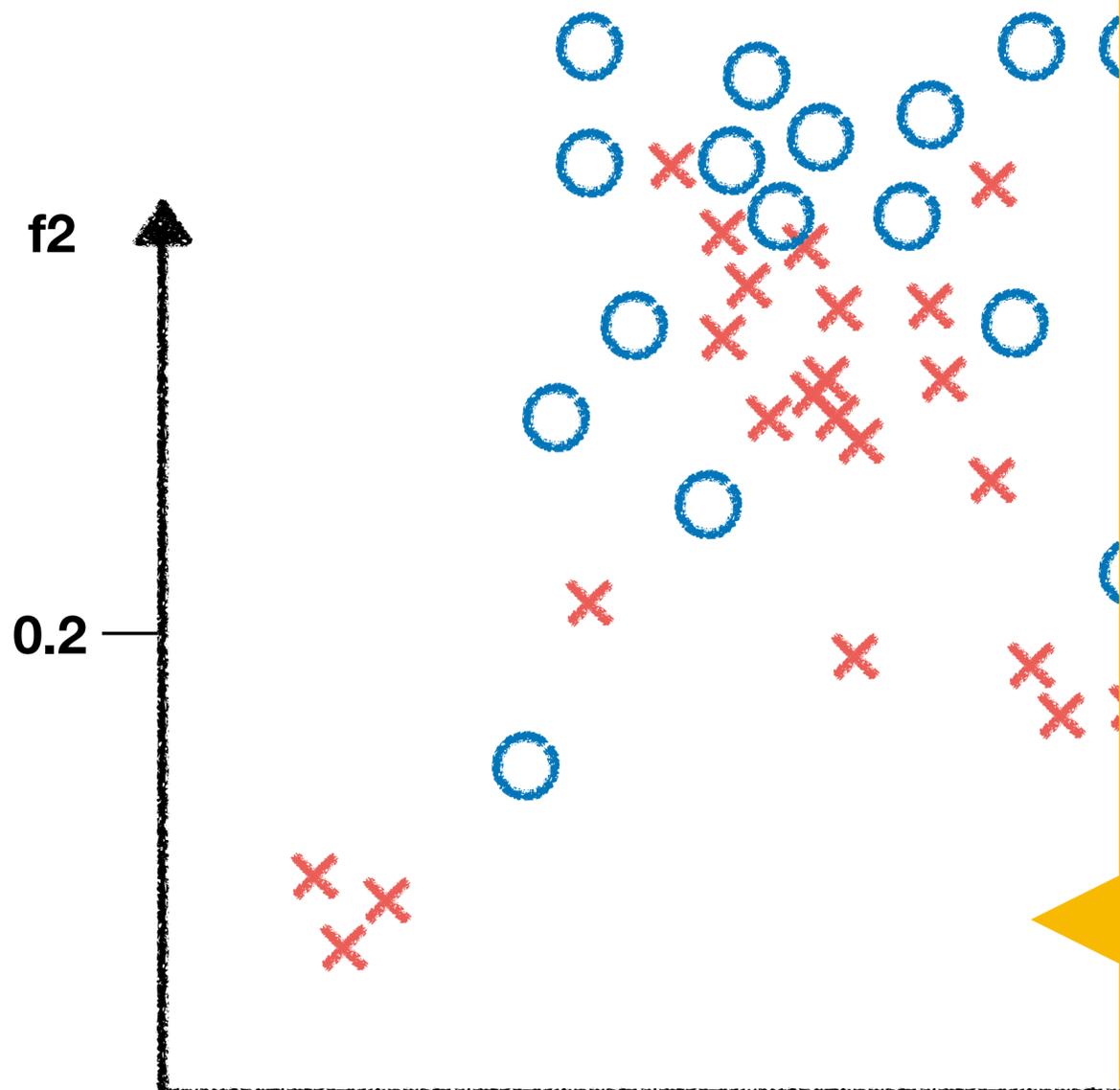


Rule based

```
If  $f_2 < 0.3$ :  
    predict  $\times$   
else:  
    If  $f_1 > 0.2$  and  $f_1 < 0.3$ :  
        predict  $\circ$   
    else:  
        ...
```



Building a new model



○ Class0

× Class1

Rule based

```
If  $f_1 < 0.1$ :  
    predict ×  
else:  
    If  $f_2 > 0.4$  and  $f_2 < 0.6$ :  
        predict ○  
    else:  
        ...
```

decision trees, rule lists, rule sets

[Breiman, Friedman, Stone, Olshen 84]

[Rivest 87]

[Muggleton and De Raedt 94]

[Wang and Rudin 15]

[Letham, Rudin, McCormick, Madigan '15]

[Hauser, Toubia, Evgeniou, Befurt, Dzyabura 10]

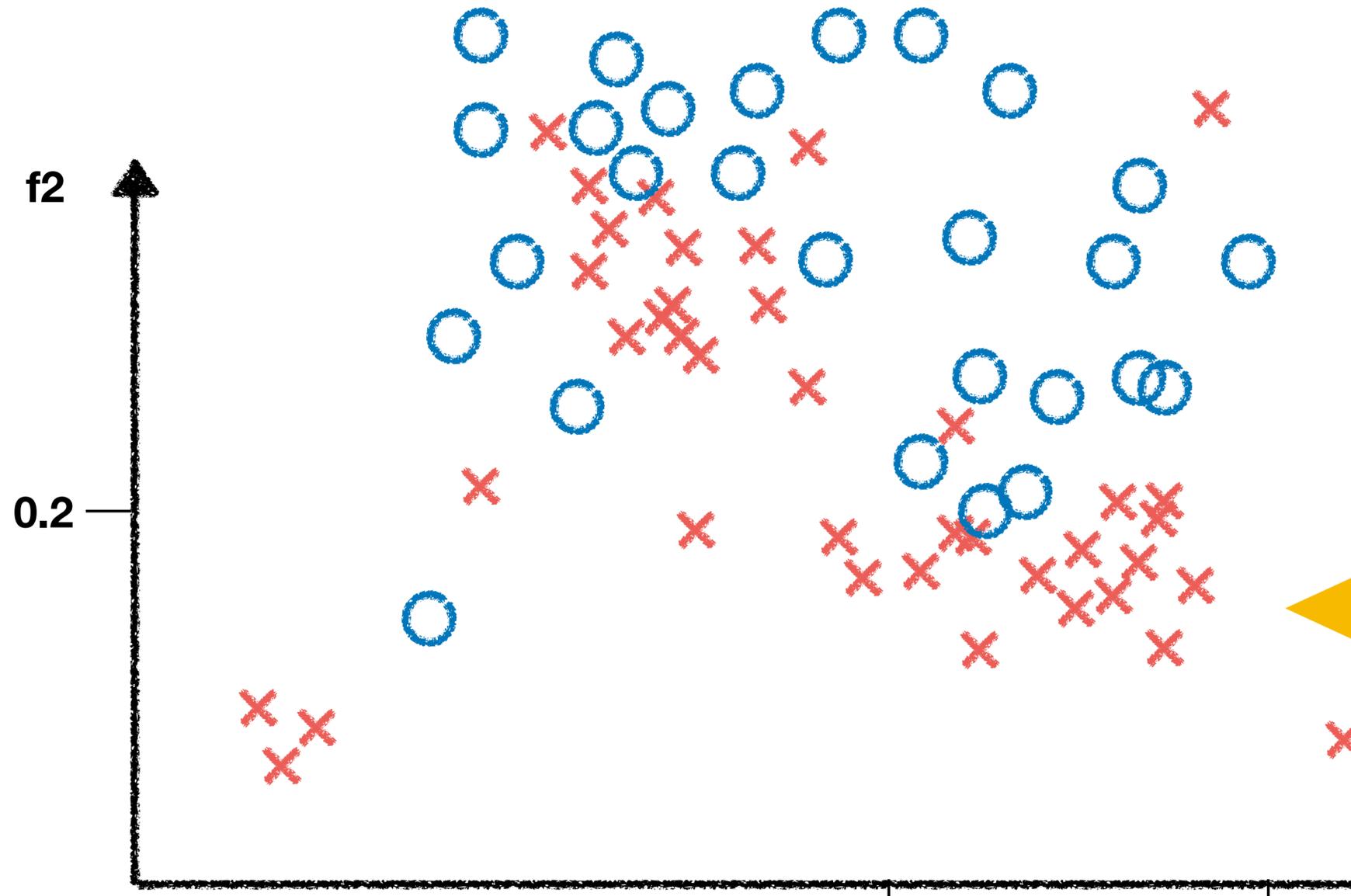
[Wang, Rudin, Doshi-Velez, Liu, Klampfl, MacNeille 17]

Learning certifiably **optimal** rule list

[Angelino, Larus-Stone, Alabi, Seltzer, Rudin '18]



Building a new model

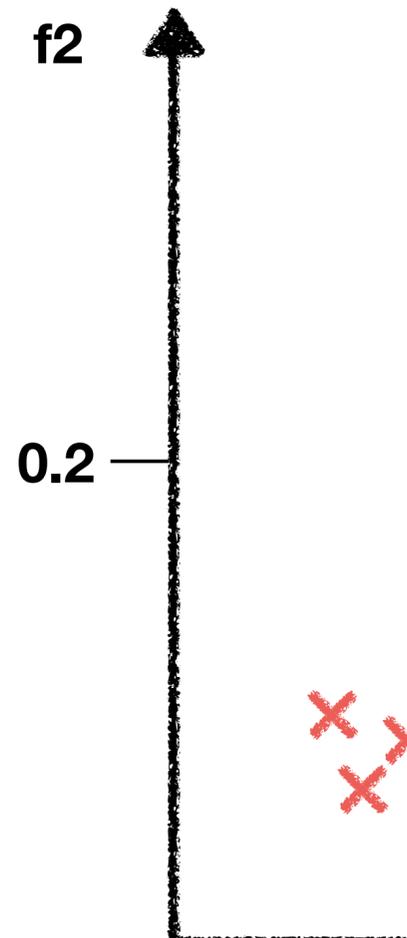


○ Class0
× Class1

Fit a simpler function
for each feature

A yellow callout box containing a diagram of a 2D coordinate system with axes $f1$ and $f2$. A blue curve is fitted to the Class 0 data points, and a pink curve is fitted to the Class 1 data points. The curves are non-linear and complex, illustrating the process of fitting a function to each feature.

Fit a simpler function



○ Class0
 × Class1

Linear model

$$y = \beta_0 + \beta_1 x_1 + \dots + \beta_n x_n$$

generalized linear model

$$g(y) = \beta_0 + \beta_1 x_1 + \dots + \beta_n x_n$$

generalized additive model

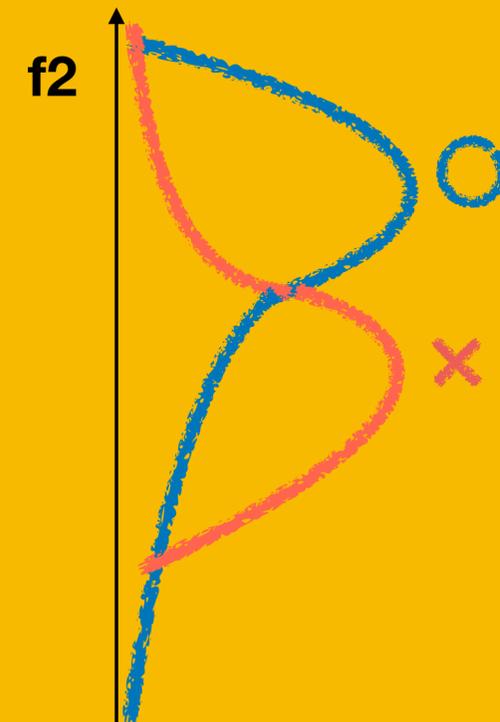
$$g(y) = f_1(x_1) + \dots + f_n(x_n)$$

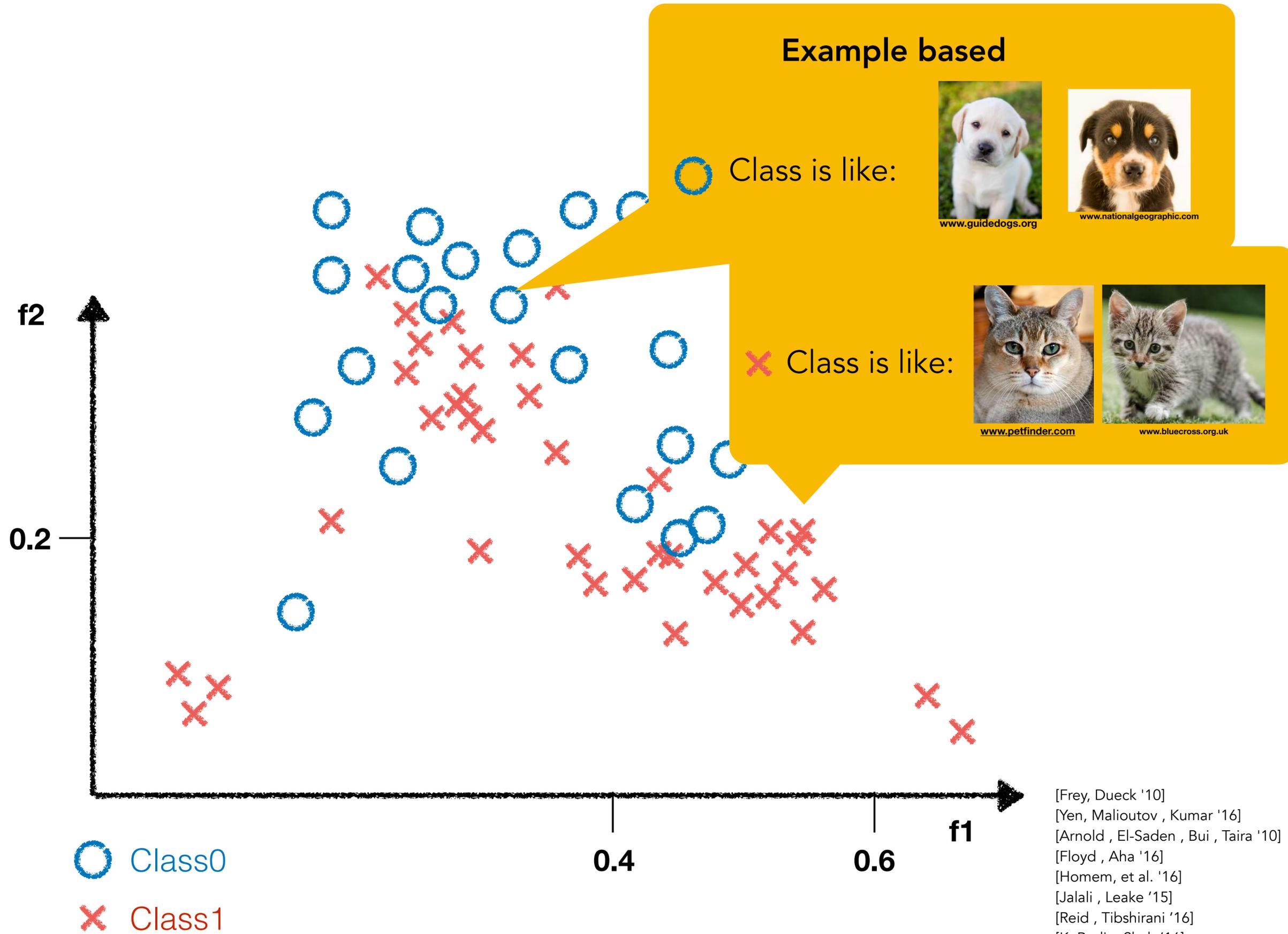
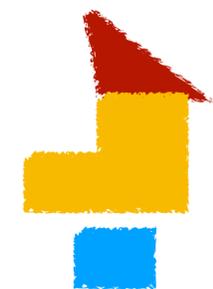
generalized additive2 model

$$g(E[y]) = \sum f_i(x_i) + \sum f_{ij}(x_i, x_j);$$

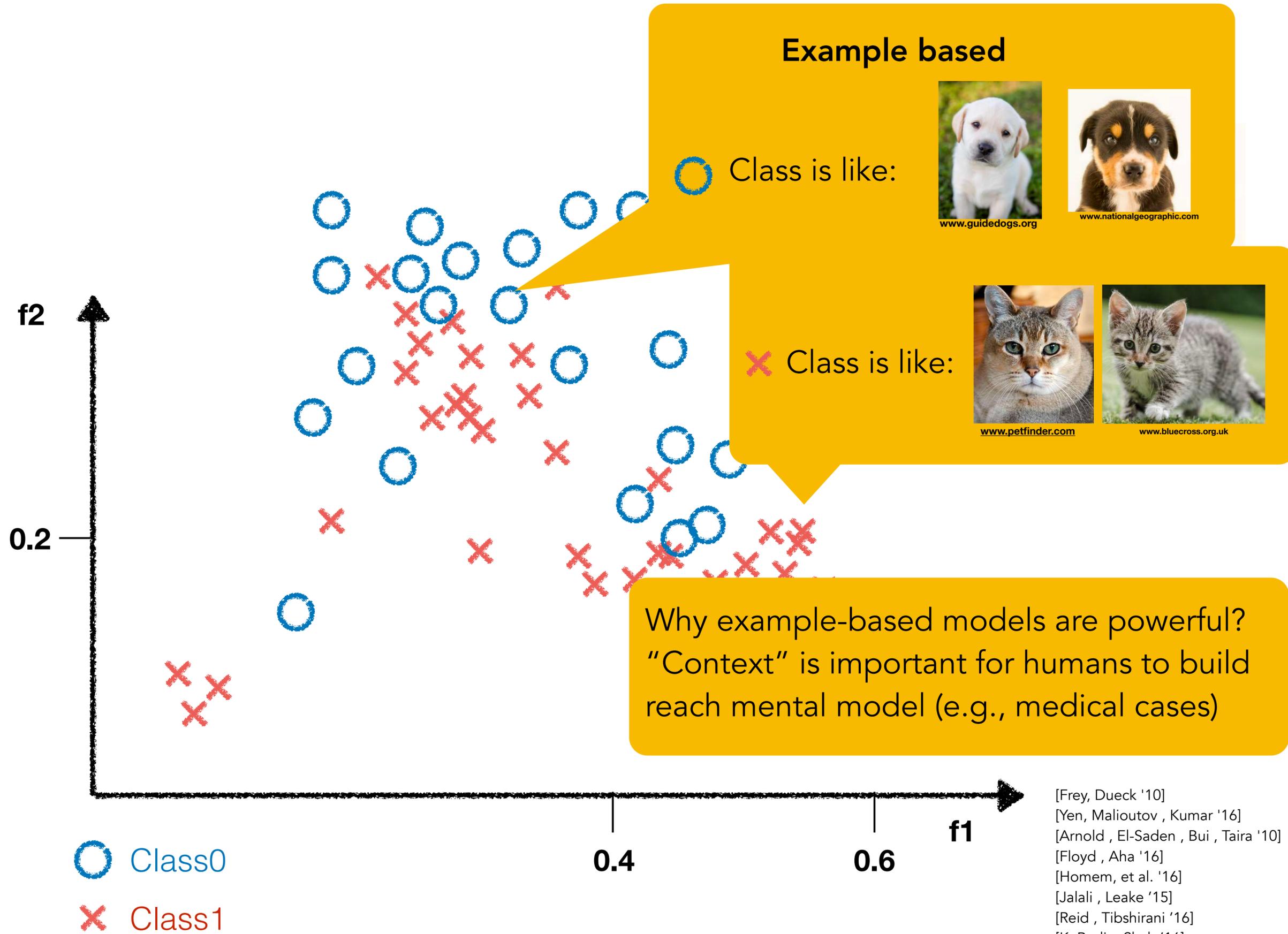
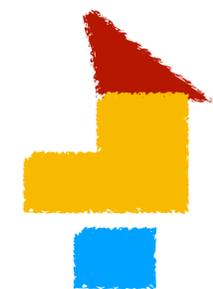
[Lou et al. '12]

Table edited from [Gehrke et al. '12]

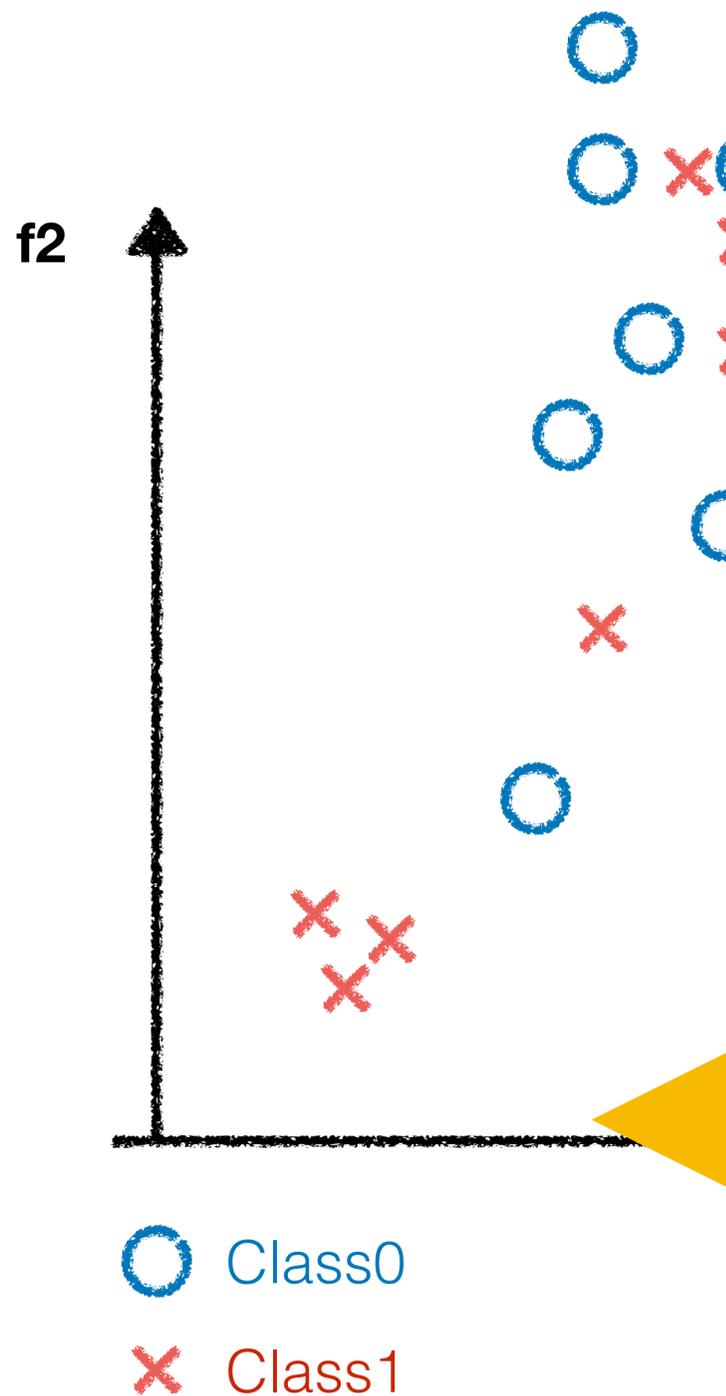
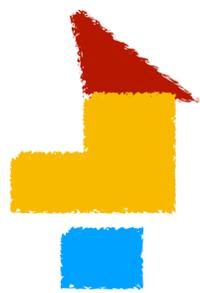




[Frey, Dueck '10]
[Yen, Malioutov , Kumar '16]
[Arnold , El-Saden , Bui , Taira '10]
[Floyd , Aha '16]
[Homem, et al. '16]
[Jalali , Leake '15]
[Reid , Tibshirani '16]
[K. Rudin, Shah '16]
[Koh, Liang '17]

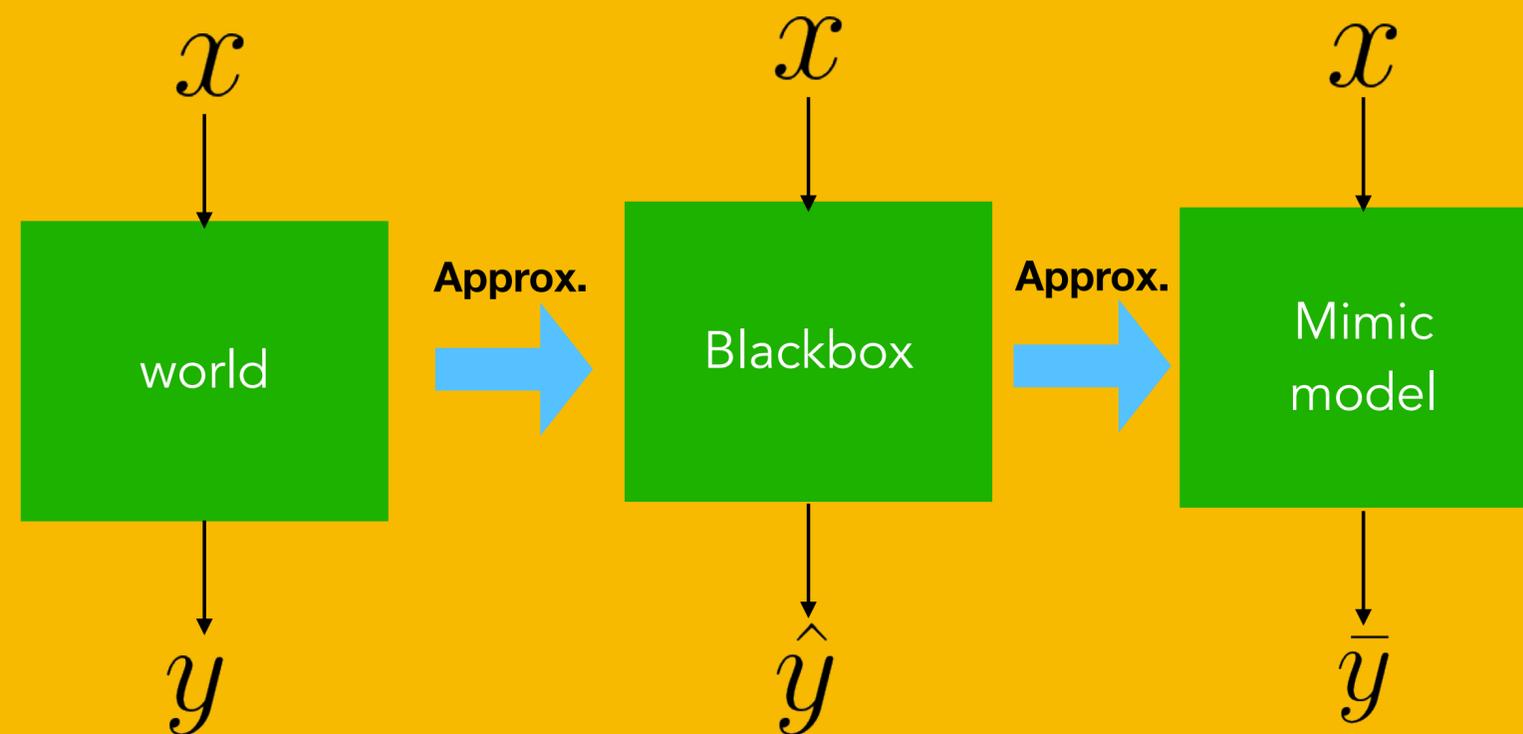


[Frey, Dueck '10]
[Yen, Malioutov, Kumar '16]
[Arnold, El-Saden, Bui, Taira '10]
[Floyd, Aha '16]
[Homem, et al. '16]
[Jalali, Leake '15]
[Reid, Tibshirani '16]
[K. Rudin, Shah '16]
[Koh, Liang '17]



Mimic models, model distillation

Building a simpler model that walks, talks, barks like the complex model.



[Bucila et al. '06]

Do Deep Nets Really Need to be Deep? [Ba et al. '14]

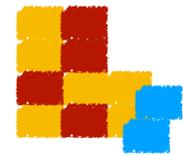
Distilling the Knowledge in a Neural Network [Hinton et al. '15] [Frosst '17]

The Lottery Ticket Hypothesis: Finding Sparse, Trainable Neural Networks

Jonathan Frankle, Michael Carbin

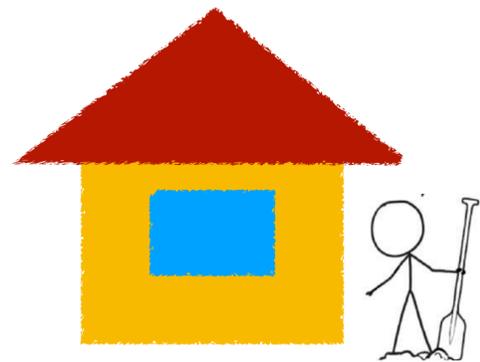
“A randomly-initialized, dense neural network contains a subnetwork that is initialized such that — when trained in isolation — it can match the test accuracy of the original network after training for at most the same number of iterations.”

Types of interpretability methods



Explaining data

$$\operatorname{argmax}_E Q(\mathbf{Explanation} | \mathbf{Human}, \mathbf{Data}, \mathbf{Task})$$



My ML



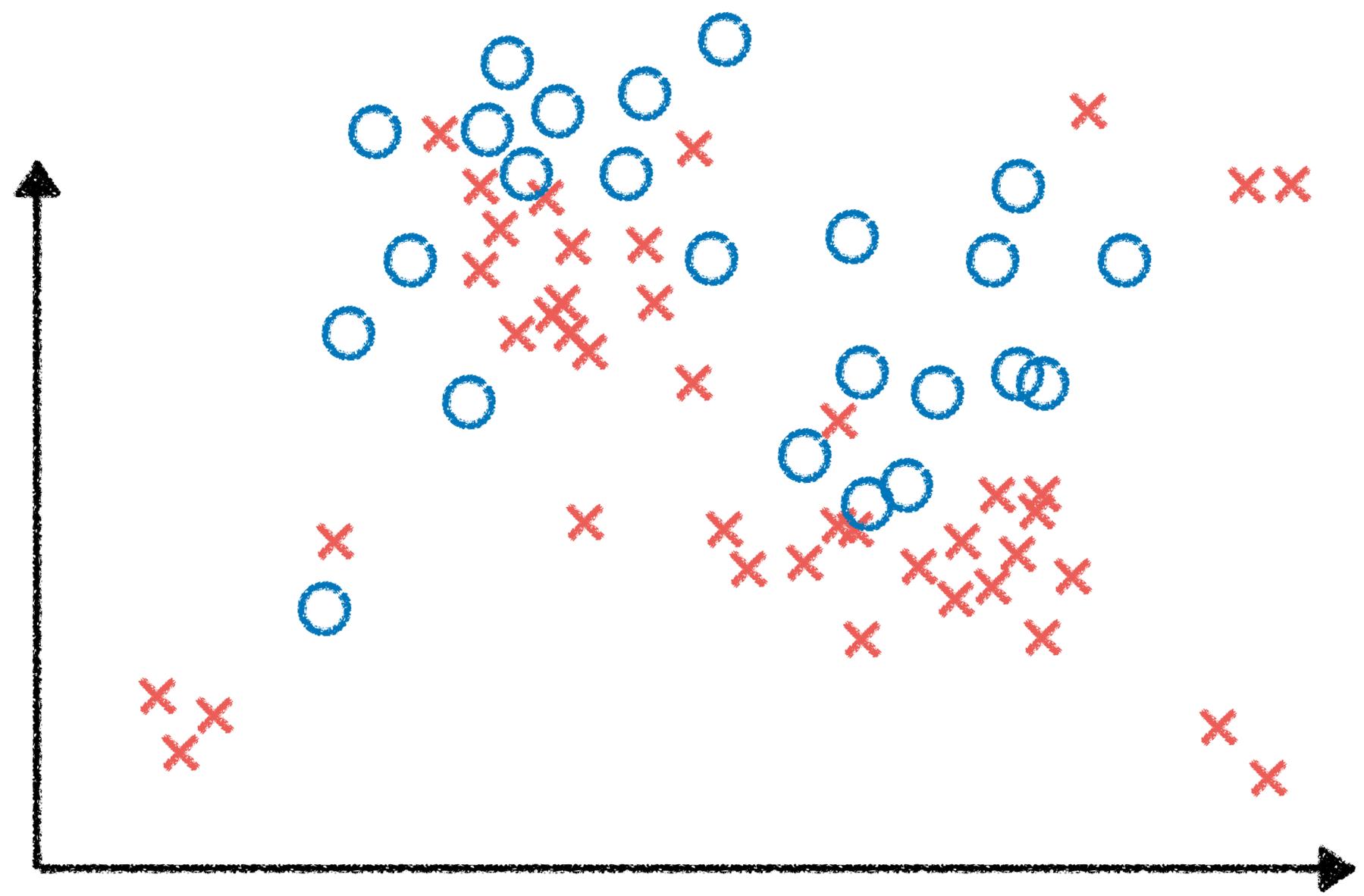
Building inherently interpretable model

$$\operatorname{argmax}_{E, M} Q(\mathbf{Explanation}, \mathbf{Model} | \mathbf{Human}, \mathbf{Data}, \mathbf{Task})$$



Post-training interpretability methods

$$\operatorname{argmax}_E Q(\mathbf{Explanation} | \mathbf{Model}, \mathbf{Human}, \mathbf{Data}, \mathbf{Task})$$

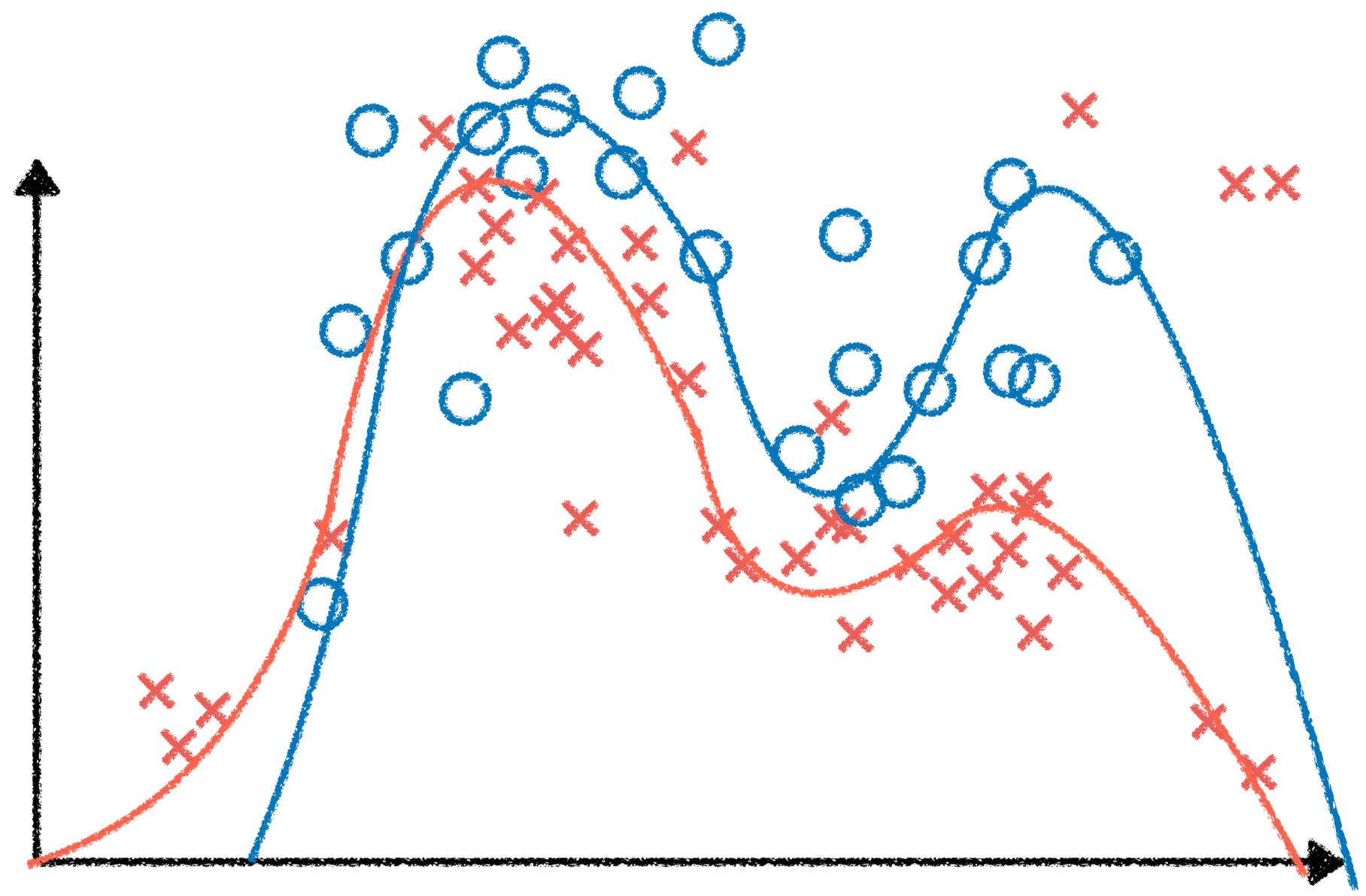


○ Class0

× Class1



After building a model

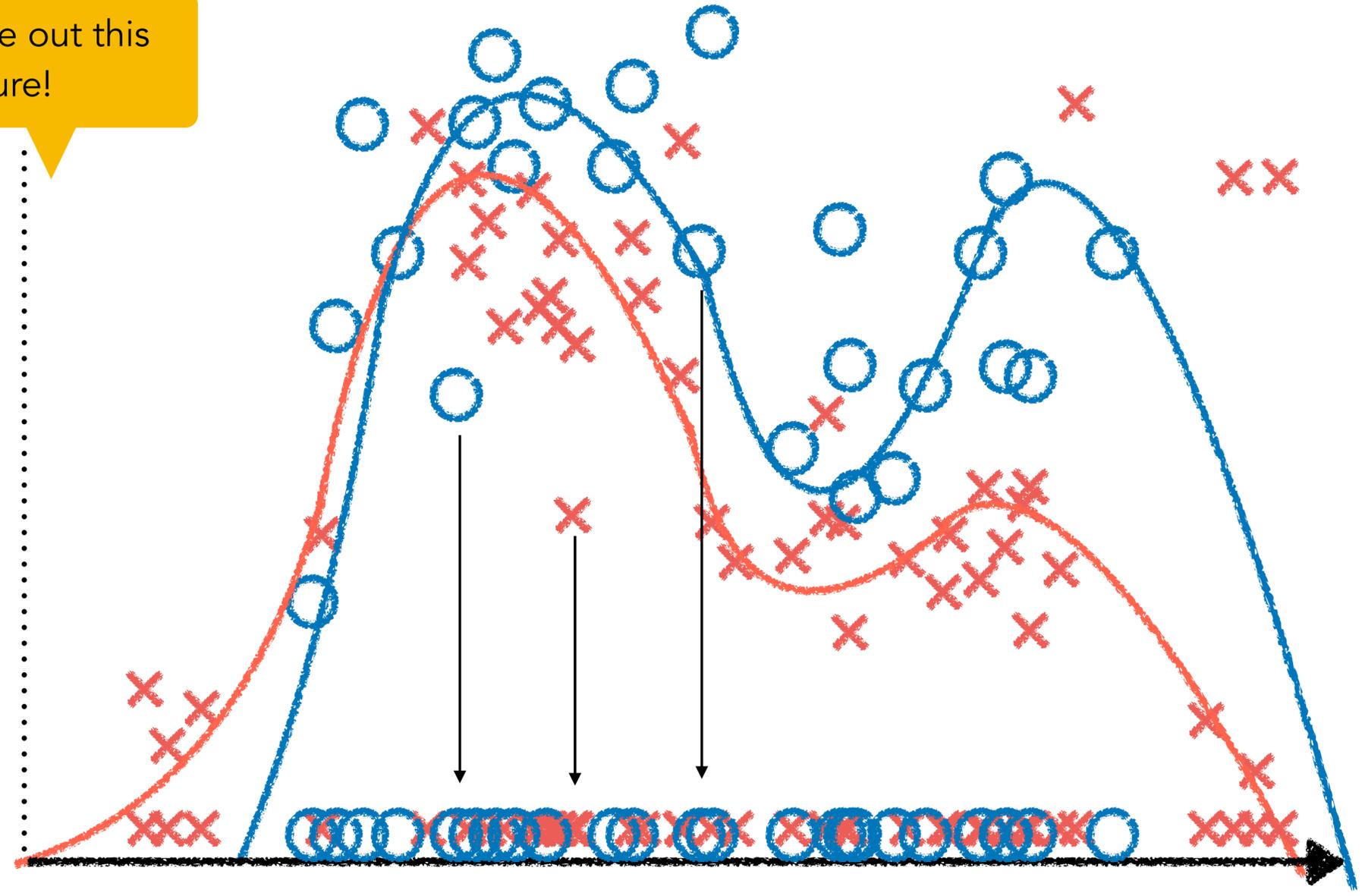


- Class0
- × Class1



After building a model

Marginalize out this feature!

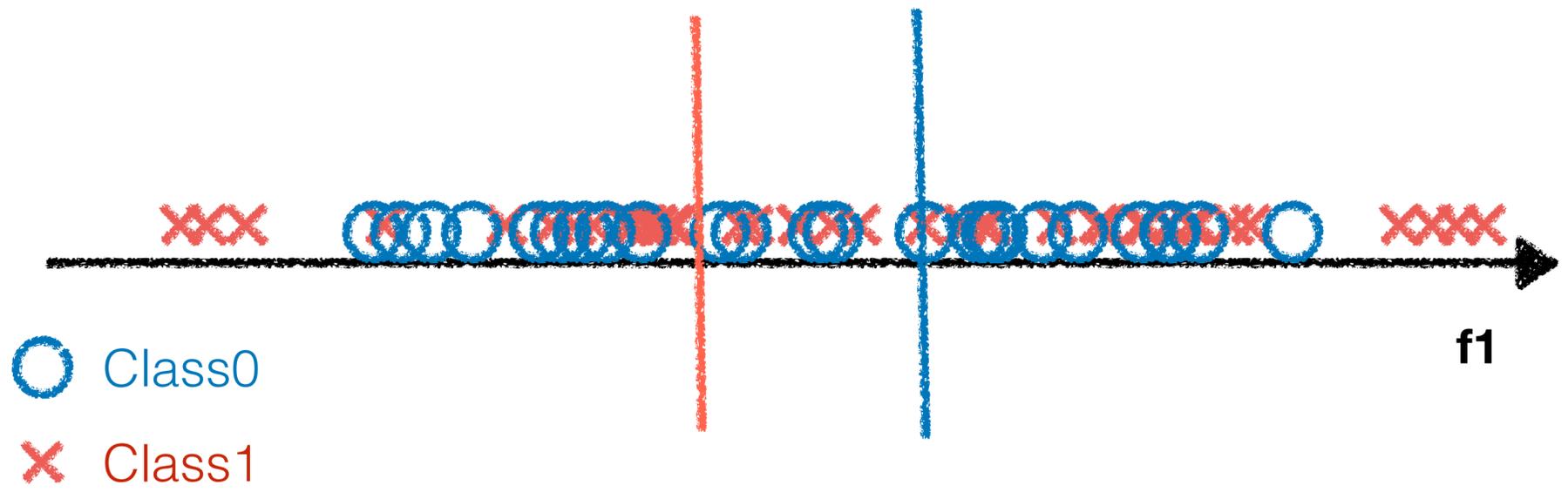


○ Class0
× Class1



After building a model

1. Ablation test: train without that feature/data points and see the impact





After building a model

Definition of importance: "how would the model's predictions change if a training input were modified?"

1. Ablation test: train without that feature/data points and see the impact

Smarter ablation Influence functions [Koh et al.'17]

To classify this image:

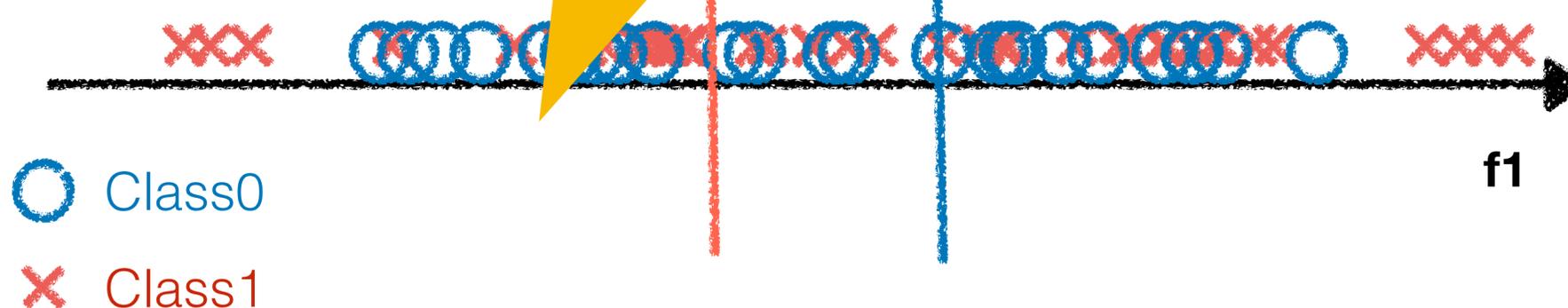


Model found these images most helpful

SVM



Inception

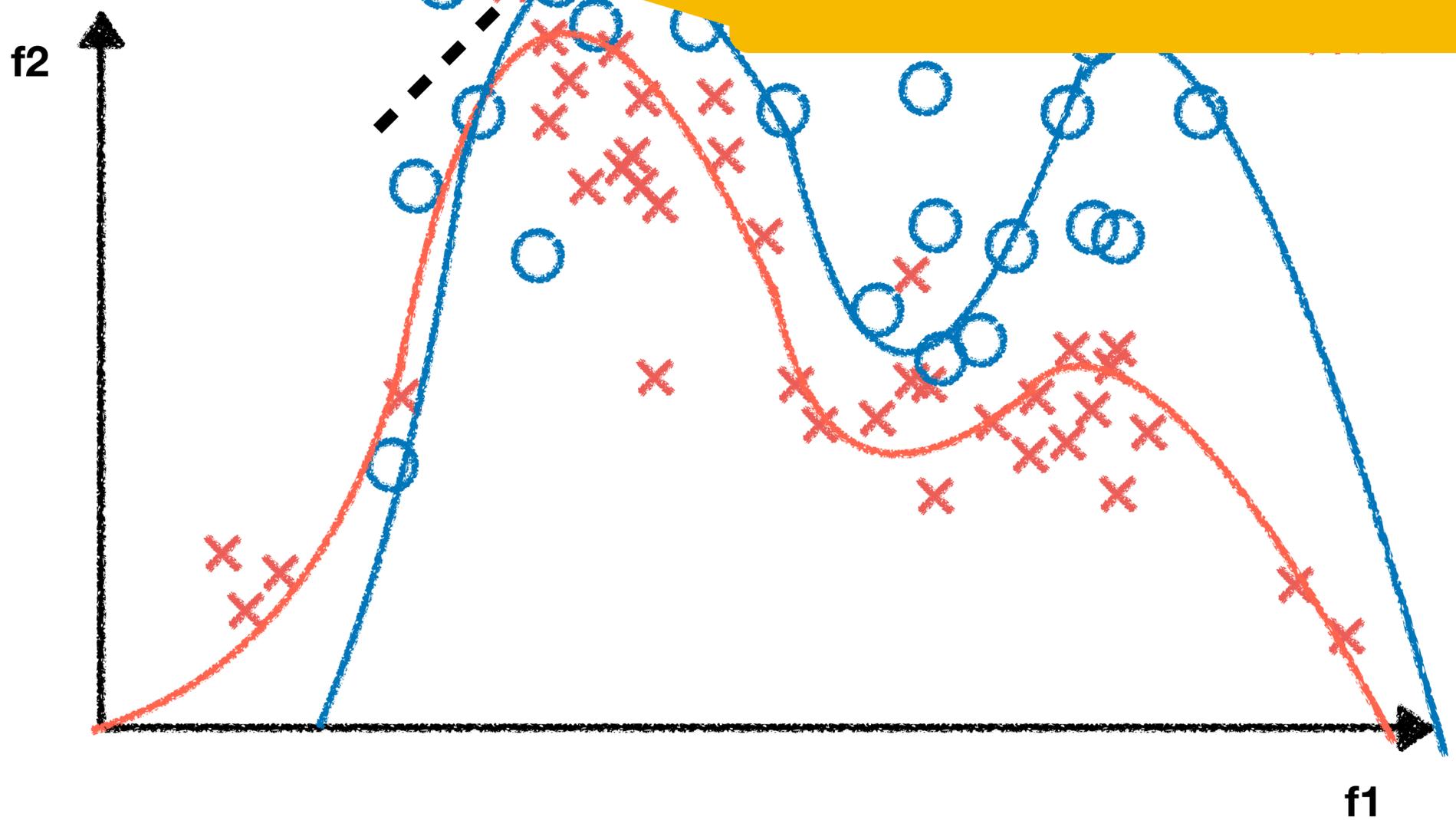




After building a model

$$\frac{\partial p(x)}{\partial f1} = \frac{\partial p(x)}{\partial x_{ij}}$$

1. Ablation test: train without that feature/data and see the impact
2. Sensitivity analysis/fitting linear function/gradient-based

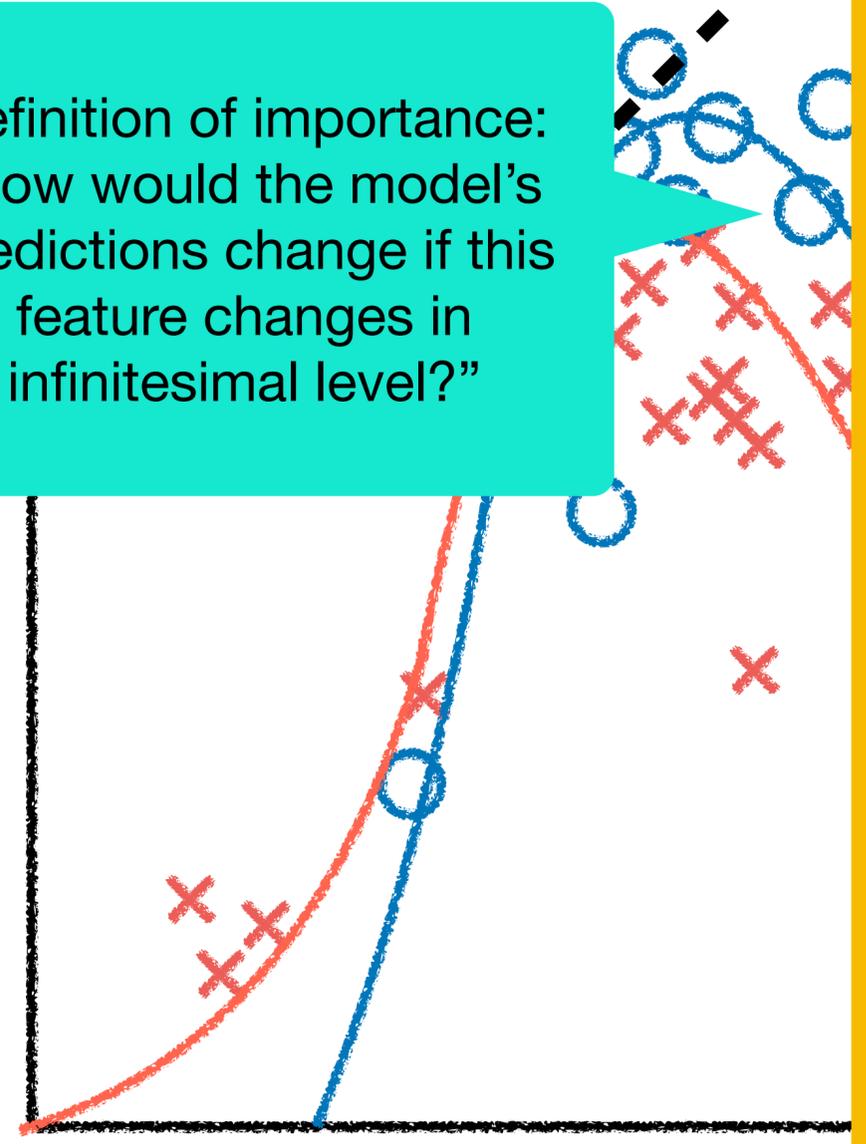




After building a model

$$\frac{\partial p(x)}{\partial x} = \frac{\partial p(x)}{\partial x}$$

Definition of importance:
“how would the model’s predictions change if this feature changes in infinitesimal level?”



1. Ablation test: train without that feature/data and see the impact
2. Sensitivity analysis/fitting linear function/gradient-based

Sensitivity analysis on model
[Ribeiro et al. '16]

Want local explanation
of the **+** data point



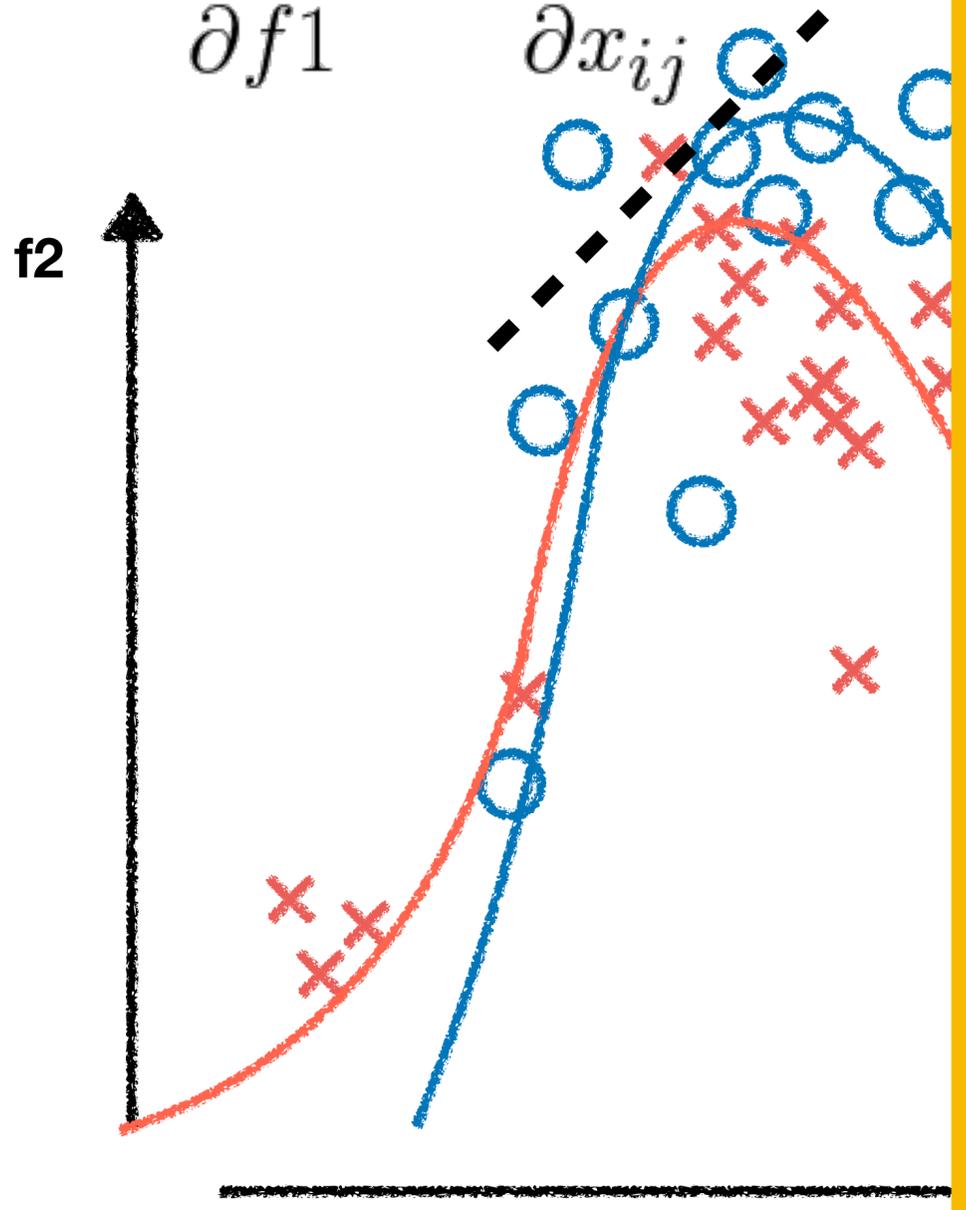
Locally fitted linear function

Many sensitivity analysis literature
[Ribeiro et al. '16] [Simonyan et al., '13] [Li et al., '16]
[Datta et al. '16] [Adler et al., '16] [Bach '15]



After building a model

$$\frac{\partial p(x)}{\partial f1} = \frac{\partial p(x)}{\partial x_{ij}}$$

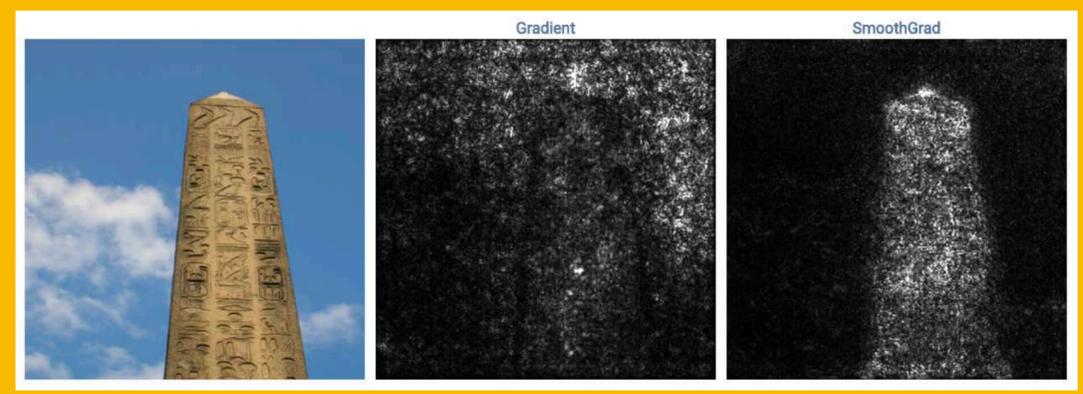


1. Ablation test: train without that feature/data and see the impact
2. Sensitivity analysis/fitting linear function/
gradient-based

Integrated gradients [Sundararajan et al. 17]



SmoothGrad [Smilkov et al. 17]



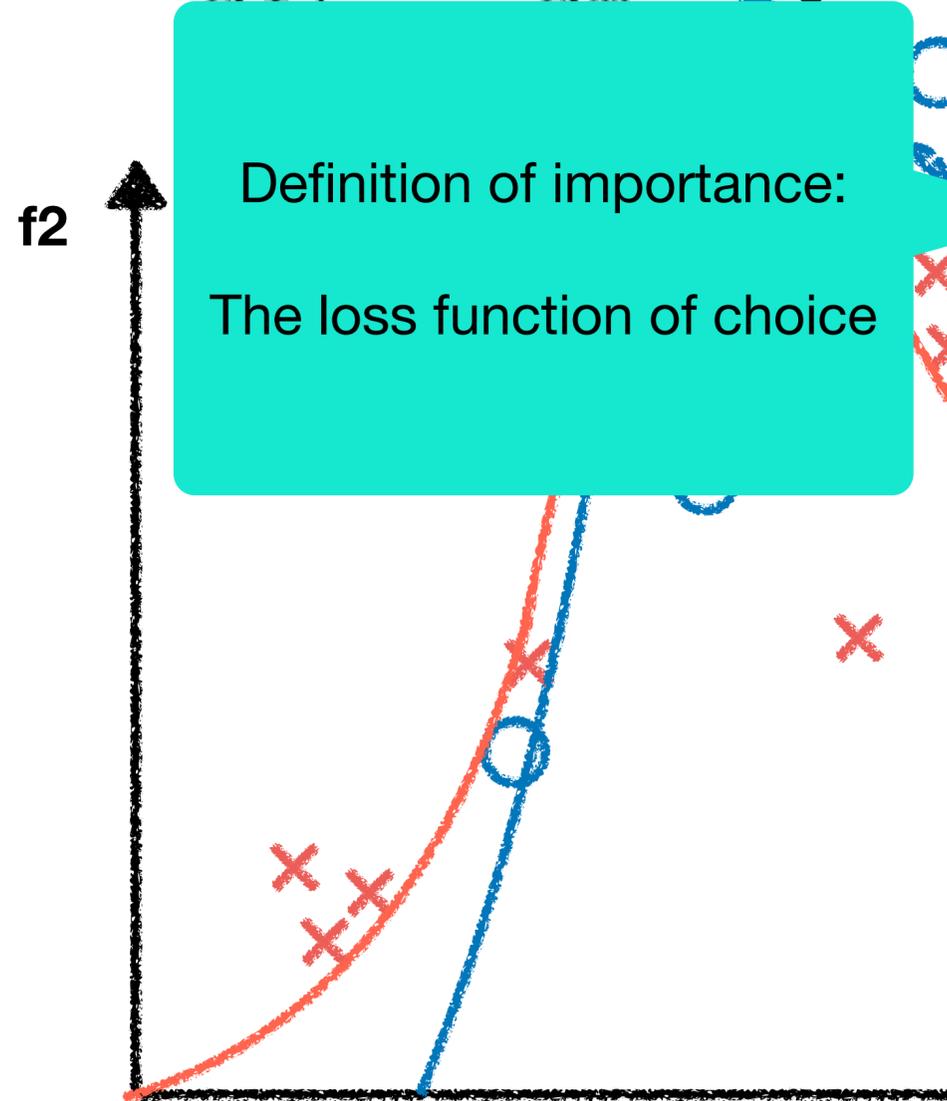
[Zeiler et al. '13] [Selvaraju et al. 16]

[Erhan 2009] [Springenberg, '14] [Shrikumar '17] and many more..



After building a model

$$\frac{\partial p(x)}{\partial f_1} = \frac{\partial p(x)}{\partial x}$$



1. Ablation test: train without that feature/data and see the impact
2. Sensitivity analysis/fitting linear function/
gradient-based
3. Optimization based methods



Figure 2: From left to right: the input image; smallest sufficient region (SSR); smallest destroying region (SDR). Regions were found using the mask optimisation procedure from [3].

- Smallest sufficient region (SSR) — smallest region of the image that alone allows a confident classification,
- Smallest destroying region (SDR) — smallest region of the image that when removed, prevents a confident classification.

[Dabkowski et al. 17]



Figure 1. An example of a mask learned (right) by blurring an image (middle) to suppress the softmax probability of its target class (left: original image; softmax scores above images).

$$\min_{m \in [0,1]^{\Lambda}} \lambda_1 \|1 - m\|_1 + \lambda_2 \sum_{u \in \Lambda} \|\nabla m(u)\|_{\beta}^{\beta} + \mathbb{E}_{\tau} [f_c(\Phi(x_0(\cdot - \tau), m))],$$

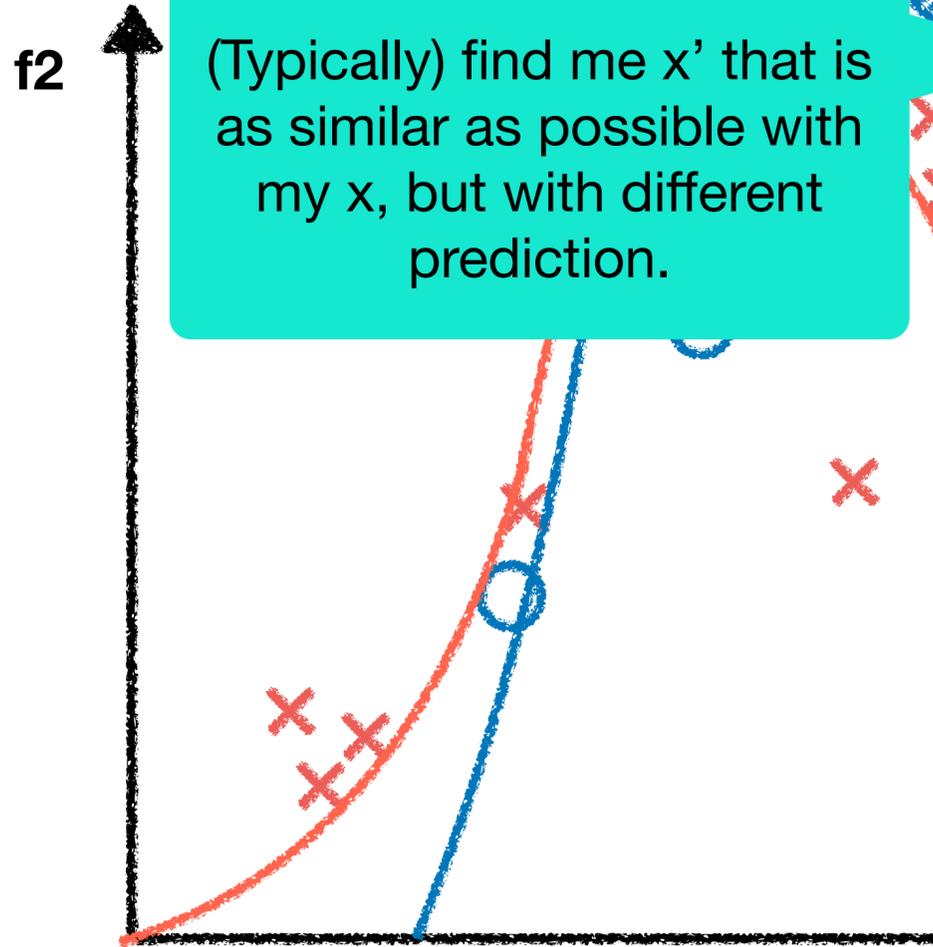
[Fong et al. 17, 18, 20]



After building a model

$$\frac{\partial p(x)}{\partial f_1} = \frac{\partial p(x)}{\partial x}$$

Definition:
 (Typically) find me x' that is as similar as possible with my x , but with different prediction.



1. Ablation test: train without that feature/data and see the impact
2. Sensitivity analysis/fitting linear function/gradient-based
3. Optimization based methods
4. Counterfactual explanations

$$\arg \min_{x'} \max_{\lambda} \lambda (f_w(x') - y')^2 + d(x_i, x')$$

[Watcher et al. 18]

$$d(x_i, x') = \sum_{k \in F} \frac{|x_{i,k} - x'_{k}|}{MAD_k}$$

$$\widetilde{\mathcal{L}}_{\mathcal{M}}(y, \bar{x}) = \mathbb{1} \left[y = \arg \max_{y'} \mathcal{M}(y' | \bar{x}) \right] \cdot \widetilde{\mathcal{M}}(y | \bar{x}).$$

Extend Watcher's framework to non-differentiable (e.g., trees)
 [Lucic et al. 21]

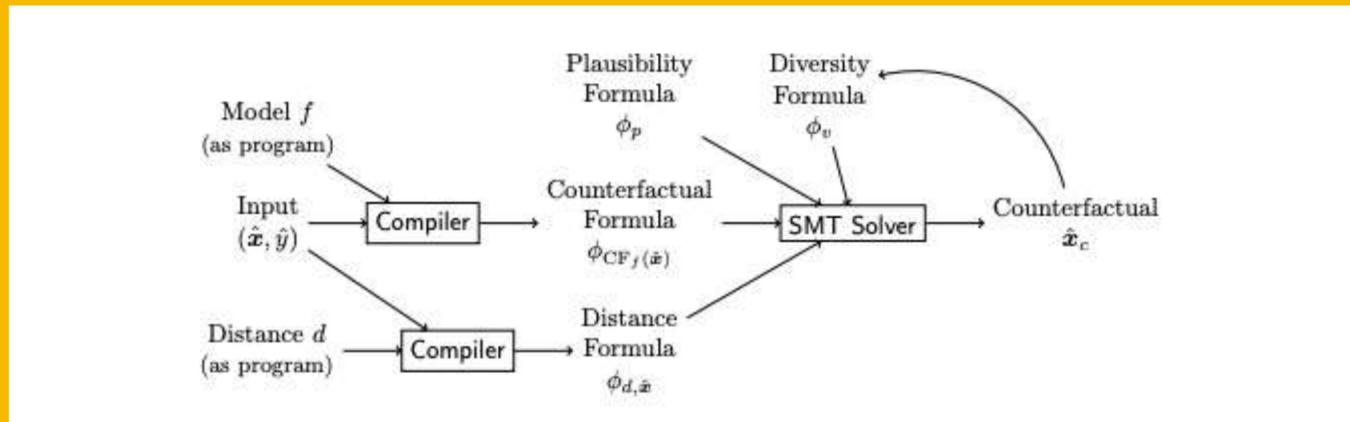


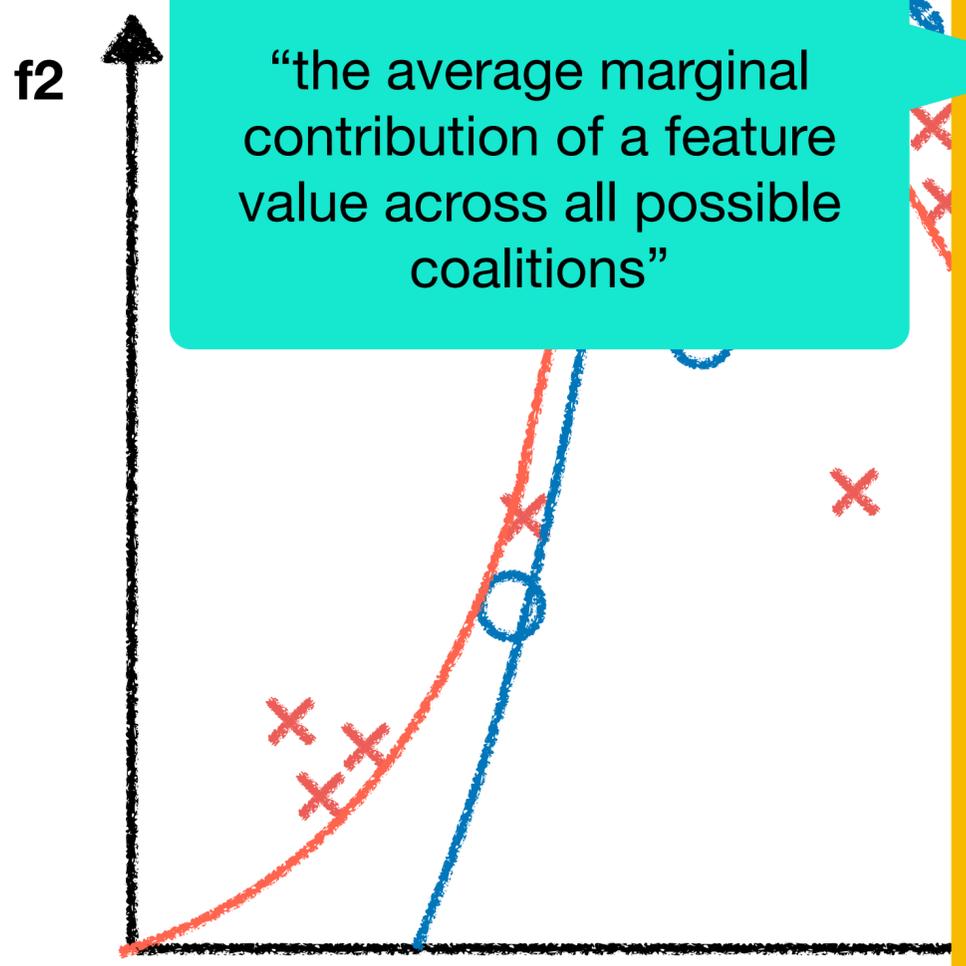
Figure 1: Architecture Overview for Model-Agnostic Counterfactual Explanations (MACE) [Karimi 20]



After building a model

$$\frac{\partial p(x)}{\partial f_1} = \frac{\partial p(x)}{\partial x}$$

Definition of importance:
"the average marginal contribution of a feature value across all possible coalitions"



1. Ablation test: train without that feature/data and see the impact
2. Sensitivity analysis/fitting linear function/gradient-based
3. Optimization based methods
4. Counterfactual explanations
5. Game theoretic approach

Shapley [Shapley 53]
how important is each player to the overall cooperation ("gain")
<-> The Shapley value is the average marginal contribution of a feature value across all possible coalitions.

gain = prediction value for x - E[all prediction values]

SHAP [Lundberg et al. 17]

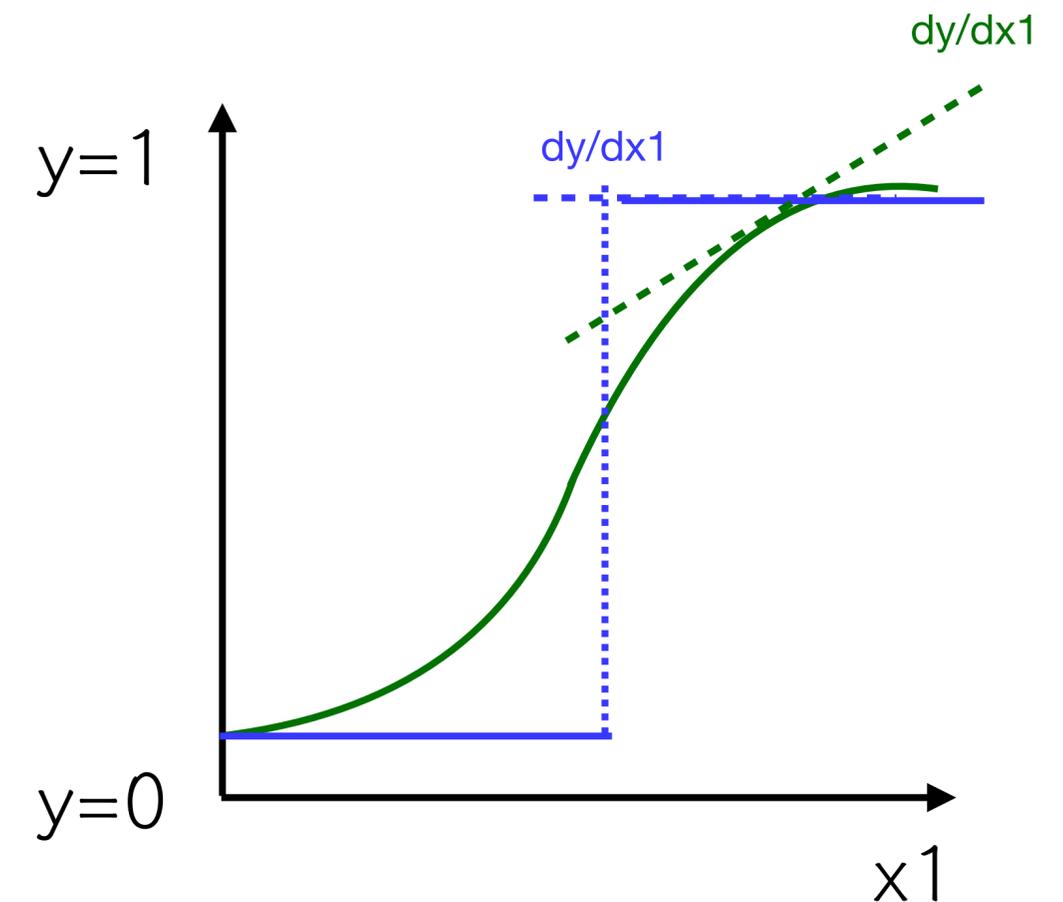
Definition 1 Additive feature attribution methods have an explanation model that is a linear function of binary variables:

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

(A)	Input	Explain 8	Explain 3	Masked
Orig. DeepLift				
New DeepLift				
SHAP				
LIME				

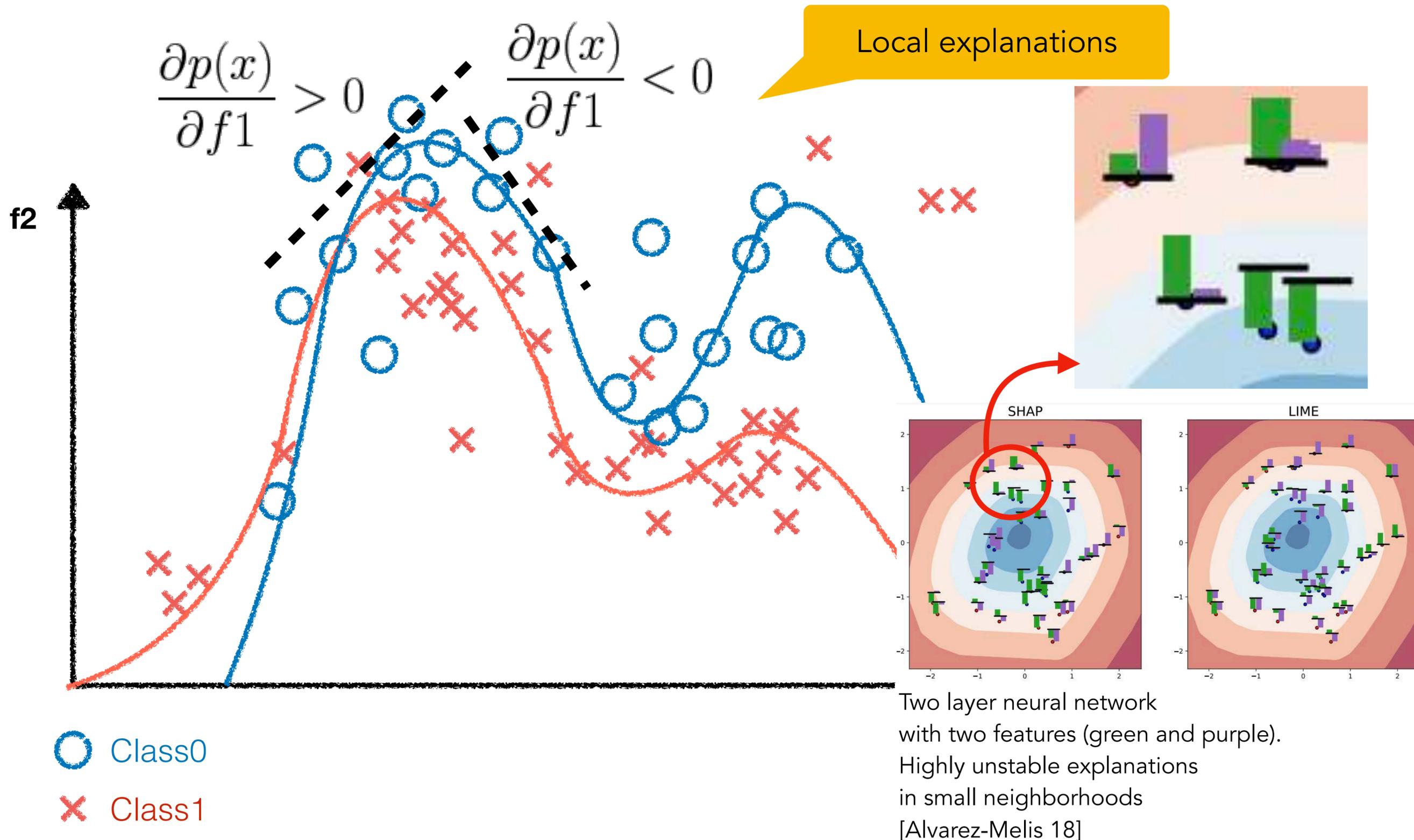
0-th order or 1-st order derivatives could lead to very different intuition

- Which feature is dominant (0-th order derivative)
 - feature x_1 is important distinction between class $y=1$ and $y=0$ for both **blue curve** and **green curve**.
- Which feature is sensitive (1-th order derivative)
 - feature x_1 is important distinction between class $y=1$ and $y=0$ for **green curve** ($dy/dx > 0$), but not for **blue curve** ($dy/dx=0$).
- Neither represents causal relationship (of course)
- What you think you want may not be what you need! -> Test with the end-task.



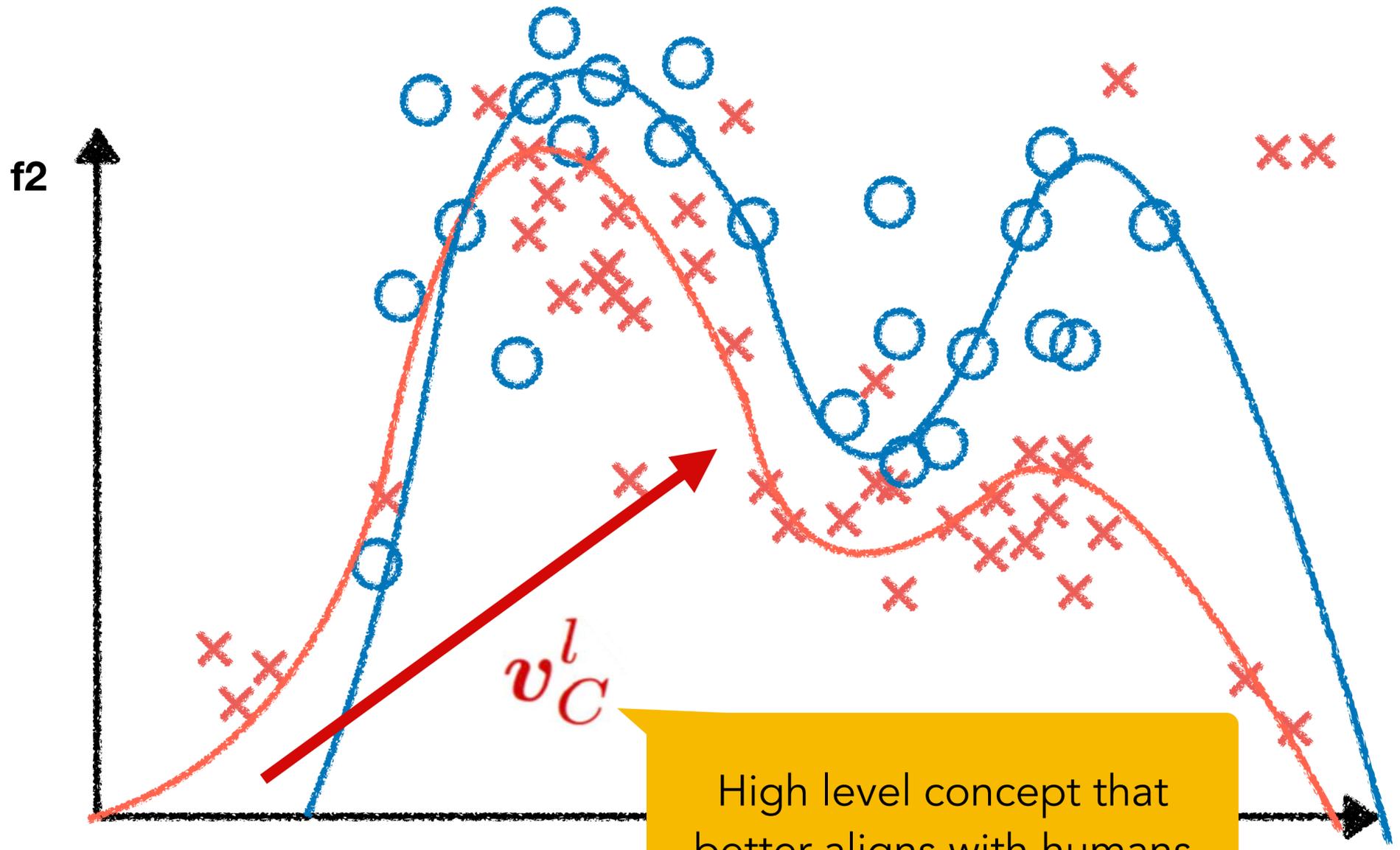


That's all good. What could go wrong?





After building a model



- Class0
- × Class1

High level concept that better aligns with humans Instead of using individual features/pixels

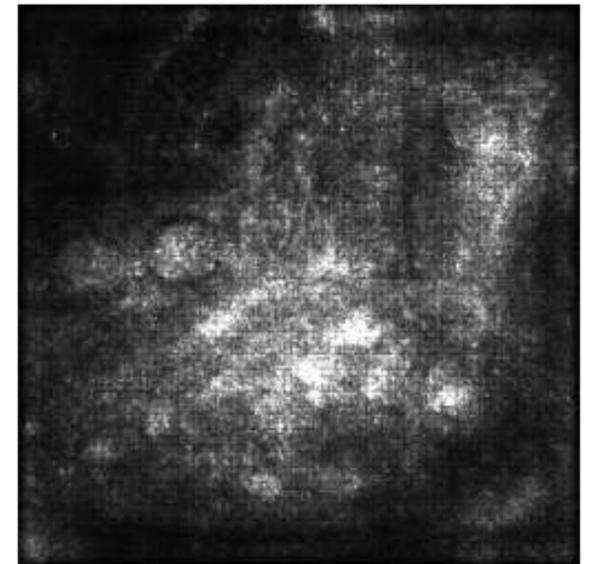
Problem: Post-training explanation

$$\operatorname{argmax}_E Q(\mathbf{Explanation} | \mathbf{Model}, \mathbf{Human}, \mathbf{Data}, \mathbf{Task})$$



→ A trained machine learning model (e.g., neural network) →

$p(z)$
popularity



VS

Why was this a popular pizza?

-  was important 0.8
-  was important 0.3
-  was important 0.1

Problem:

Post-training explanation

$$\operatorname{argmax}_E Q(\mathbf{Explanation} | \mathbf{Model}, \mathbf{Human},$$



A trained machine learning model (e.g., neural network)

$p(z)$
popularity

Quantitative explanation:
how much a **concept** (e.g., gender, race) was important for a **prediction** in a trained model.

...even if the **concept** was not part of the training.

Why was this a popular pizza?



was important 0.8

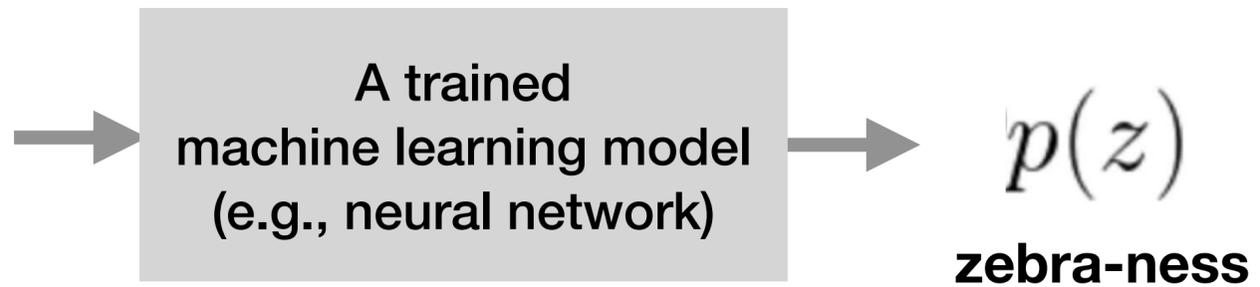


was important 0.3



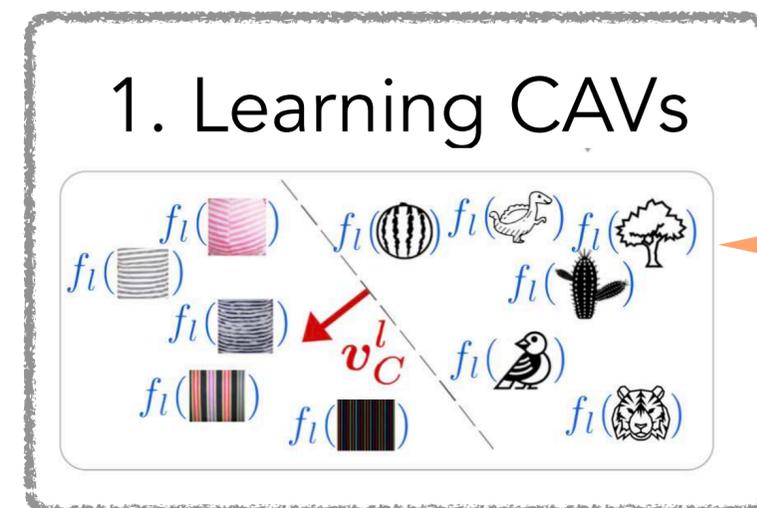
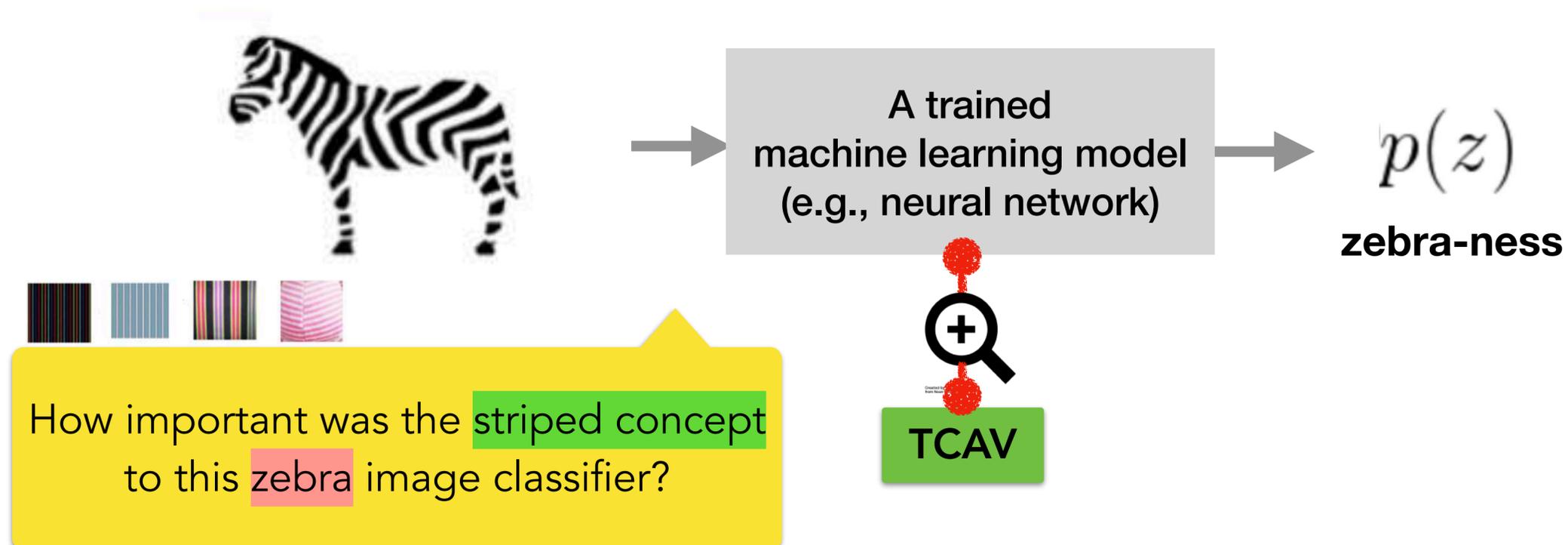
was important 0.1

TCAV: Testing with Concept Activation Vectors



How important was the striped concept to this zebra image classifier?

TCAV: Testing with Concept Activation Vectors



1. How to define concepts?

Defining concept activation vector (CAV)

Inputs:

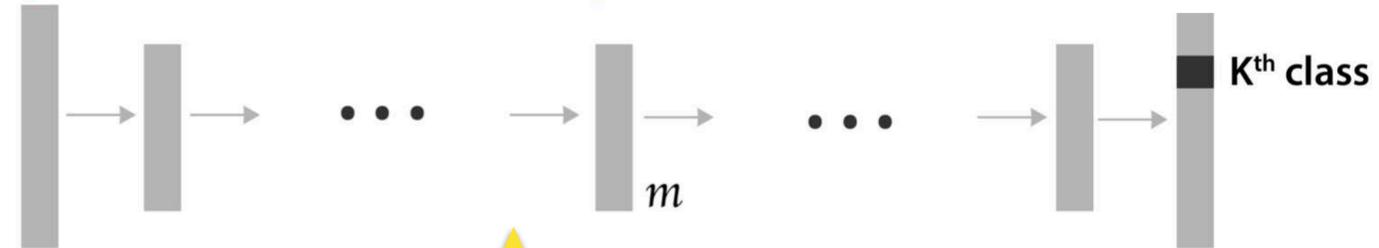
a



Examples of
concepts

Random
images

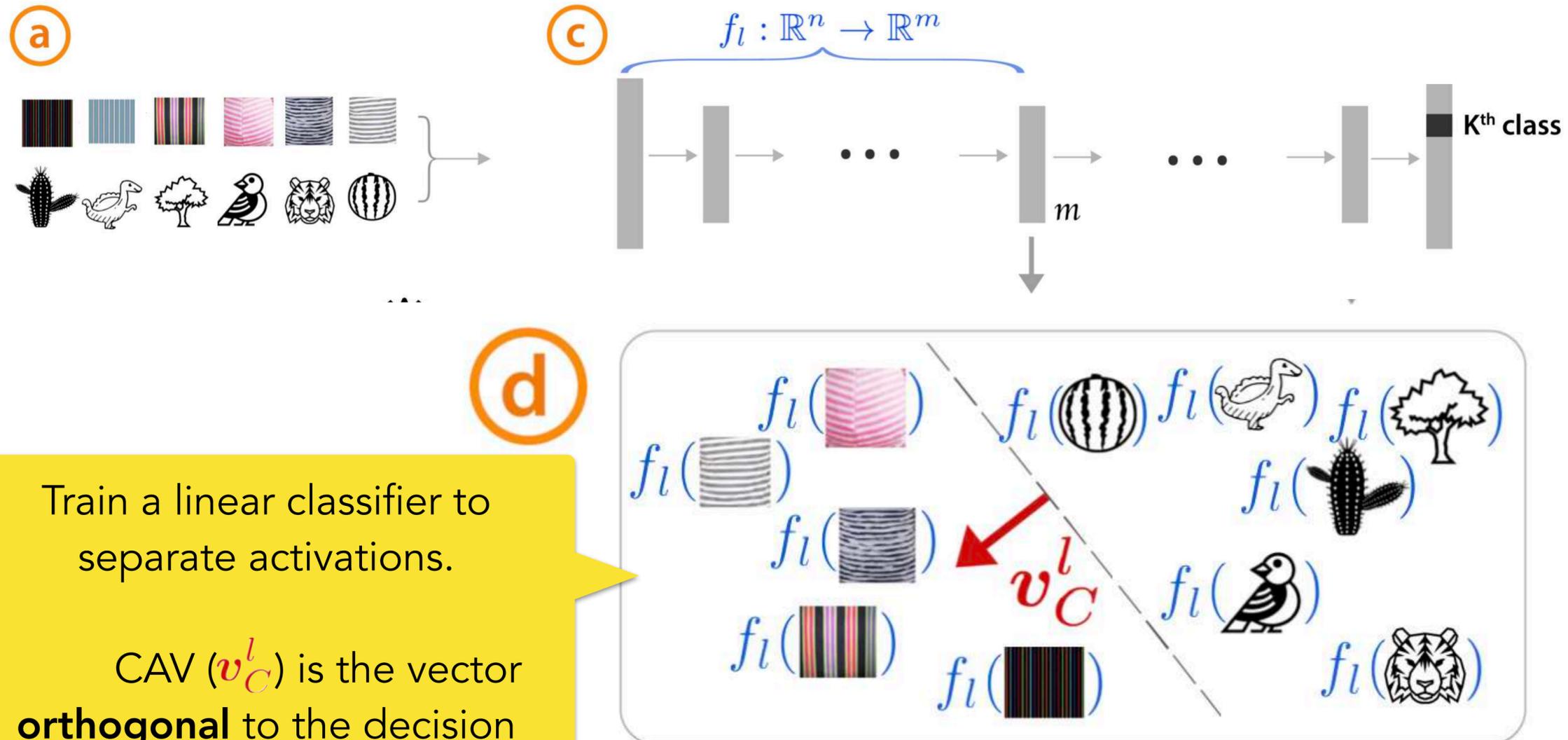
$$f_l : \mathbb{R}^n \rightarrow \mathbb{R}^m$$



A trained network under investigation
and
Internal tensors

Defining concept activation vector (CAV)

Inputs:

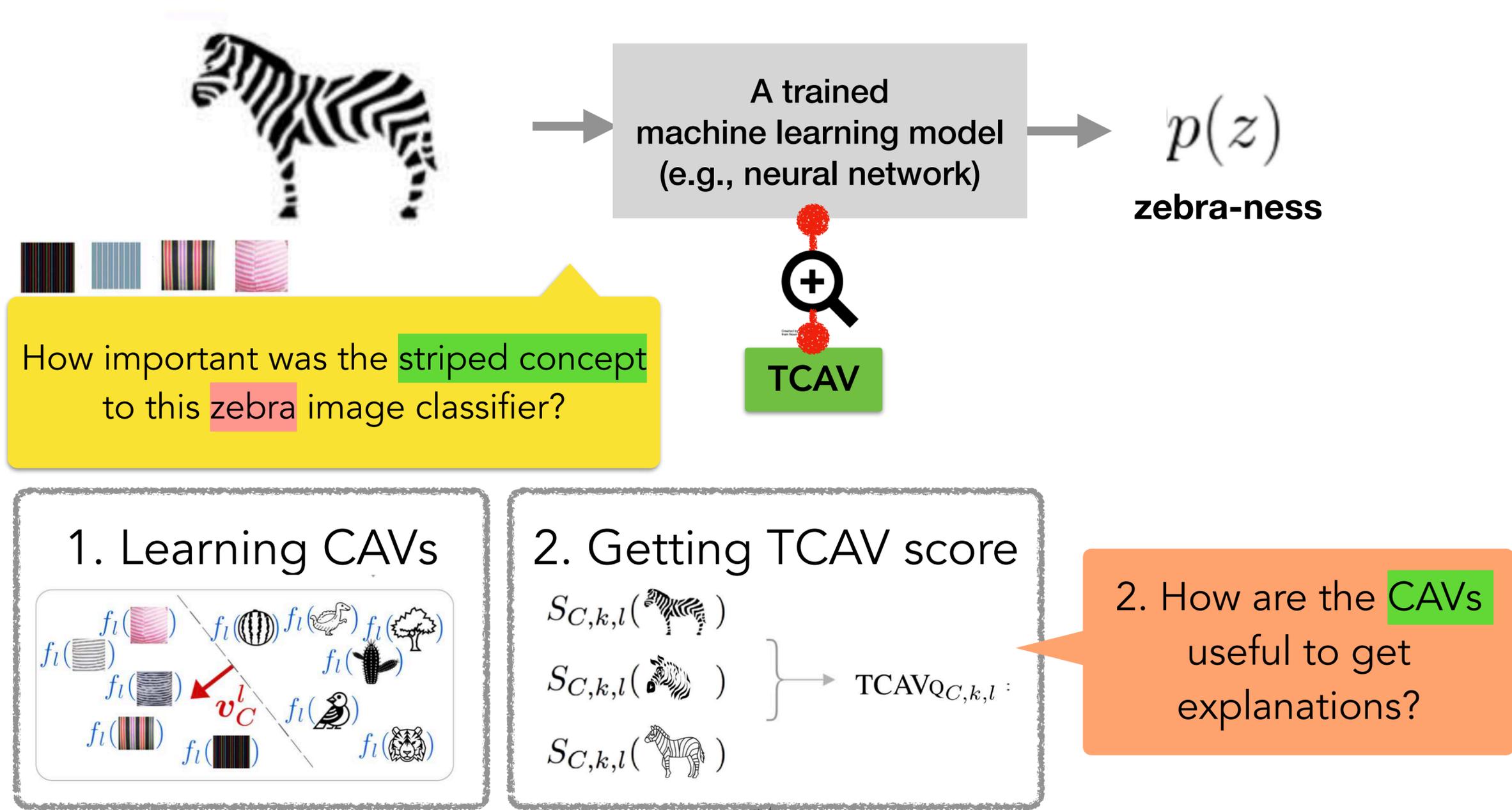


Train a linear classifier to separate activations.

CAV (v_C^l) is the vector **orthogonal** to the decision boundary.

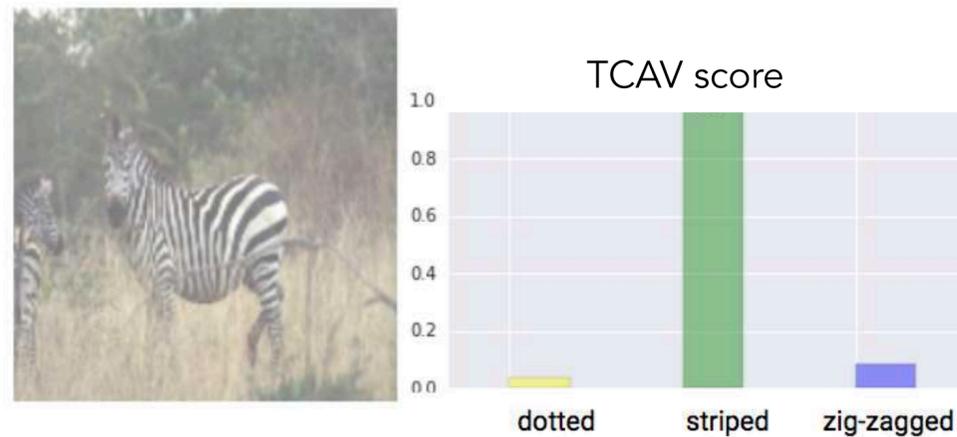
[Smilkov '17, Bolukbasi '16, Schmidt '15]

TCAV: Testing with Concept Activation Vectors



TCAV core idea: Derivative with CAV to get prediction sensitivity

TCAV

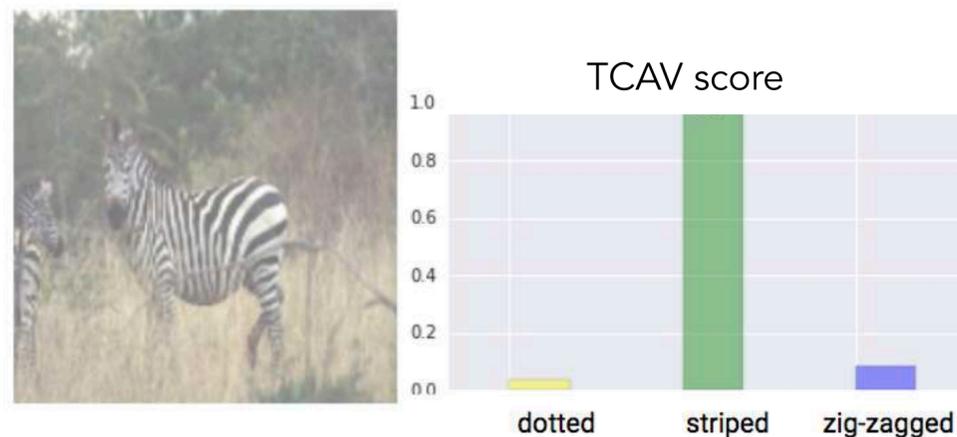


$$\begin{aligned} \text{zebra-ness} &\rightarrow \frac{\partial p(z)}{\partial \mathbf{v}_C^l} = S_{C,k,l}(\mathbf{x}) \\ \text{striped CAV} &\rightarrow \end{aligned}$$

Directional derivative with CAV

TCAV core idea: Derivative with CAV to get prediction sensitivity

TCAV



$$\begin{aligned} \text{zebra-ness} &\rightarrow \frac{\partial p(z)}{\partial \mathbf{v}_C^l} = S_{C,k,l}(\mathbf{x}) \\ \text{striped CAV} &\rightarrow \end{aligned}$$

Directional derivative with CAV

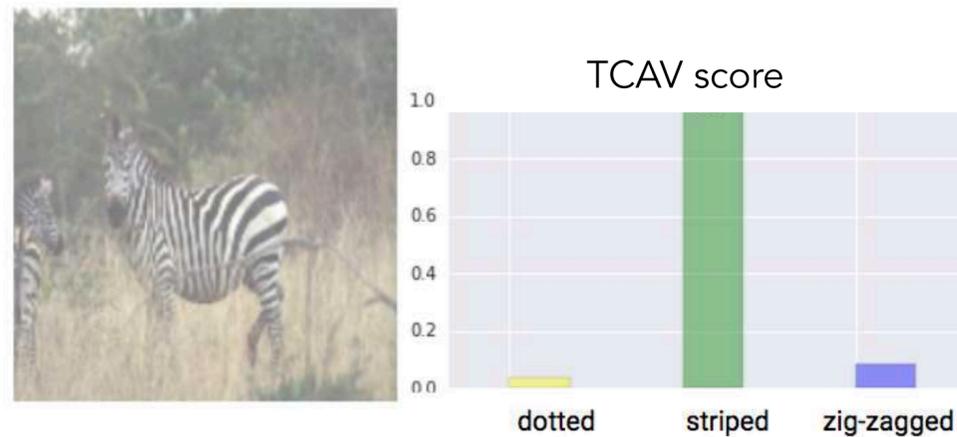
One definition of explanation:

Tell me how **sensitive** the prediction is when we slightly **change** each concept.

TCAV core idea:

Derivative with CAV to get prediction sensitivity

TCAV

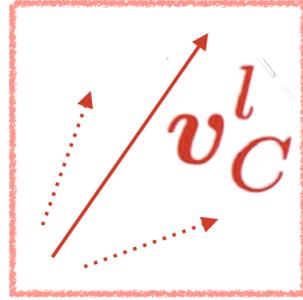


$$\begin{aligned}
 &S_{C,k,l}(\text{zebra}) \\
 &S_{C,k,l}(\text{zebra}) \\
 &S_{C,k,l}(\text{zebra}) \\
 &S_{C,k,l}(\text{zebra})
 \end{aligned}
 \left. \vphantom{\begin{aligned} &S_{C,k,l}(\text{zebra}) \\ &S_{C,k,l}(\text{zebra}) \\ &S_{C,k,l}(\text{zebra}) \\ &S_{C,k,l}(\text{zebra}) \end{aligned}} \right\}$$

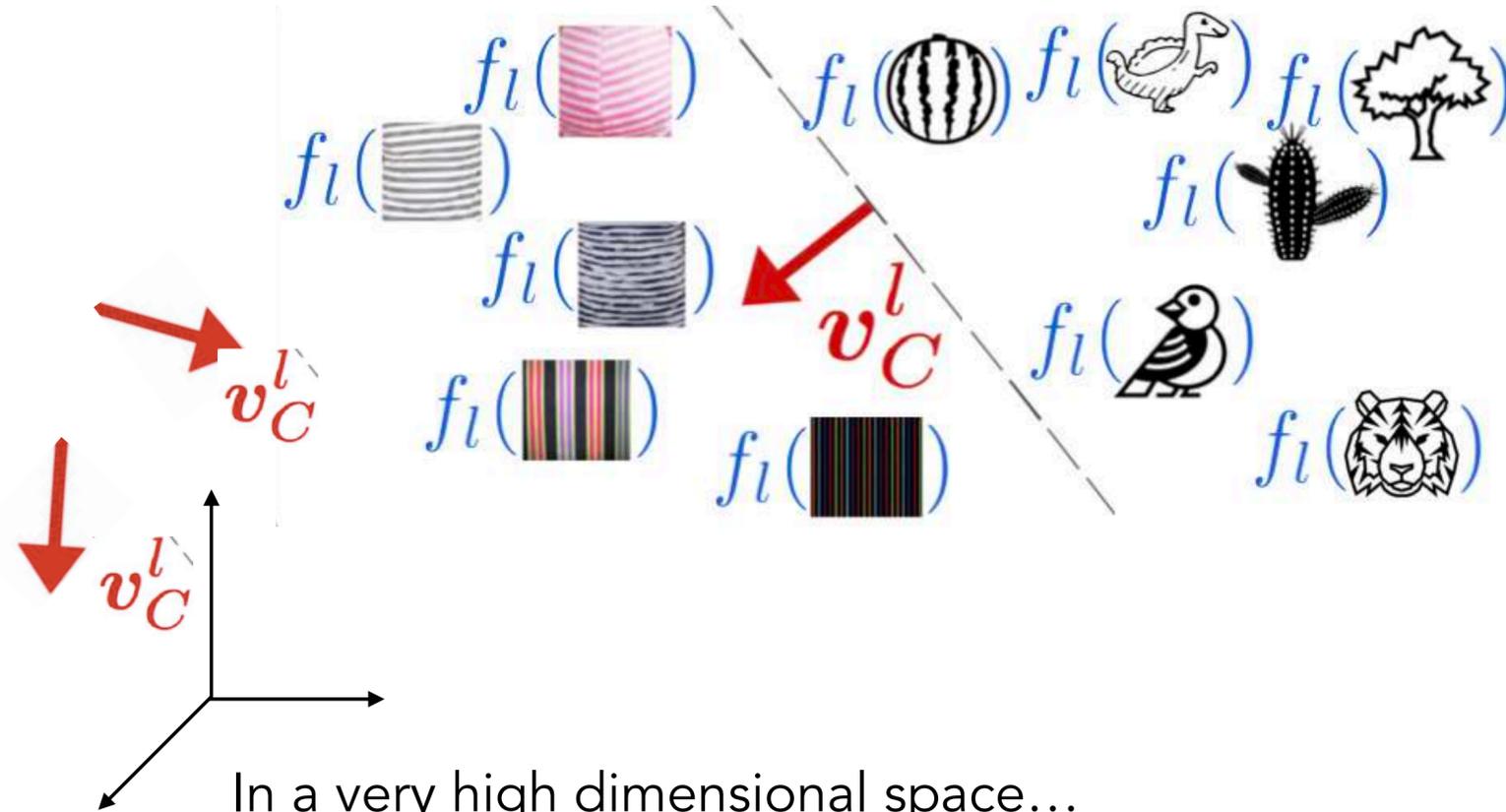
$$\begin{aligned}
 \text{zebra-ness} &\rightarrow \frac{\partial p(z)}{\partial \mathbf{v}_C^l} = S_{C,k,l}(\mathbf{x}) \\
 \text{striped CAV} &\rightarrow \frac{\partial p(z)}{\partial \mathbf{v}_C^l} = S_{C,k,l}(\mathbf{x})
 \end{aligned}$$

$$\text{TCAV}_{Q_{C,k,l}} = \frac{|\{\mathbf{x} \in X_k : S_{C,k,l}(\mathbf{x}) > 0\}|}{|X_k|}$$

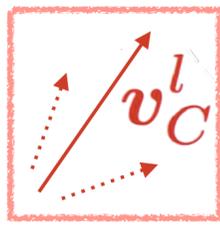
Directional derivative with CAV



Is this CAV legit?

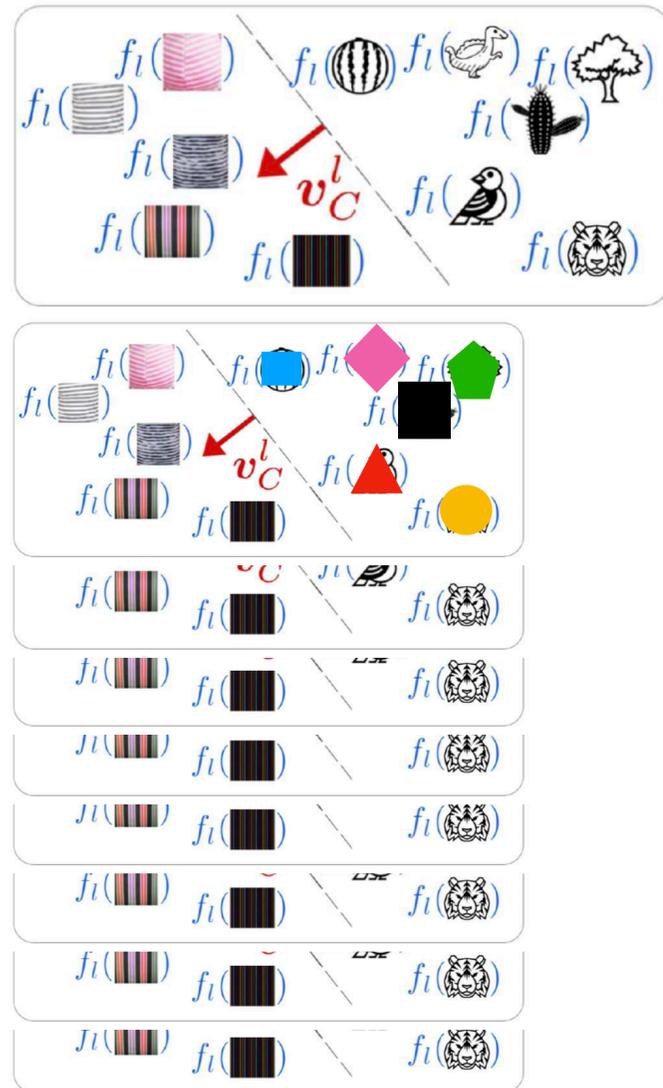


In a very high dimensional space...
funky things can happen.



Quantitative validation:

Guarding against spurious CAV



Zebra

→ $TCAV_{QC,k,l} :$

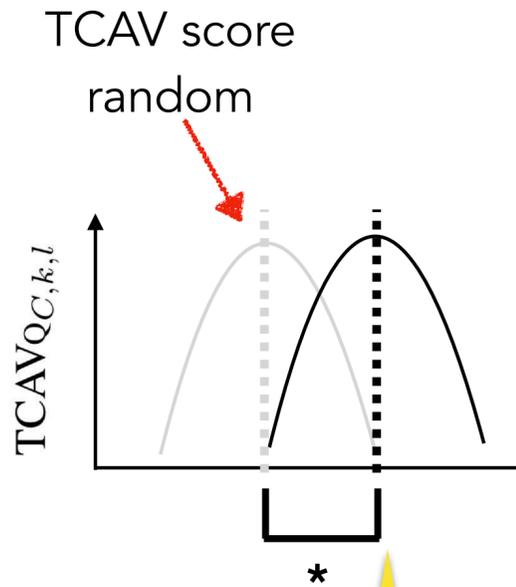
⋮

→ $TCAV_{QC,k,l} :$

→ $TCAV_{QC,k,l} :$

→ $TCAV_{QC,k,l} :$

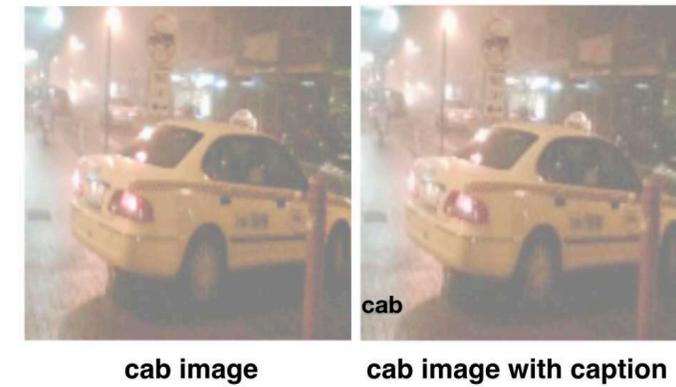
⋮



Check the distribution of $TCAV_{QC,k,l}$ is statistically different from random using t-test

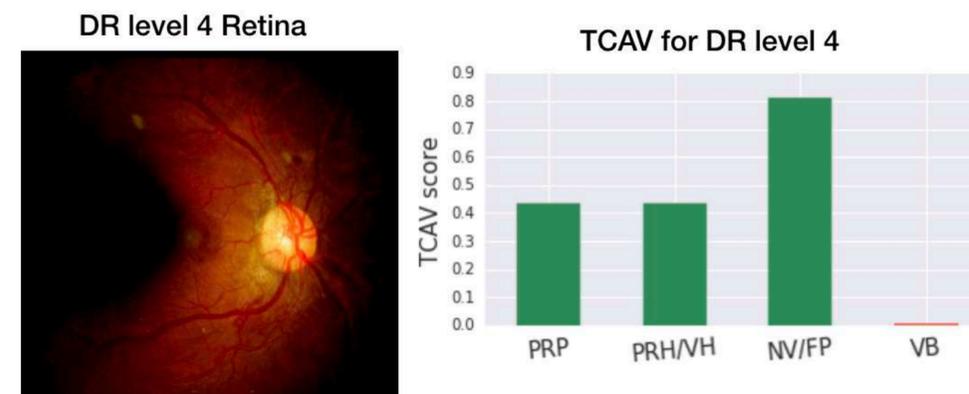
Results

1. Sanity check experiment



2. Biases in Inception V3 and GoogleNet

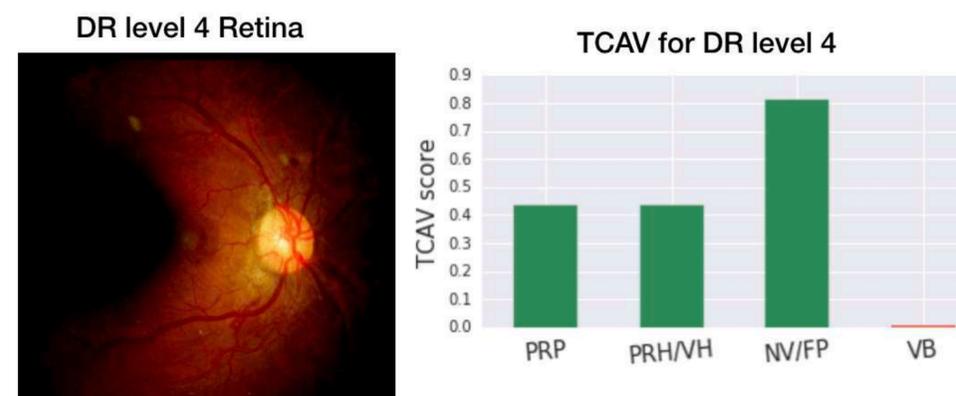
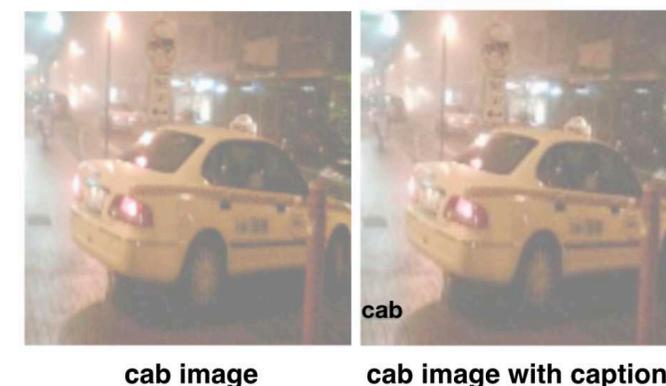
3. Domain expert confirmation from Diabetic Retinopathy



Real!

Results

1. Sanity check experiment
2. Biases in Inception V3 and GoogleNet
3. Domain expert confirmation from Diabetic Retinopathy



Global and Local Interpretability for Cardiac MRI Classification

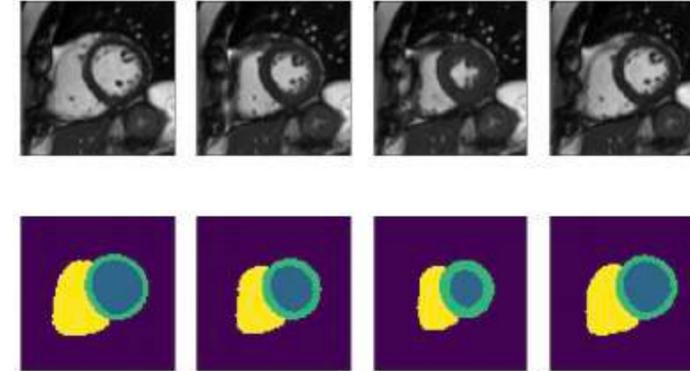
James R. Clough, Ilkay Oksuz, Esther Puyol-Antón, Bram Ruijsink,
Andrew P. King, and Julia A. Schnabel

School of Biomedical Engineering & Imaging Sciences, King's College London, UK
james.clough@kcl.ac.uk

CAV	Description	$\nabla_{\tilde{y}} \cdot \mathbf{v}_c > 0$	$\langle \nabla_{\tilde{y}} \cdot \mathbf{v}_c \rangle$
Low EF	Ejection Fraction	78.2%	0.0417
Low PER	Peak Ejection Rate	88.8%	0.0770
Low PFR	Peak Filling Rate	99.6%	0.1560
Low APFR	Atrial Peak Filling Rate	58.2%	0.0048
High LVT	Variance of LV wall thickening	63.4%	0.0156

Table 1: The sensitivity of the classifier to clinical biomarkers of poor cardiac health. A biomarker with no relevance would have $\nabla_{\mathbf{z}} \tilde{y} \cdot \mathbf{v}_c = 0$ on average.

Interpreting a jointly trained
VAE+classification model.



Global and Local Interpretability for Cardiac MRI Classification

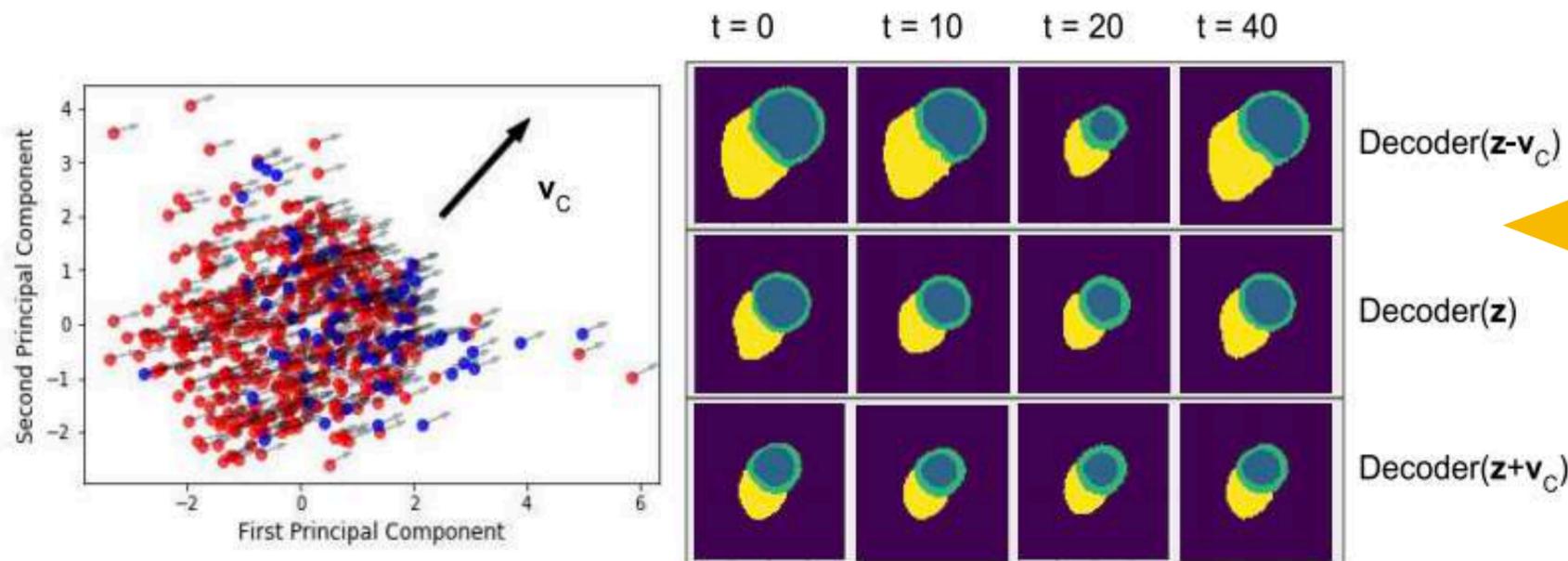
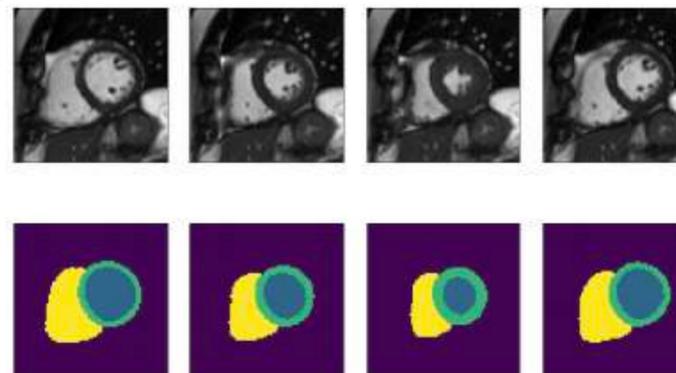
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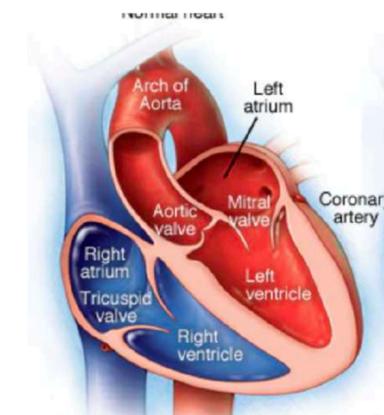
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Interpreting a jointly trained VAE+classification model.



Can generate images with more/less LV (left ventricle) concept



Global and Local Interpretability for Cardiac MRI Classification

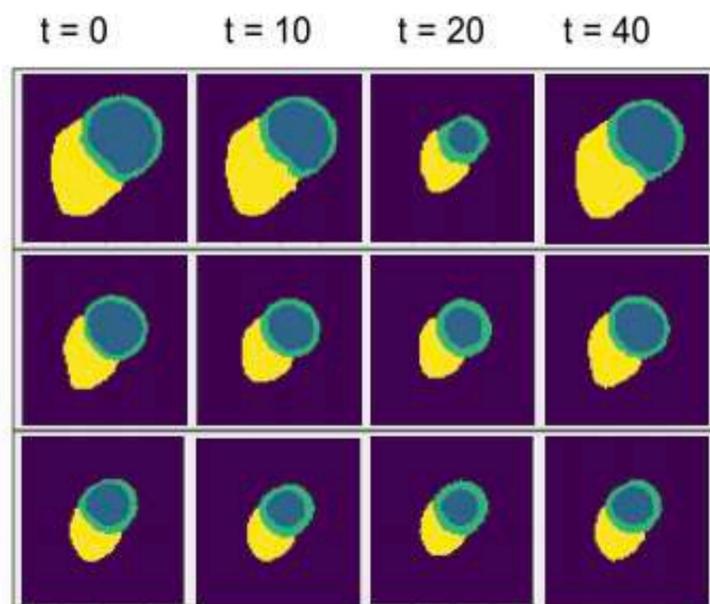
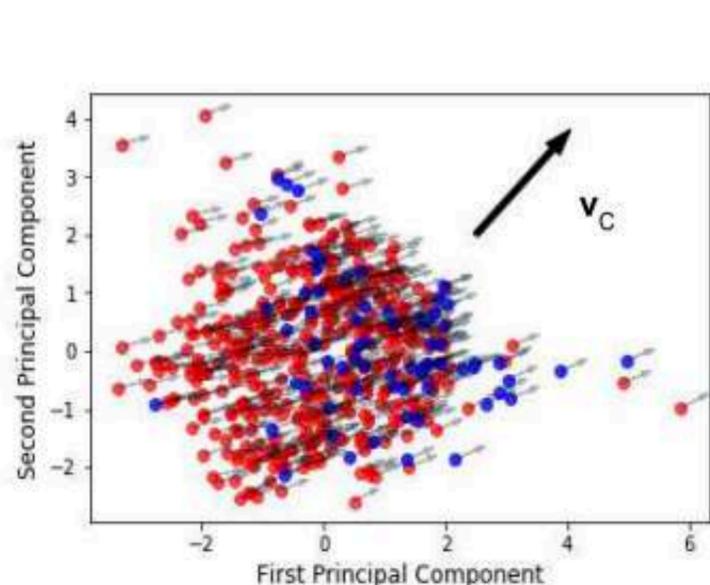
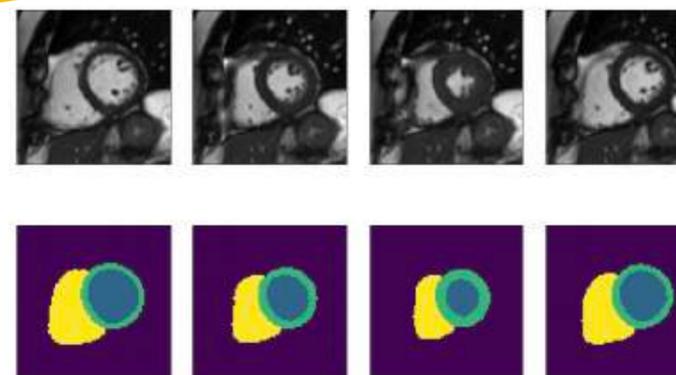
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School of Biomedical Engineering & Imaging Sciences, King's College London, UK
james.clough@kcl.ac.uk

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Interpreting a jointly trained VAE+classification model.

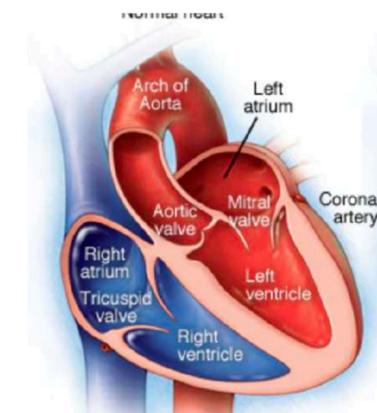


Decoder($\mathbf{z}-\mathbf{v}_c$)

Decoder(\mathbf{z})

Decoder($\mathbf{z}+\mathbf{v}_c$)

Can generate images with more/less LV (left ventricle) concept



Interpretable models do not just offer clinicians a well-calibrated estimate of the likelihood of disease. Interpretability using known biomarkers allows the model's prediction to be placed in the context of current medical knowledge and clinical decision-making guidelines, which is a key part of translation into clinical practice.

Concept-based model explanations for Electronic Health Records

Diana Mincu
Google Research
London, UK

Sebastien Baur
Google Health
London, UK

Anne Mottram
DeepMind
London, UK

Eric Loreaux
Google Health
Palo Alto, CA, USA

Ivan Protsyuk
Google Health
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Nenad Tomasev
Deepmind
London, UK

Jessica Schrouff*
Google Research
London, UK
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Shaobo Hou
DeepMind
London, UK

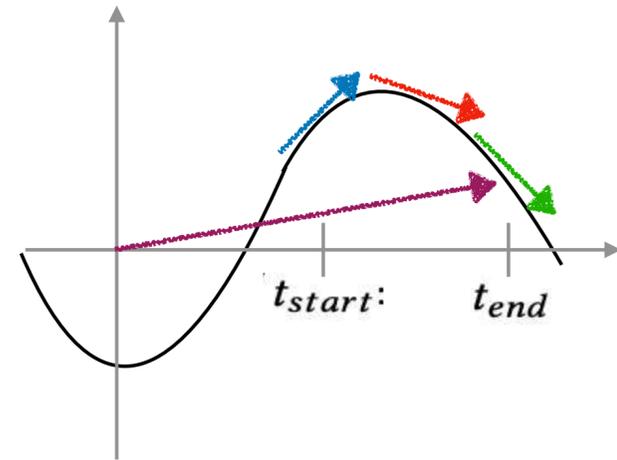
Martin Seneviratne
Google Health
London, UK

Alan Karthikesalingam
Google Health
London, UK

TCAV for RNNs

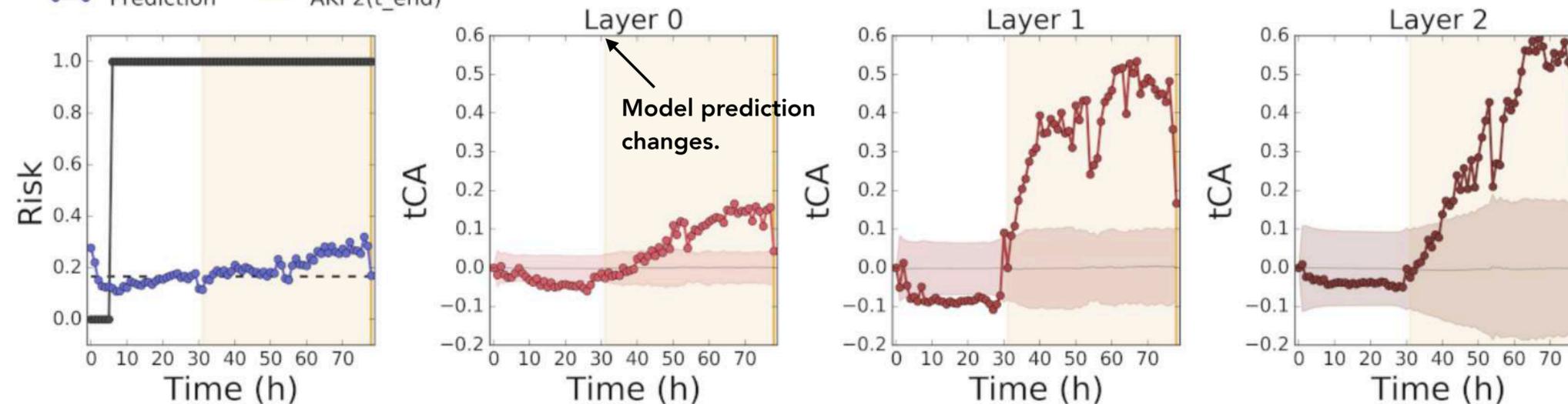
Presence of a concept in one data point

$$tCA_C(\vec{x}_t) = \frac{\vec{a}_t^T}{\|\vec{a}_t\|_2} \vec{v}_C$$



- $CAV_{t_{end}}$
- $CAV_{t_{start}:t_{end}}$
- $CAV_{t_{end}-t_{start}}$

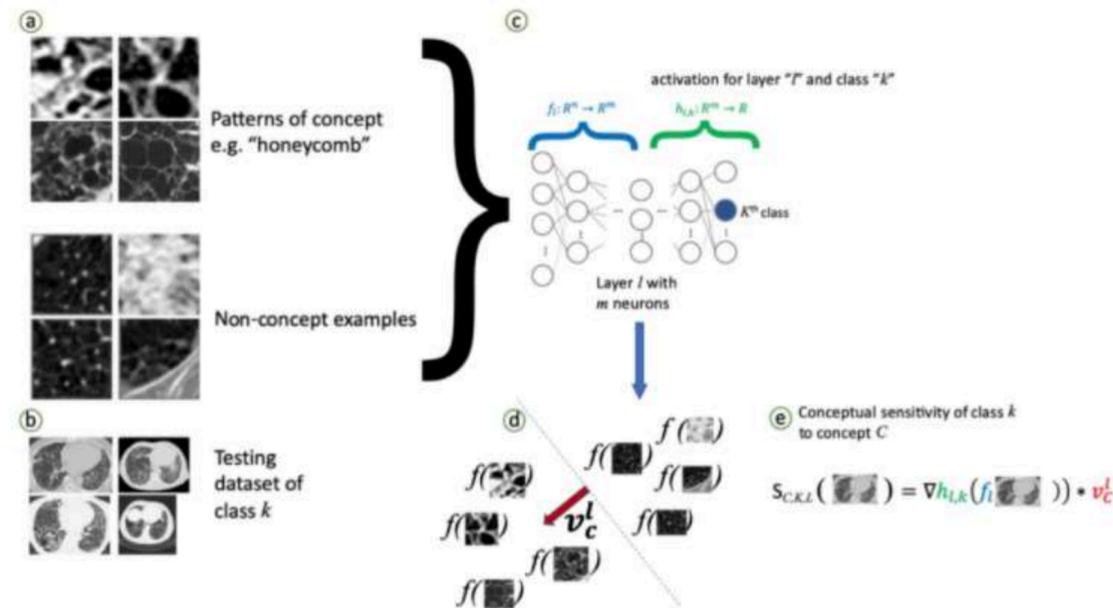
d —●— Target - - Decision
 —●— Prediction — AKI 2(t_end)



Radiology: Artificial Intelligence

On the Interpretability of Artificial Intelligence in Radiology: Challenges and Opportunities

Mauricio Reyes, Raphael Meier, Sérgio Pereira, Carlos A. Silva, Fried-Michael Dahlweid, Hendrik von Tengg-Kobligk, Ronald M. Summers, Roland Wiest



UBS: A Dimension-Agnostic Metric for Concept Vector Interpretability Applied to Radiomics

Authors: Hugo Yeche, Justin Harrison, Tess Berthier

Authors and affiliations

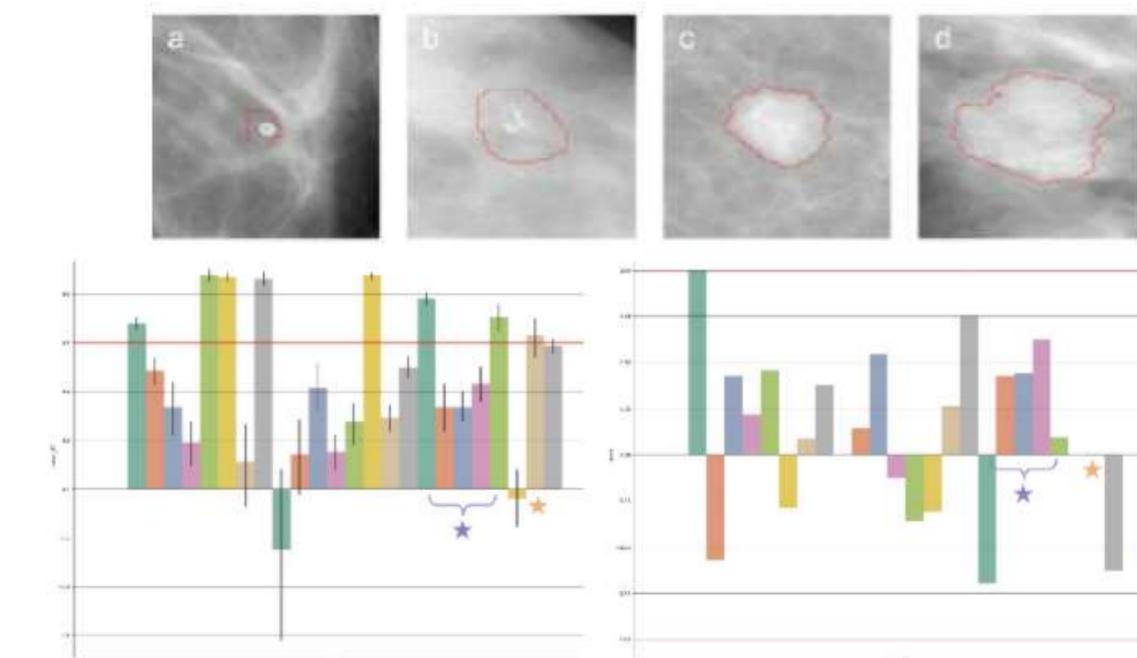
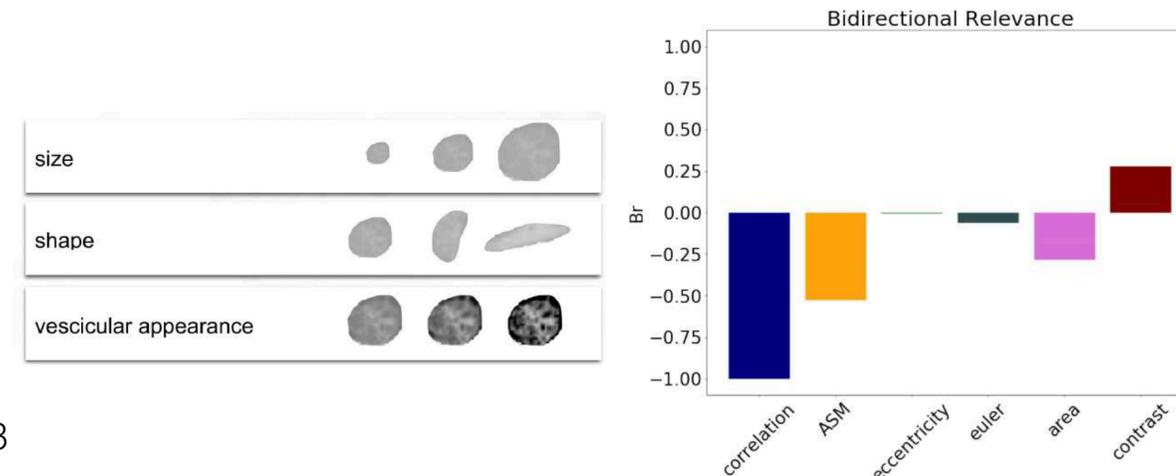


Fig. 4. Results at layer fire6/concat of SqueezeNet for GLCM radiomics, showing R^2 scores (left) and Br scores (right) for calcification prediction.

[Submitted on 9 Apr 2019]

Regression Concept Vectors for Bidirectional Explanations in Histopathology

Mara Graziani, Vincent Andrearczyk, Henning Müller



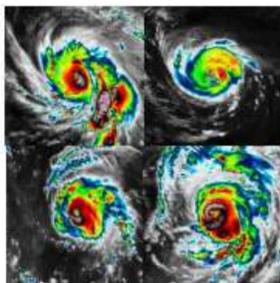


Interpretable AI for Deep-Learning-Based Meteorological Applications

Eric B. Wendoloski, Ingrid C. Guch
The Aerospace Corporation

Importance of Eye Structure to Cat. 4 Prediction

Gather known Cat. 4 Images



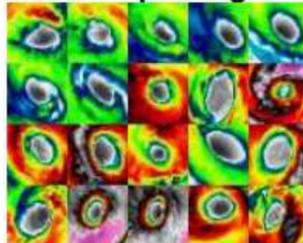
Calculate gradient of model loss for HU4 class w.r.t. activations from final layer

Gradient vectors point in direction of decreasing probability of correct class identification

Gradient vectors (GV)



Concept images



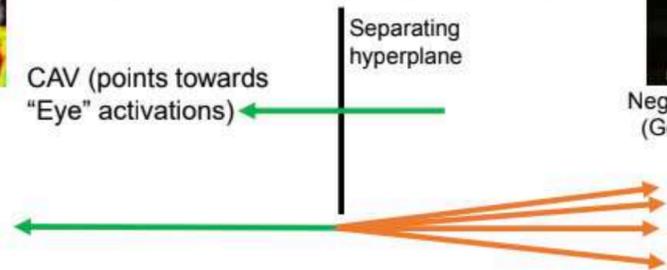
Determine Concept Activation Vector (CAV)

1. Gather concept images / negative images
2. Gather layer activations for the above
3. Train linear classifier on activations
4. Repeat while varying negative images

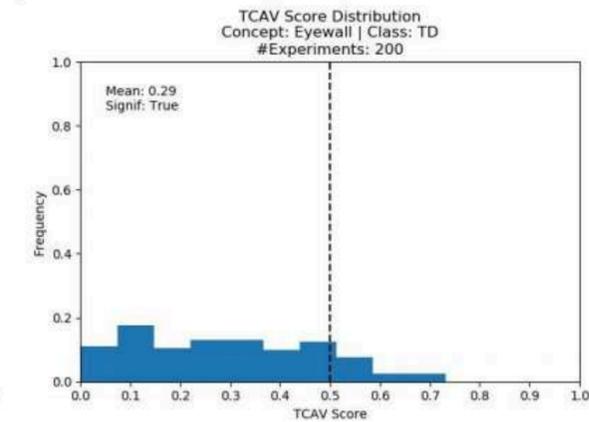
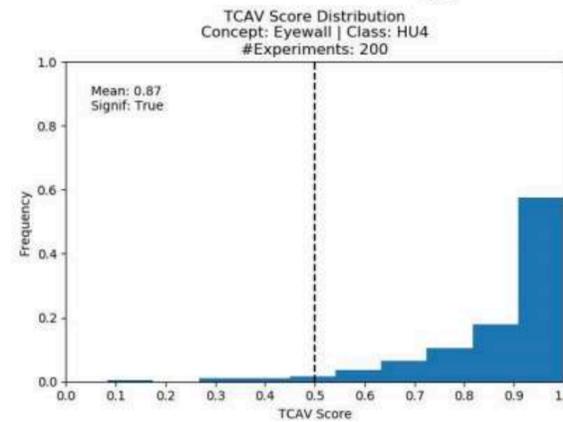
Negative images



Negative images from ALOI (Geusebroek et al. 2005)



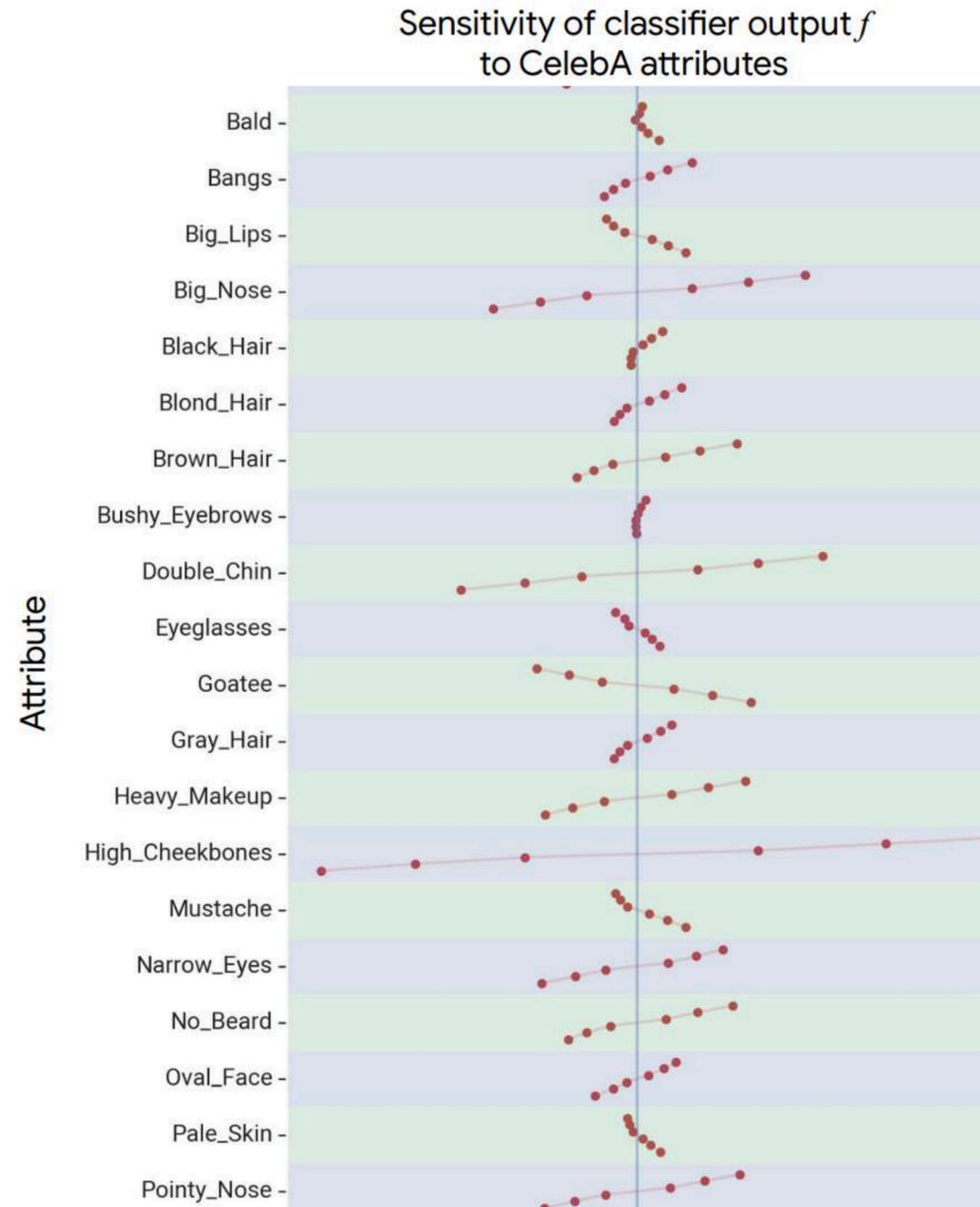
- CAV tending to point in opposite direction of GVs tends to point in direction of increasing probability of correct class identification



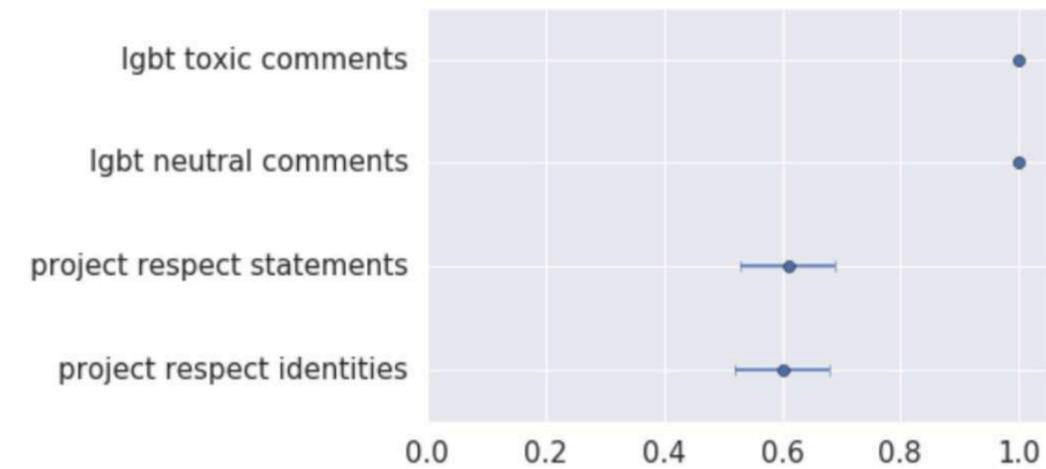
Negative Images had to be on black background (similar to concept images)

Follow up work on ML fairness @Google with non-image data

Language model

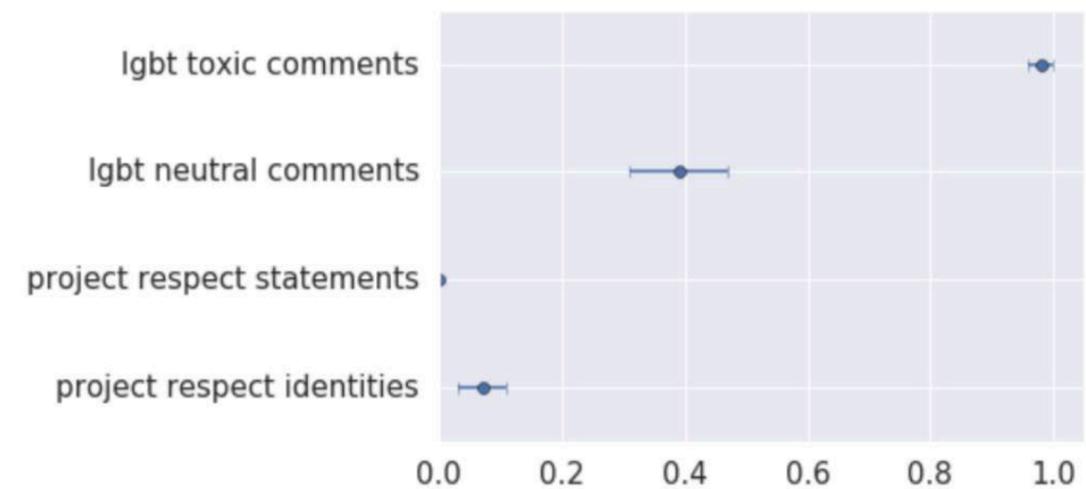


[Denton et al. 19]



(a) TOXICITY@1

↓ Unbiasing



(b) TOXICITY@6

[Hutchinson et al. 19]

What if concepts are confounded/overlap?

Published as a conference paper at ICLR 2021

DEBIASING CONCEPT-BASED EXPLANATIONS WITH CAUSAL ANALYSIS

Mohammad Taha Bahadori, David E. Heckerman
 {bahadorm, heckerma}@amazon.com

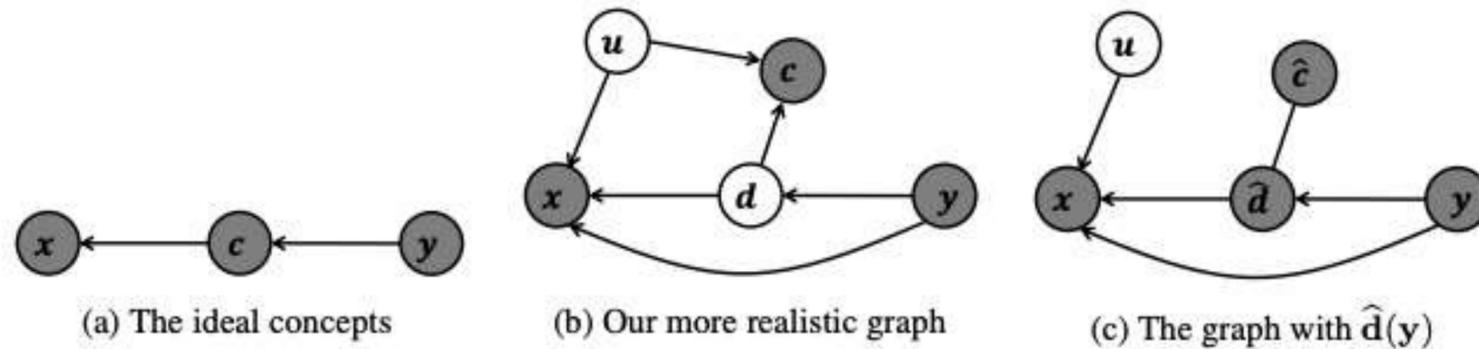


Figure 2: (a) The ideal view of the causal relationships between the features x , concepts c , and labels y . (b) In a more realistic setting, the unobserved confounding variable u impacts both x and c . The shared information between x and y go through the discriminative part of the concepts d . We also model the completeness of the concepts via a direct edge from the features x to the labels y . (c) When we use $\hat{d}(y) = E[c|y]$ in place of d and c , we eliminate the confounding link $u \rightarrow c$.

2020 Nature Machine Intelligence

Concept Whitening for Interpretable Image Recognition

Zhi Chen¹ Yijie Bei² Cynthia Rudin^{1,2}

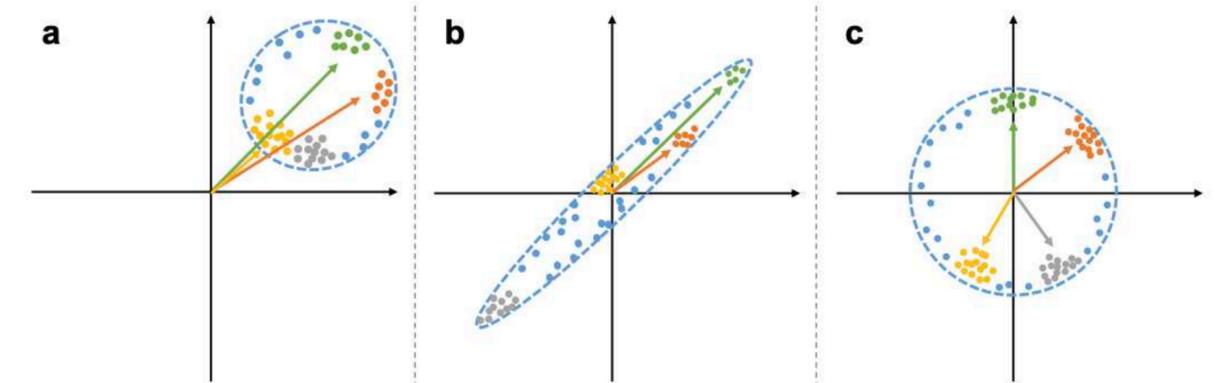


Figure 1. Possible data distributions in the latent space. **a**, the data are not mean centered; **b** the data are standardized but not decorrelated; **c** the data are whitened. In both **a** and **b**, unit vectors are not valid for representing concepts.

Debugging GAN
with concepts

GAN DISSECTION: VISUALIZING AND UNDERSTANDING GENERATIVE ADVERSARIAL NETWORKS

David Bau^{1,2}, Jun-Yan Zhu¹, Hendrik Strobelt^{2,3}, Bolei Zhou⁴,
Joshua B. Tenenbaum¹, William T. Freeman¹, Antonio Torralba^{1,2}
¹Massachusetts Institute of Technology, ²MIT-IBM Watson AI Lab,
³IBM Research, ⁴The Chinese University of Hong Kong

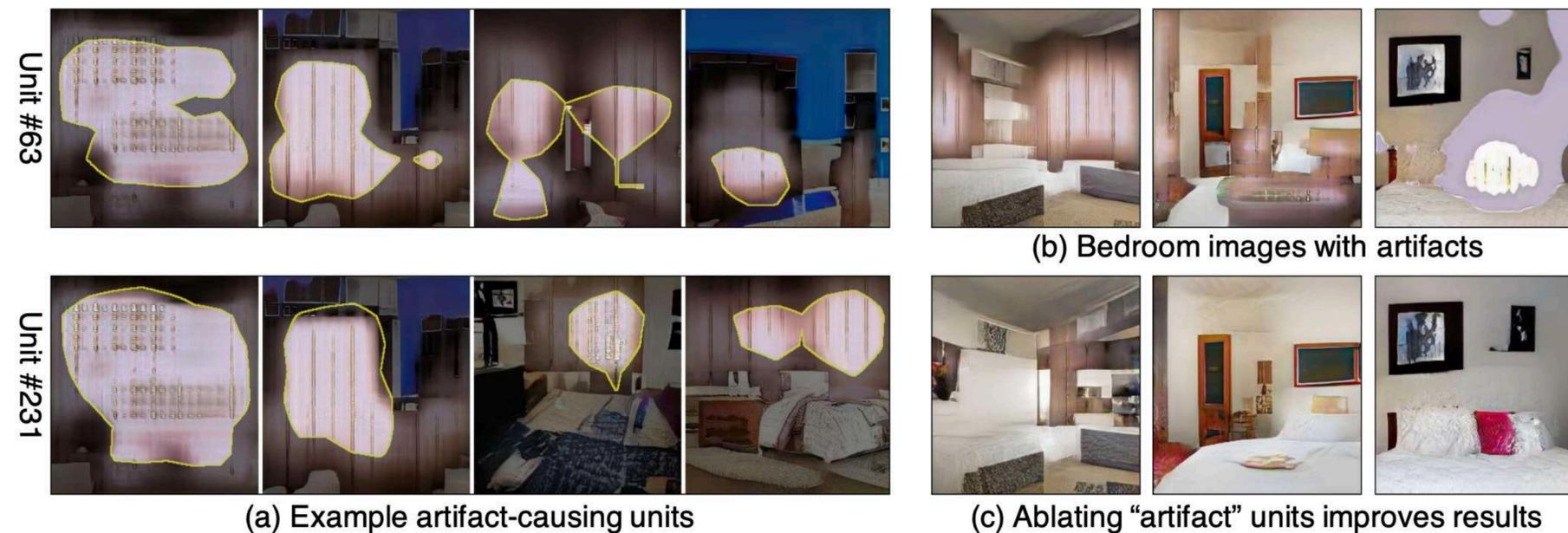
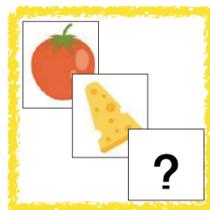


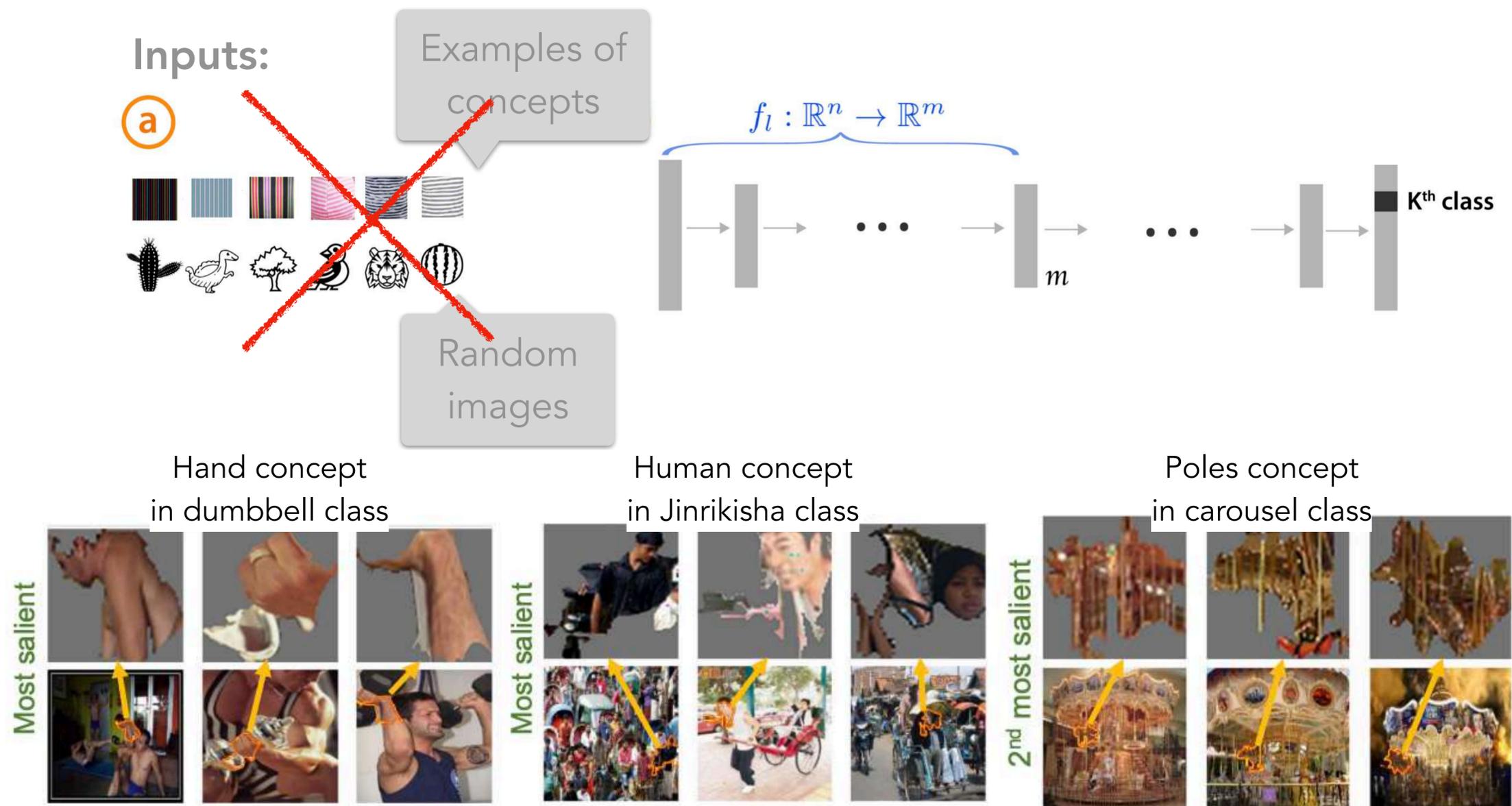
Figure 8: (a) We show two example units that are responsible for visual artifacts in GAN results. There are 20 units in total. By ablating these units, we can fix the artifacts in (b) and significantly improve the visual quality as shown in (c).

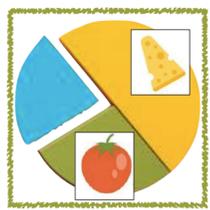


Automatically learning CAVs

[Ghorbani et al. NeurIPS 19]

Segment training images into patches, cluster them to discover new concepts (and rigorously validate them).

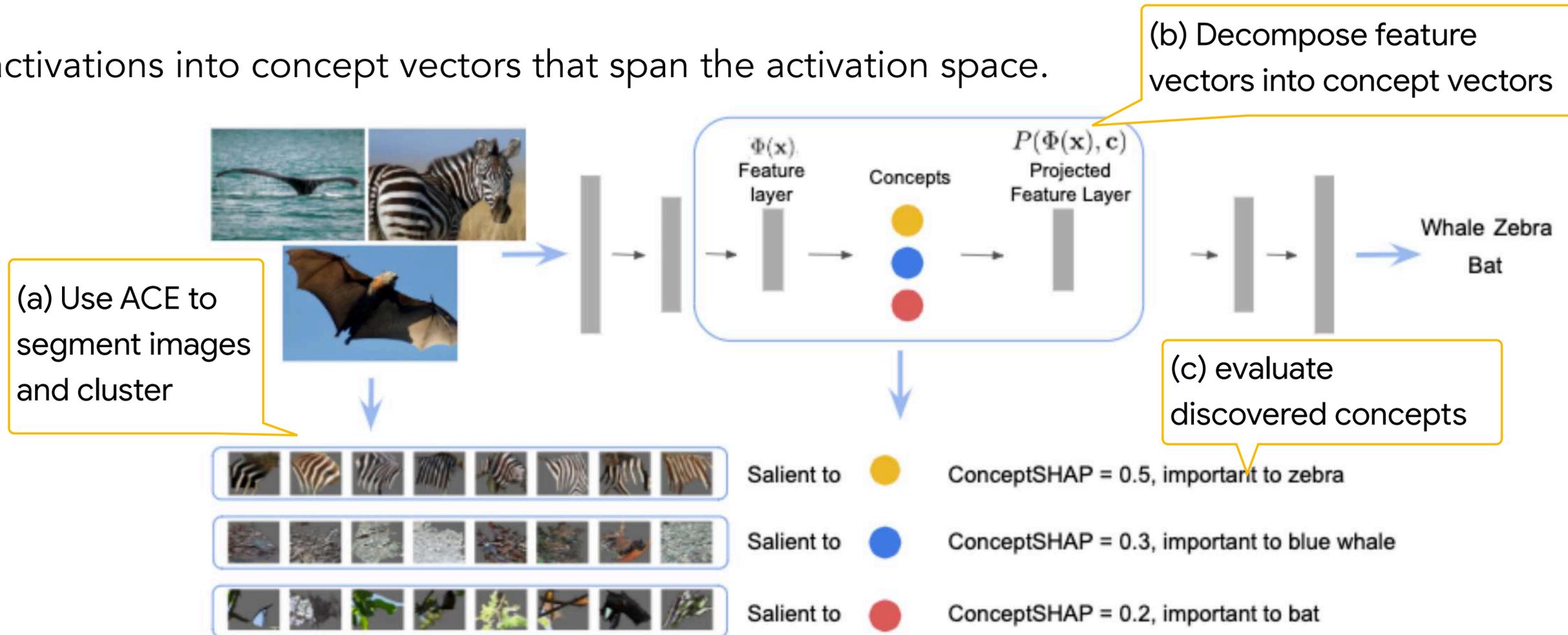




Discovering "complete" set of concepts

[Yeh et al. Neurips 20]

Decompose activations into concept vectors that span the activation space.



Completeness:

The relative prediction accuracy if I only had this concept.

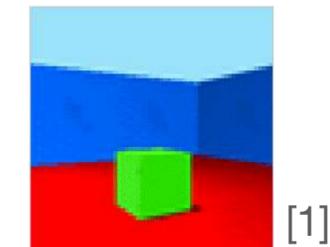
$$\frac{\mathbb{E}_{\mathbf{x}, y \sim V} [\mathbb{1}[y = \arg \max_{y'} P(y' | \mathbb{E}[z_{1:T}], h)]] - R}{\mathbb{E}_{\mathbf{x}, y \sim V} [\mathbb{1}[y = \arg \max_{y'} P(y' | \mathbf{x}_{1:T}, f)]] - R},$$

Why this metric?

Under simple assumptions, this metric is equivalent to top k PCA vectors.

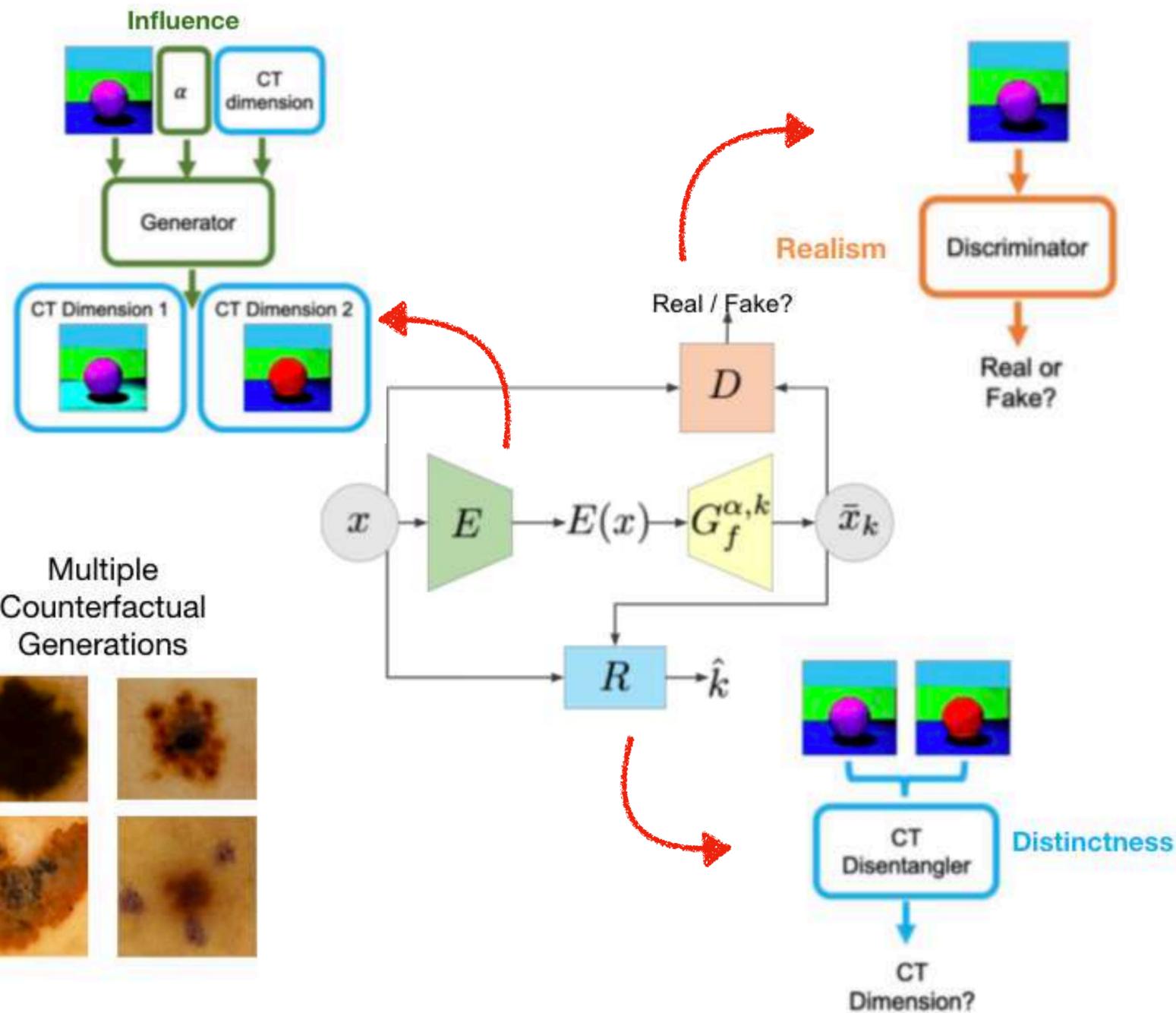
DISSECT: Disentangled Simultaneous Explanations via Concept Traversals

[Ghandeharioun et al. 2021]



[1]

Joint train a generative model to produce multiple counterfactual concepts

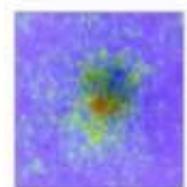


Heatmaps Segmentation Masks Retrieval Based Counterfactual Generation



Query: Benign

Is this skin lesion Melanoma?



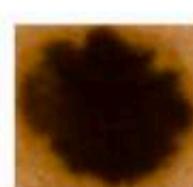
e.g. [1-4]



e.g. [5, 6]

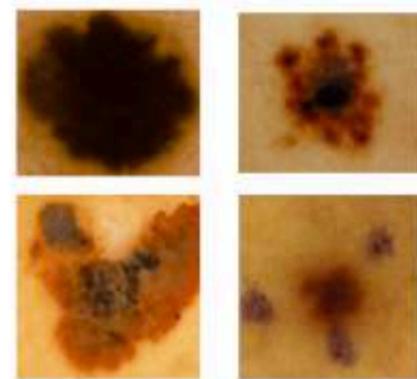


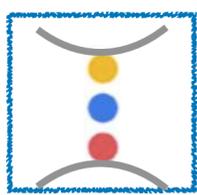
e.g. [7]



e.g. [8, 9]

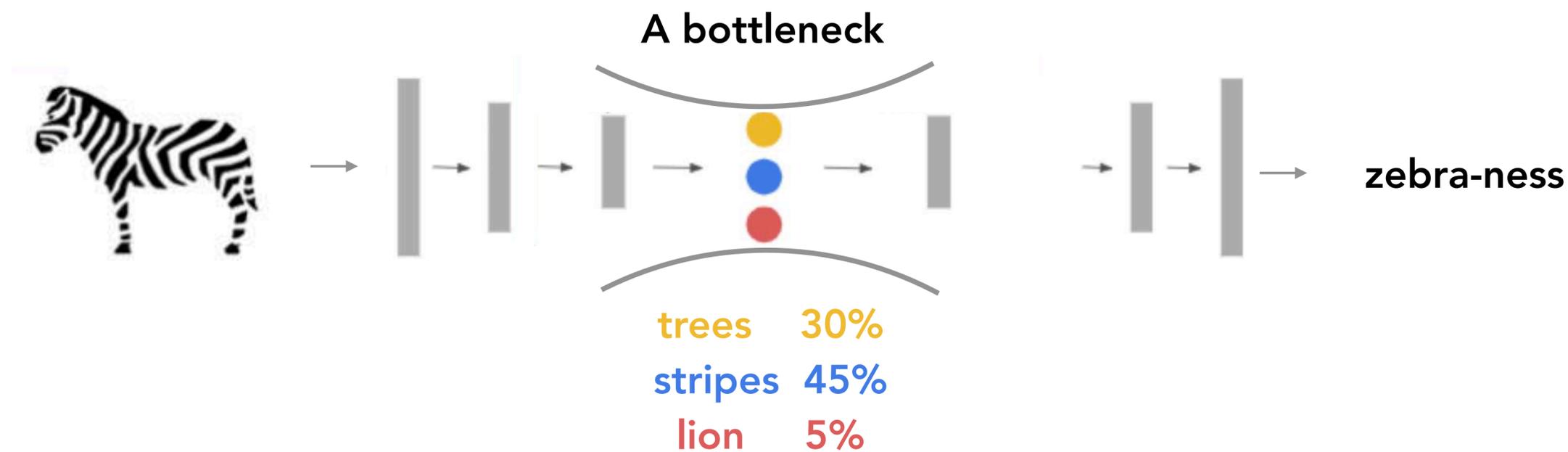
Multiple Counterfactual Generations





Concept bottleneck models

[Goh et al., ICML 20]

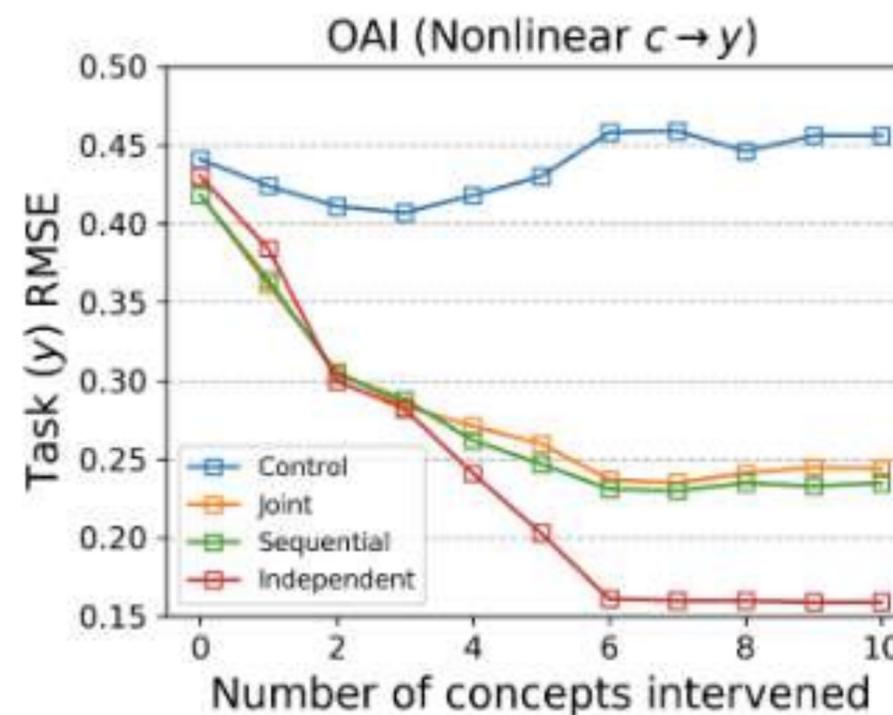


Train a model with concepts as neurons in the middle.

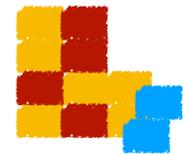
Bonus: we can **interact** and **control** the model



Based on my expertise,
symptom X should not
contribute to the diagnosis.

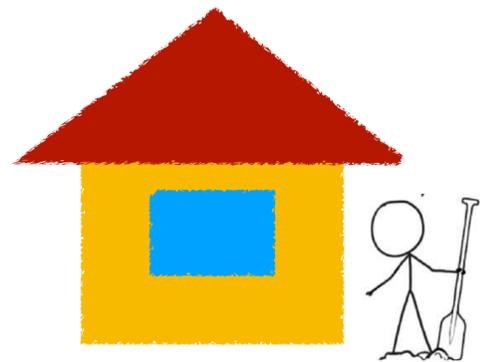


Types of interpretability methods



Explaining data

$$\operatorname{argmax}_E Q(\mathbf{Explanation} | \mathbf{Human}, \mathbf{Data}, \mathbf{Task})$$



My ML



Building inherently interpretable model

$$\operatorname{argmax}_{E, M} Q(\mathbf{Explanation}, \mathbf{Model} | \mathbf{Human}, \mathbf{Data}, \mathbf{Task})$$



Post-training interpretability methods

$$\operatorname{argmax}_E Q(\mathbf{Explanation} | \mathbf{Model}, \mathbf{Human}, \mathbf{Data}, \mathbf{Task})$$

Things that aren't covered but important - science

- Science of it - studying models as a scientific object

IMAGENET-TRAINED CNNs ARE BIASED TOWARDS TEXTURE; INCREASING SHAPE BIAS IMPROVES ACCURACY AND ROBUSTNESS

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Felix A. Wichmann*
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Wieland Brendel*
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wieland.brendel@bethgelab.org



(a) Texture image	(b) Content image	(c) Texture-shape cue conflict
81.4% Indian elephant	71.1% tabby cat	63.9% Indian elephant
10.3% indri	17.3% grey fox	26.4% indri
8.2% black swan	3.3% Siamese cat	9.6% black swan

Figure 1: Classification of a standard ResNet-50 of (a) a texture image (elephant skin: only texture cues); (b) a normal image of a cat (with both shape and texture cues), and (c) an image with a texture-shape cue conflict, generated by style transfer between the first two images.

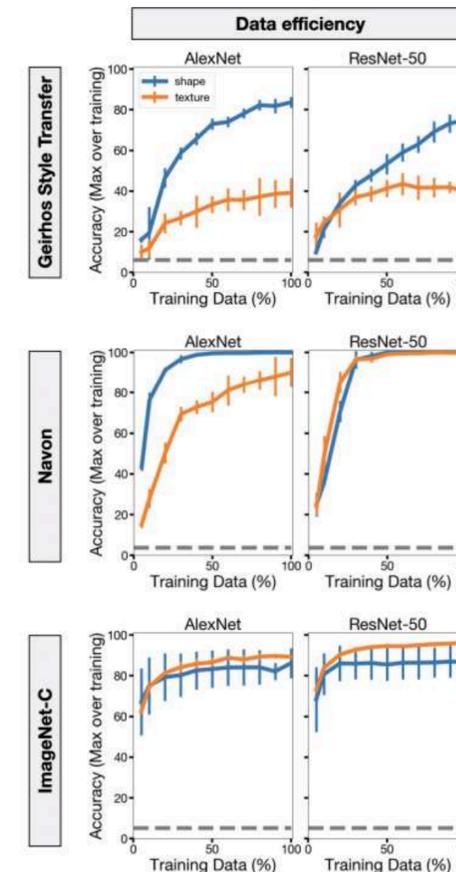
The Origins and Prevalence of Texture Bias in Convolutional Neural Networks

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Ting Chen
Google Research, Toronto
iamtingchen@google.com

Simon Kornblith
Google Research, Toronto
skornblith@google.com

4 CNNs can learn shape as easily as texture



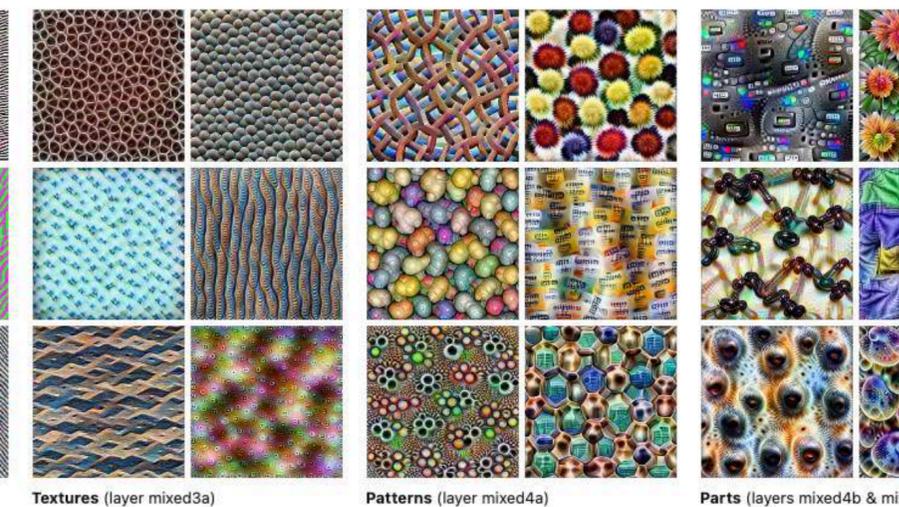
Things that aren't covered but important - science

- Science of it - studying models as a scientific object

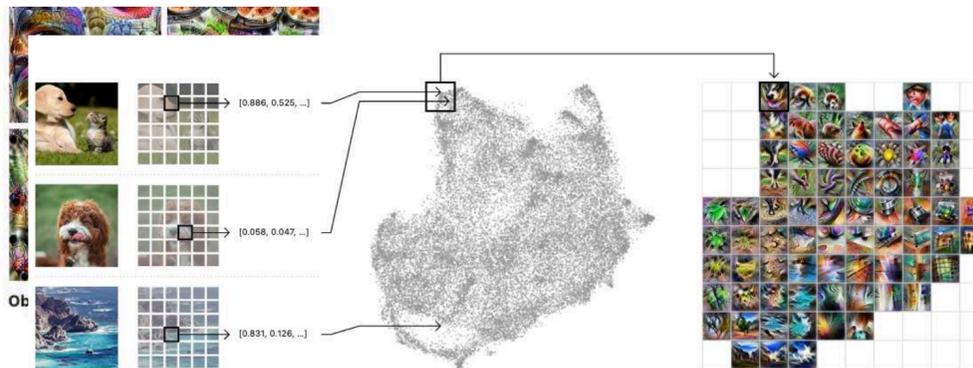
ABOUT PRIZE SUBMIT

Feature Visualization

How neural networks build up their understanding of images



Exploring Neural Networks with Activation Atlases



Feature visualization allows us to see how GoogLeNet [1], trained on the ImageNet [2] dataset, builds up its understanding of images over many layers. Visualizations of all channels are available in the [appendix](#).

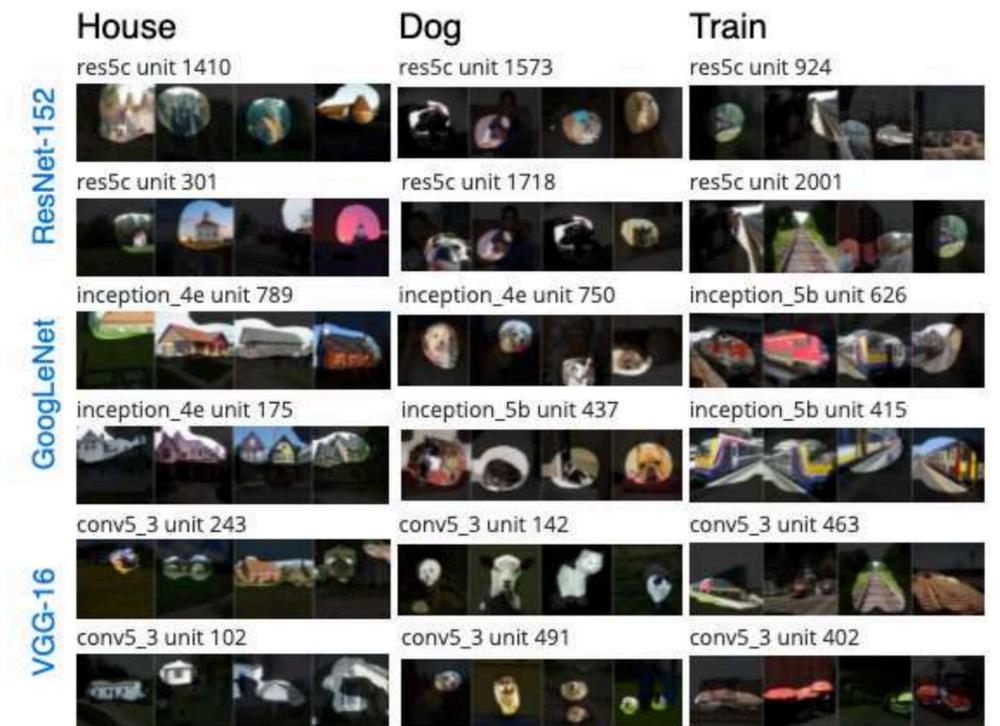
AUTHORS: Chris Olah, Alexander Mordvintsev, Ludwig Schubert
 AFFILIATIONS: Google Brain Team, Google Research, Google Brain Team
 PUBLISHED: Nov. 7, 2017
 DOI: 10.23915/distill.00007

A randomized set of one million images is fed through the network, collecting one random spatial activation per image. The activations are fed through UMAP to reduce them to two dimensions. They are then plotted, with similar activations placed near each other. We then draw a grid and average the activations that fall within a cell and run feature inversion on the averaged activation. We also optionally size the grid cells according to the density of the number of activations that are averaged within.

AUTHORS: Shan Carter, Zan Armstrong, Ludwig Schubert, Ian Johnson, Chris Olah
 AFFILIATIONS: Google Brain Team, Google Accelerated Science, OpenAI, Google Cloud, OpenAI
 PUBLISHED: March 6, 2019
 DOI: 10.23915/distill.00015

Network Dissection: Quantifying Interpretability of Deep Visual Representations

David Bau*, Bolei Zhou*, Aditya Khosla, Aude Oliva, and Antonio Torralba
 CSAIL, MIT



ResNet-152

GoogLeNet

VGG-16

That's a wrap!



- What and why



- !Caution!: Things to be careful when using and developing interpretability methods

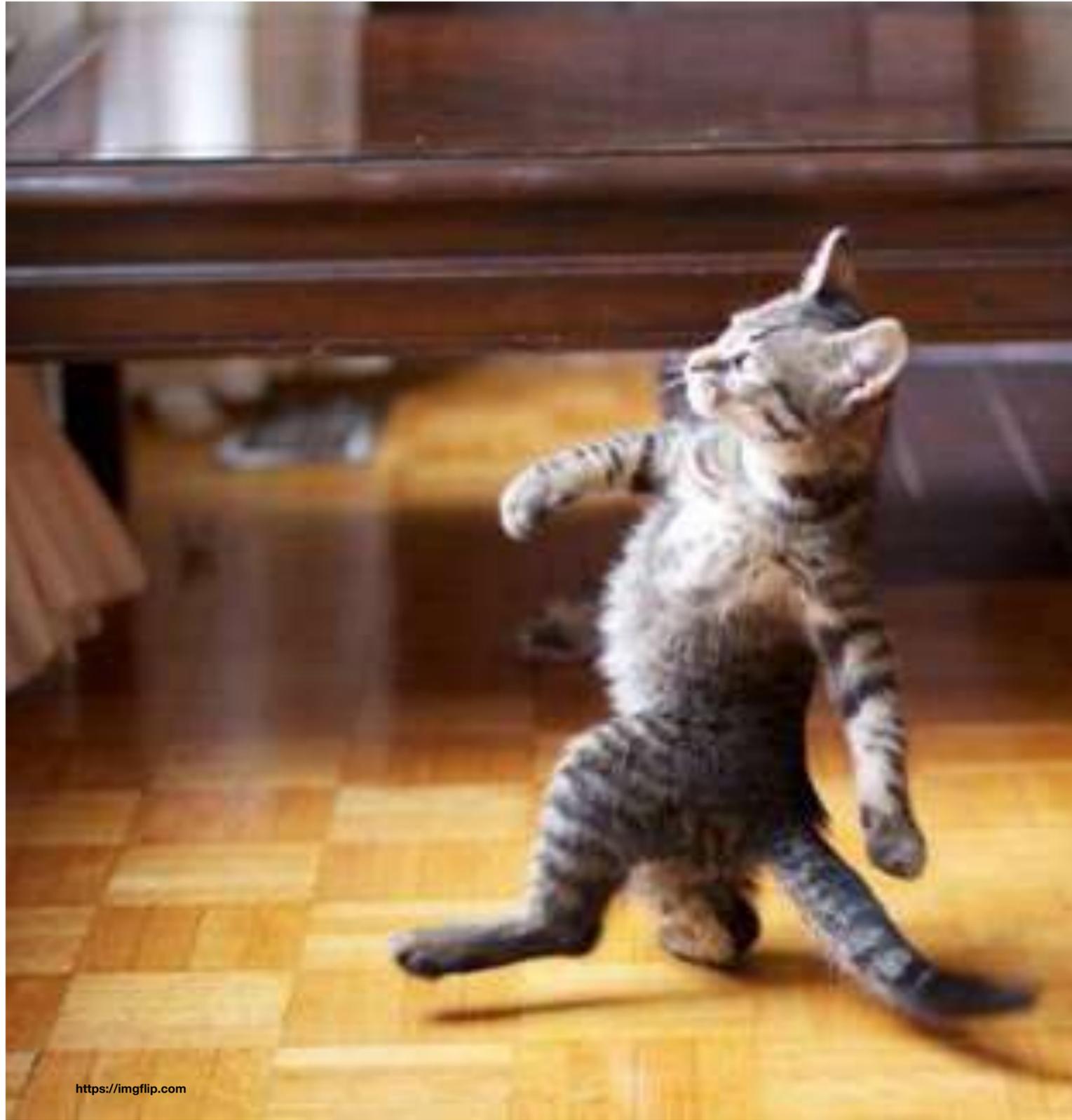


- Evaluate: How to evaluate interpretability methods



- Methods: 3 types of methods and examples





Backups

Other domains

[Submitted on 10 Aug 2021]

Post-hoc Interpretability for Neural NLP: A Survey

[Andreas Madsen](#), [Siva Reddy](#), [Sarath Chandar](#)

Radiology: Artificial Intelligence

On the Interpretability of Artificial Intelligence in Radiology: Challenges and Opportunities

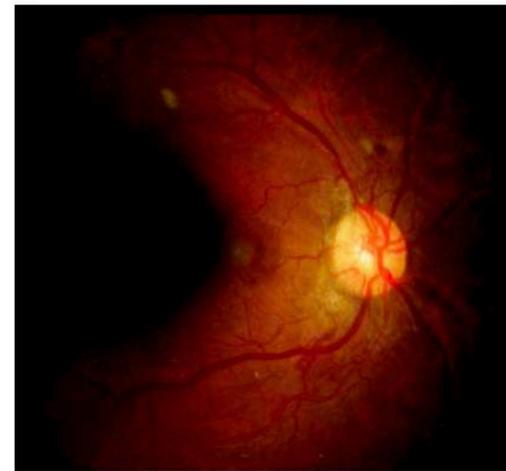
[Mauricio Reyes](#) ✉, [Raphael Meier](#), [Sérgio Pereira](#), [Carlos A. Silva](#), [Fried-Michael Dahlweid](#), [Hendrik von Tengg-Kobligk](#), [Ronald M. Summers](#), [Roland Wiest](#)

Ok, great but...

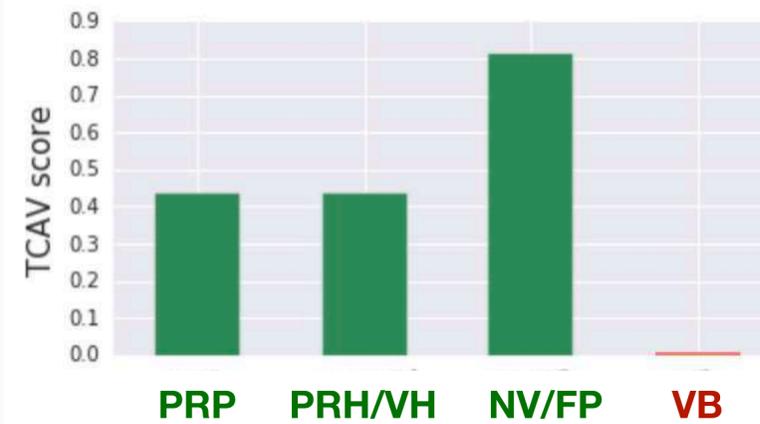
What if I don't have concepts?

Prediction class	Prediction accuracy
DR level 4	High

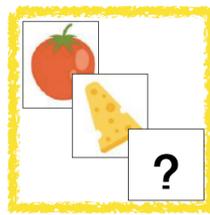
Example



TCAV scores



I don't have these!
Can we automate this?

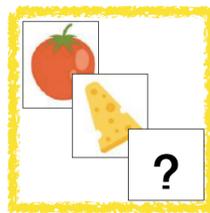


Automatically learning CAVs

[Ghorbani et al. NeurIPS 19]

Amirata Ghorbani





Automatically learning CAVs

[Ghorbani et al. NeurIPS 19]

Inputs:

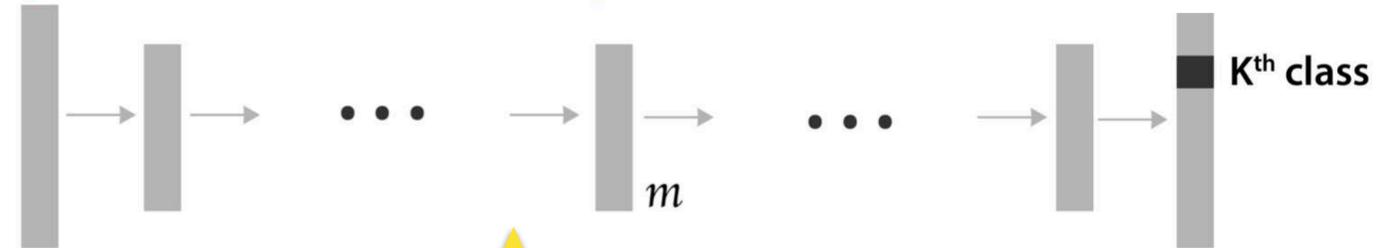
a



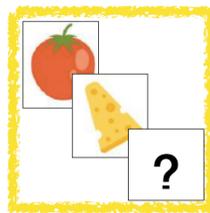
Examples of concepts

Random images

$$f_l : \mathbb{R}^n \rightarrow \mathbb{R}^m$$

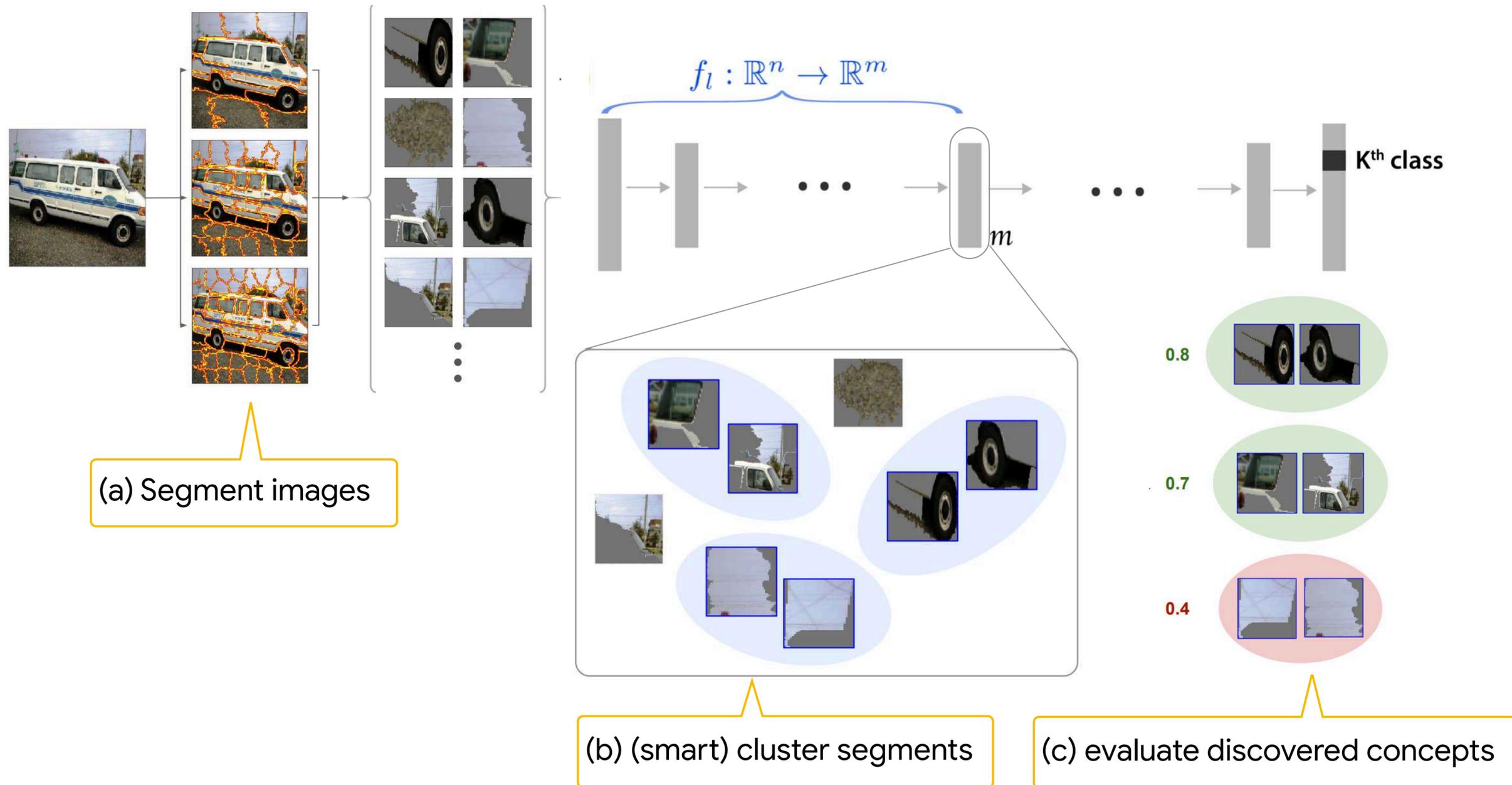


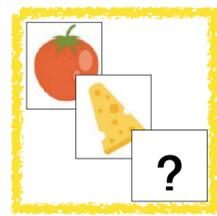
A trained network under investigation and Internal tensors



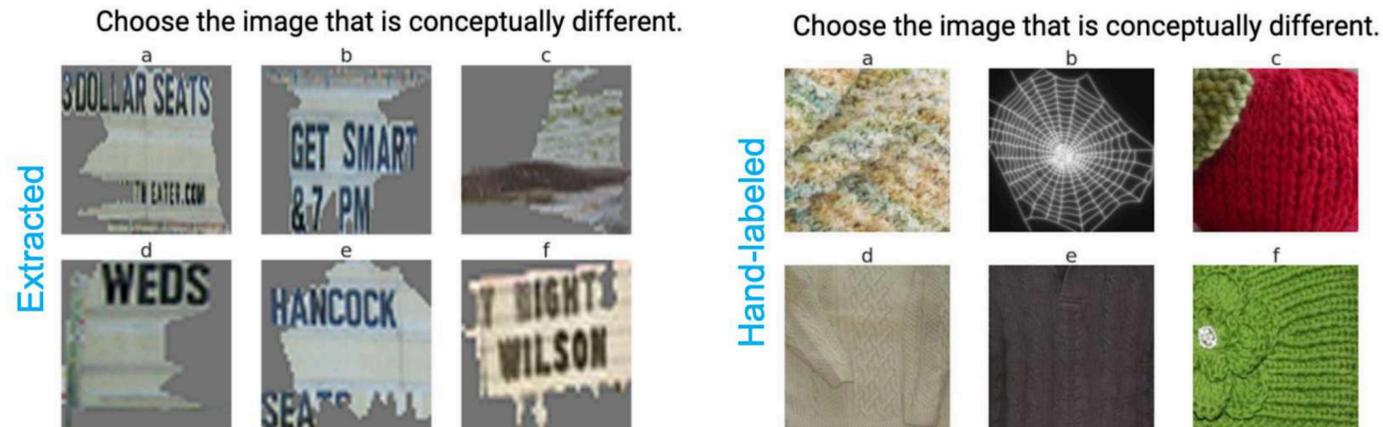
Automatic Concept-based Explanations (ACE)

[Ghorbani et al. NeurIPS 19]



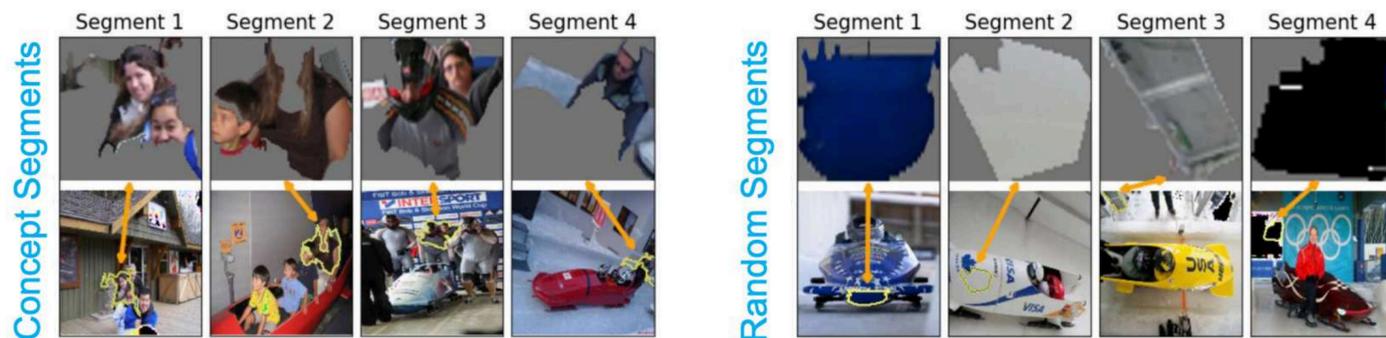


Validating with human experiments: Intruder and meaning test



Experiment 1: Identifying intruder concept

Look at the following two groups of segments. In each group, you should look at the top row. Each image in the top row is a zoomed-in version of another image shown on the bottom row. Now the question is that which of the groups seems more meaningful to you.

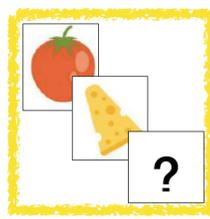


Which groups of images is more meaningful to you? right left

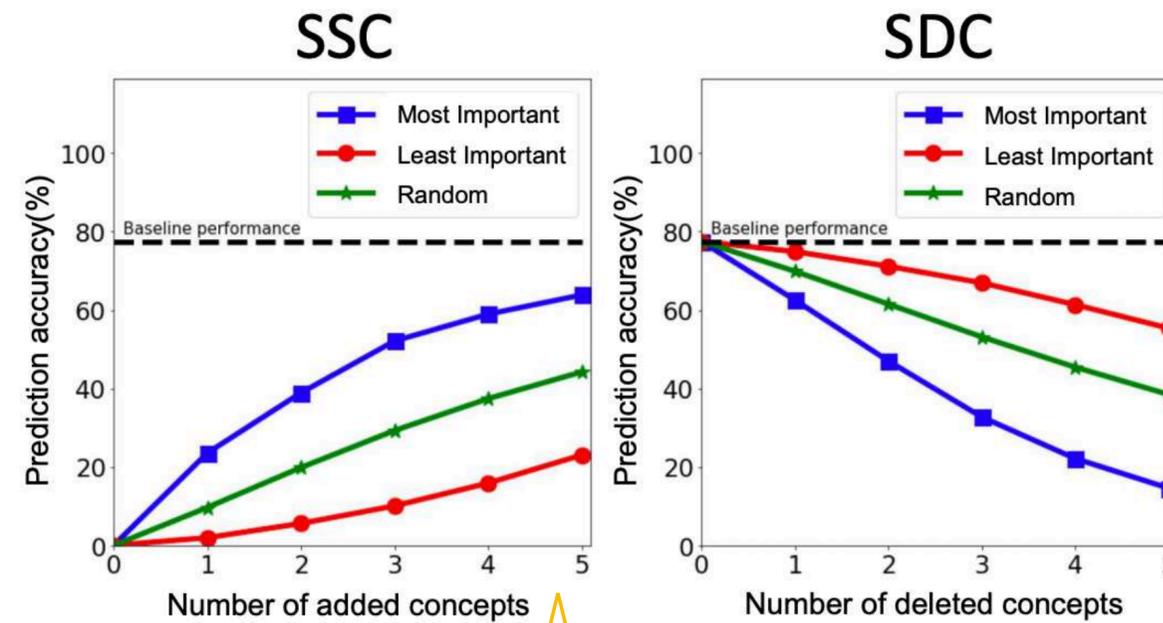
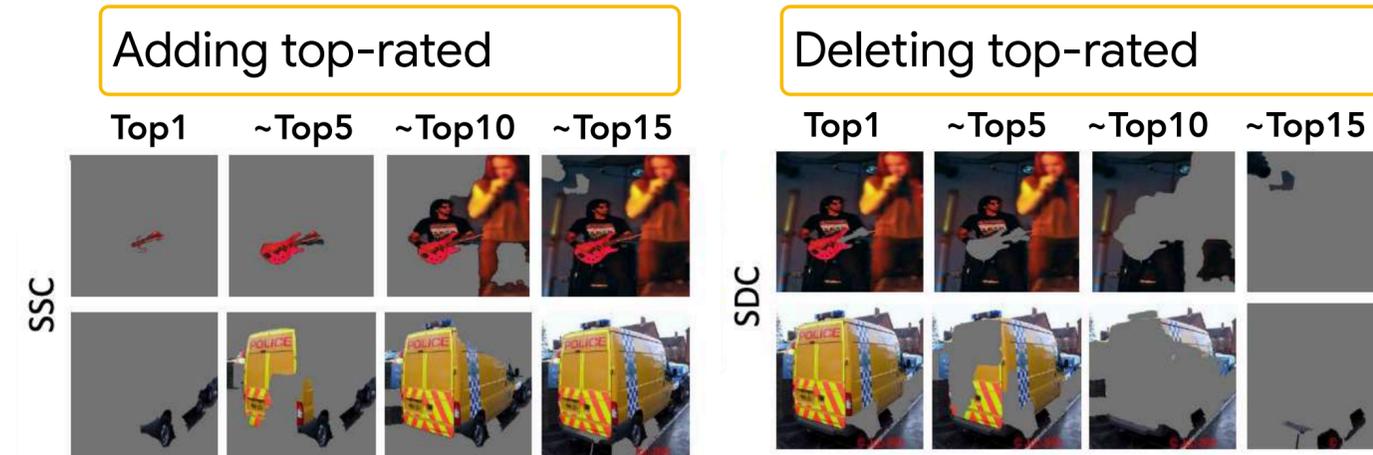
If possible please describe the chosen row in one word.

Experiment 2: Identifying the meaning of concept

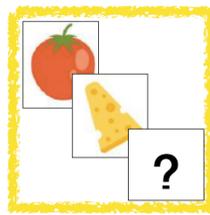
- Exp1: Intruder test
 - Task: Identify an odd one out
 - Discovered concepts: 99%, similar to hand-labeled dataset, 97%
- Exp2: Meaning test
 - Task: Select between discovered concepts vs random segments and name them.
 - Correctly chosen 95% of time
 - 56% used the same name and 77% named the same or top two terms (e.g., human, face)



Validating importance: Addition and deletion test

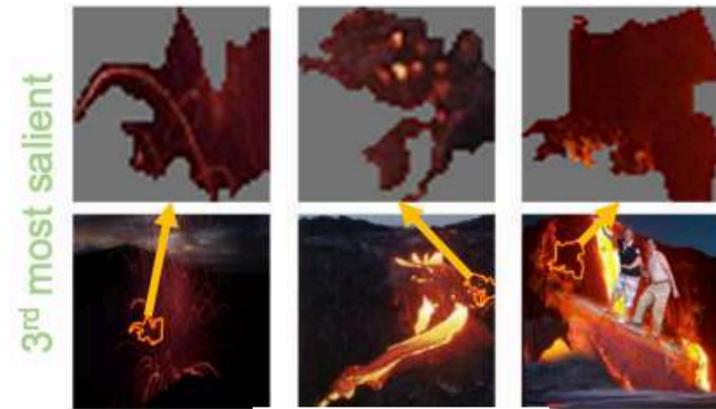


Adding the top5 discovered concepts achieves 80% of the original accuracy



Qualitative results: Surprises and non-surprises

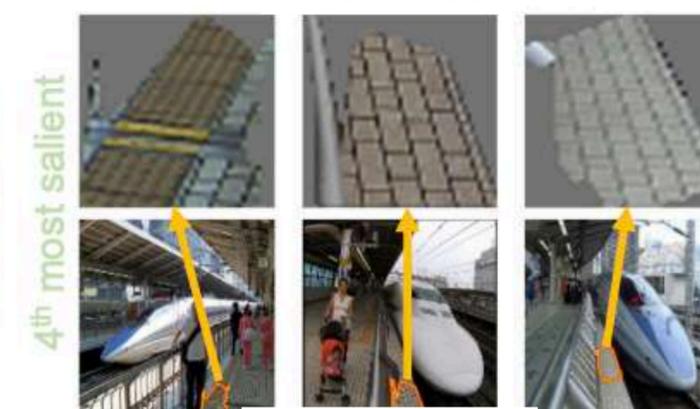
Lava concept
in volcano class



Letters concept
in cinema class

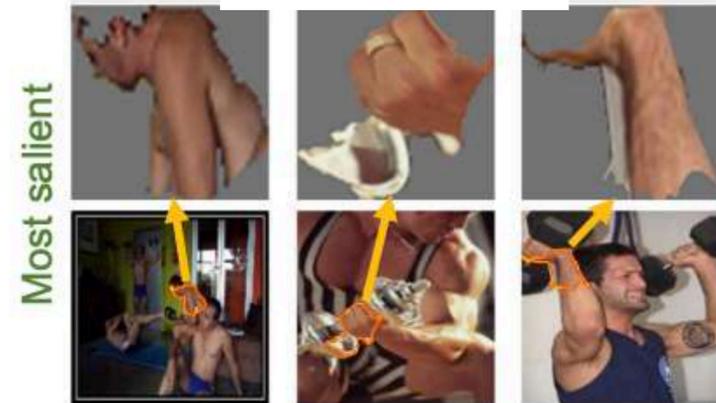


Pavement concept
in train class



This may not work
in Korea?

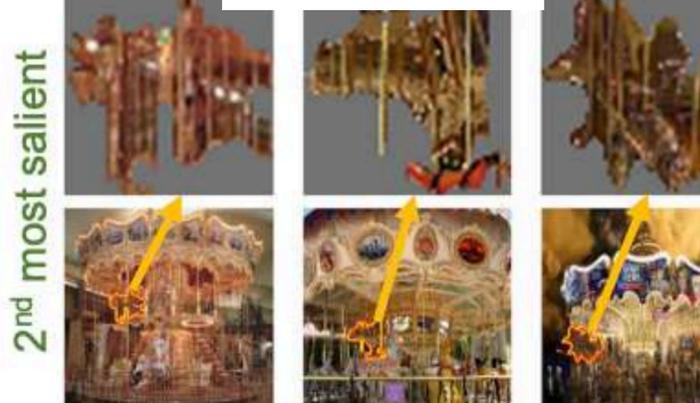
Hand concept
in dumbbell class



Human concept
in Jinrikisha class



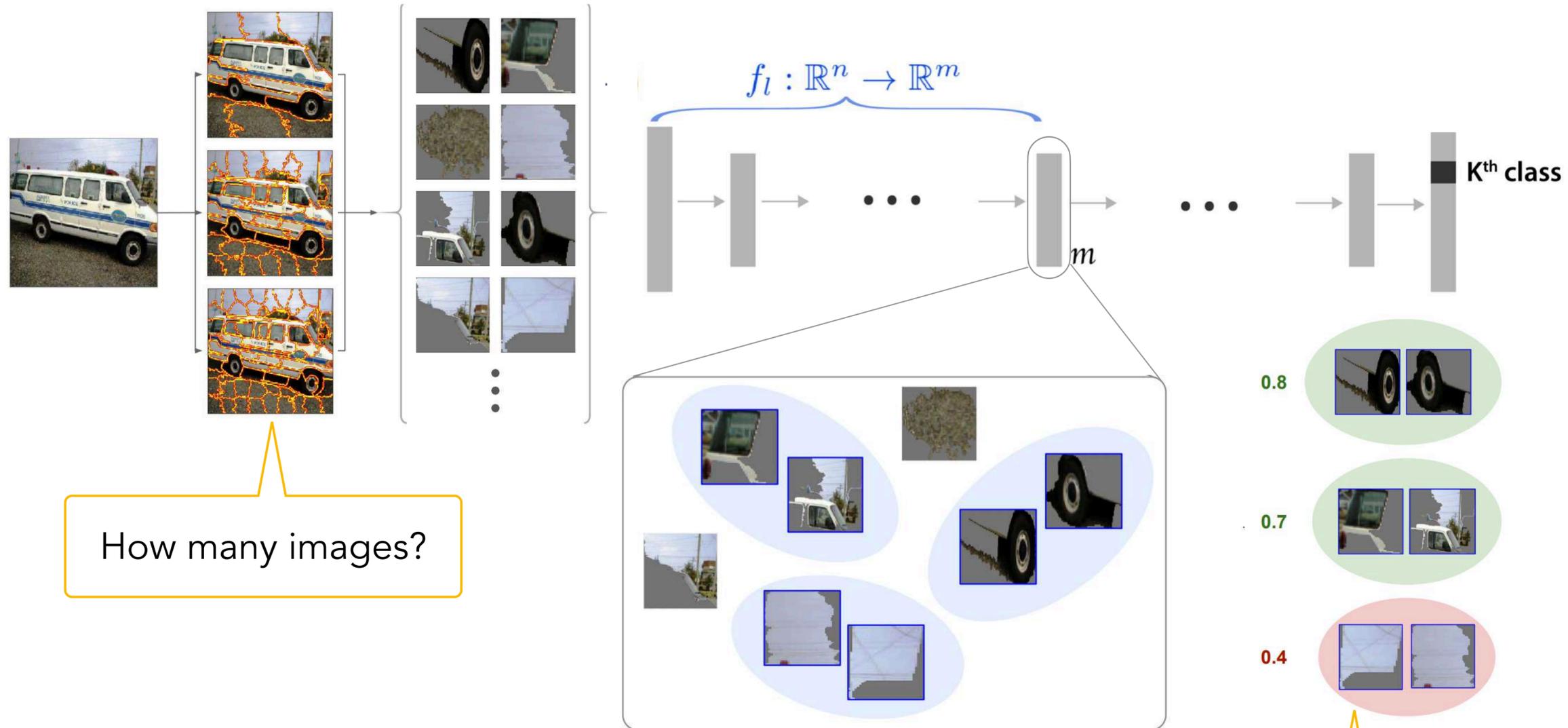
Poles concept
in carousel class



Hands are not dumbbells...

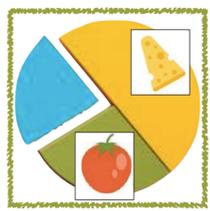
Ok, great but...

When do you stop?



How many images?

Are these concepts "enough"?

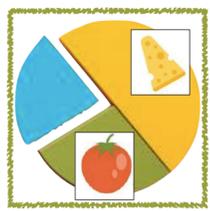


Discovering “complete” set of concepts

[Yeh, Arik, Ravikumar, Pfister, K. Neurips 20]

Chih-Kuan Yeh

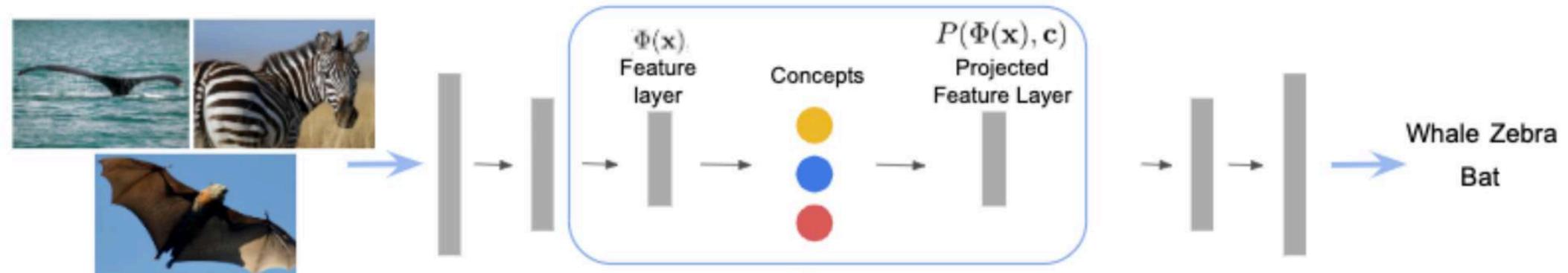


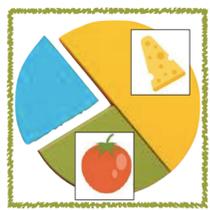


Discovering "complete" set of concepts

[Yeh, Arik, Ravikumar, Pfister, K. Neurips 20]

Decompose activations into concept vectors that span the activation space.





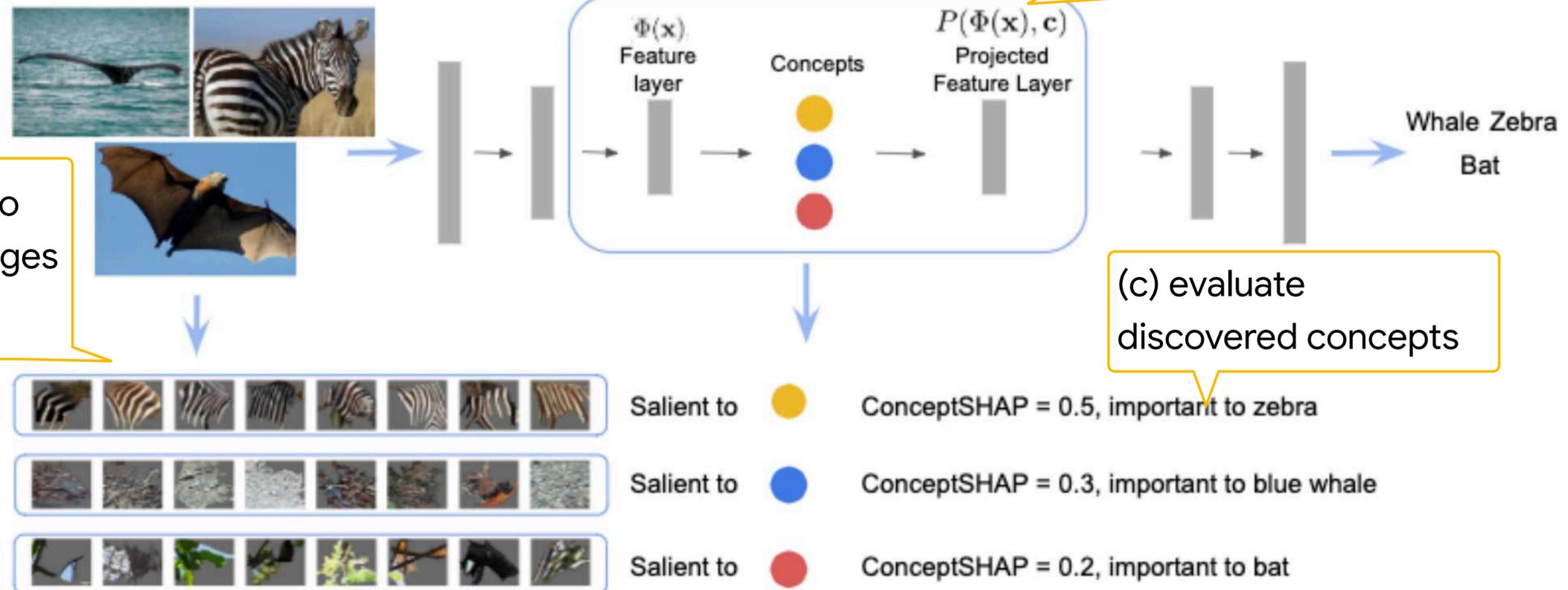
Discovering "complete" set of concepts

[Yeh, Arik, Ravikumar, Pfister, K. Neurips 20]

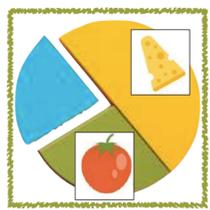
Decompose activations into concept vectors that span the activation space

(b) Decompose feature vectors into concept vectors

(a) Use ACE to segment images and cluster



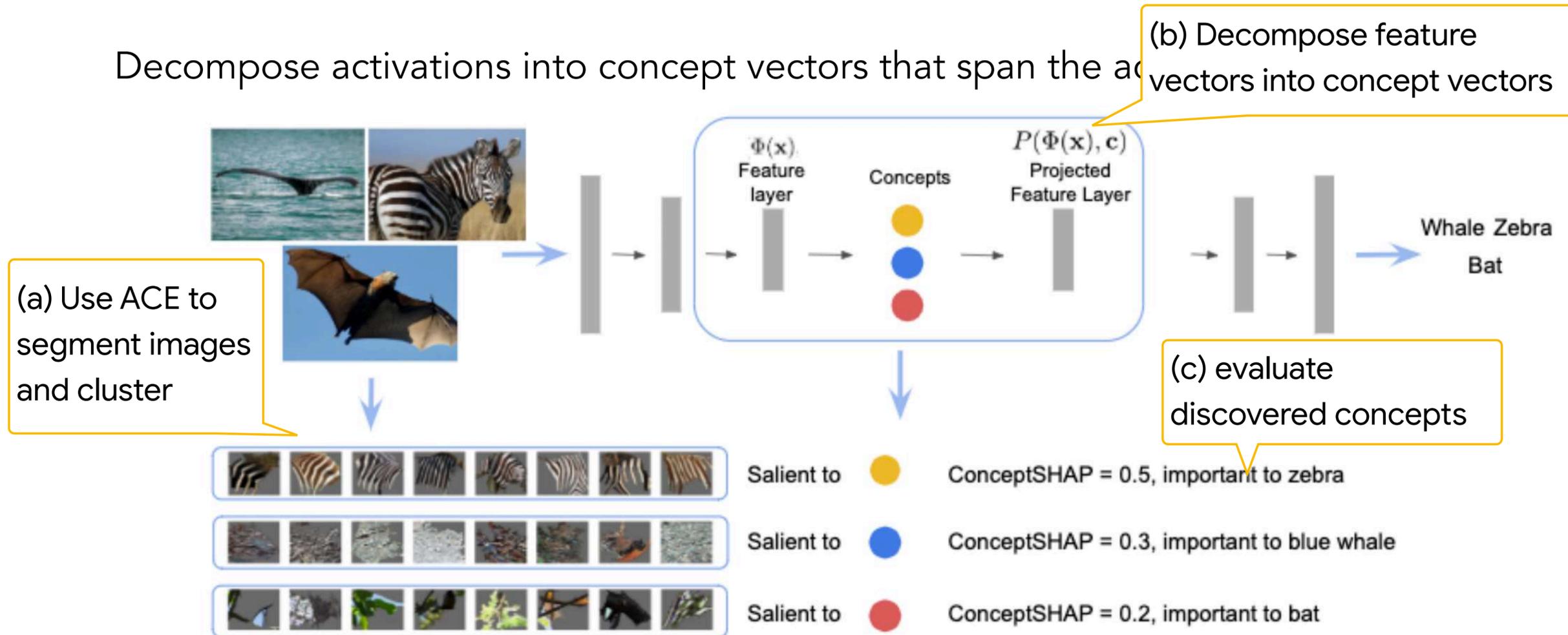
(c) evaluate discovered concepts



Discovering "complete" set of concepts

[Yeh, Arik, Ravikumar, Pfister, K. Neurips 20]

Decompose activations into concept vectors that span the activation space



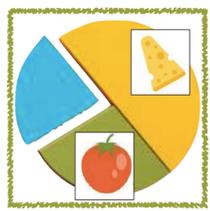
Completeness:

The relative prediction accuracy if I only had this concept.

$$\frac{\mathbb{E}_{\mathbf{x}, y \sim V} [\mathbb{1}[y = \arg \max_{y'} P(y' | \mathbb{E}[z_{1:T}], h)]] - R}{\mathbb{E}_{\mathbf{x}, y \sim V} [\mathbb{1}[y = \arg \max_{y'} P(y' | \mathbf{x}_{1:T}, f)]] - R}$$

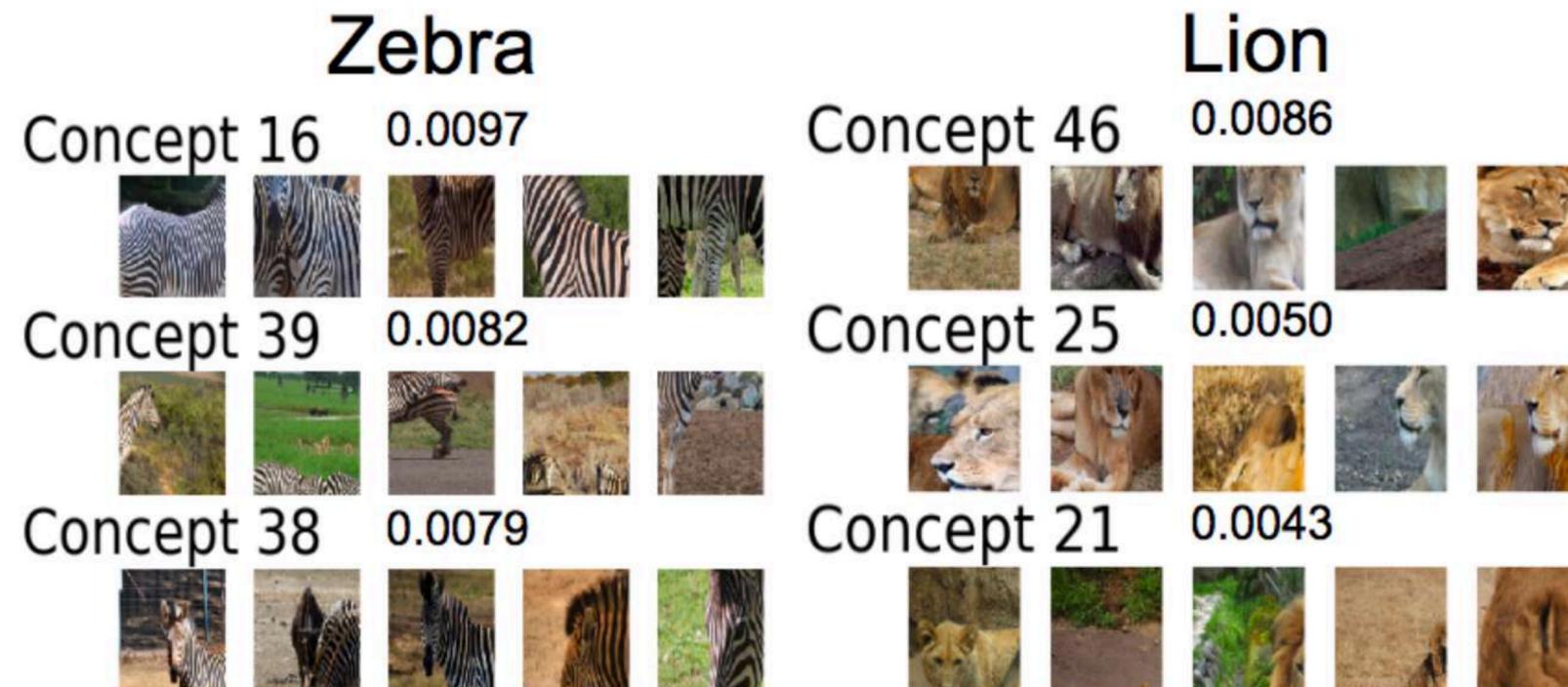
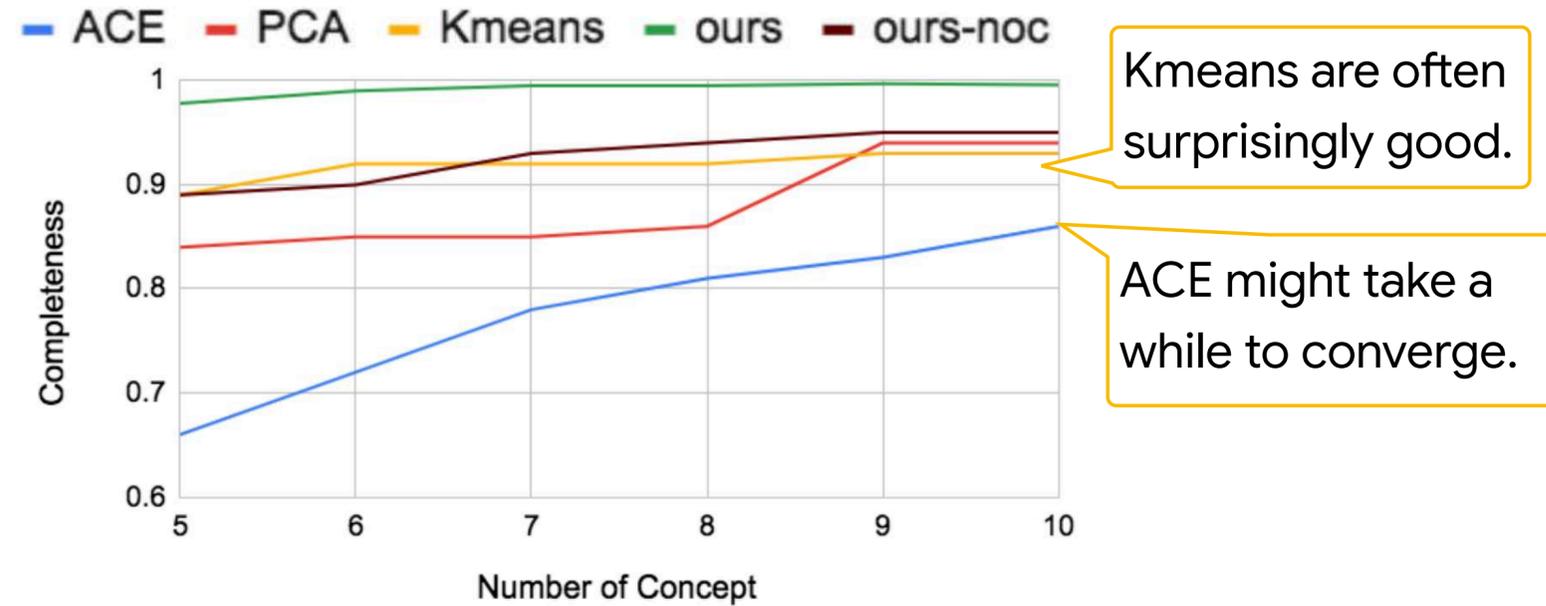
Why this metric?

Under simple assumptions, this metric is equivalent to top k PCA vectors.



Discovering "complete" set of concepts

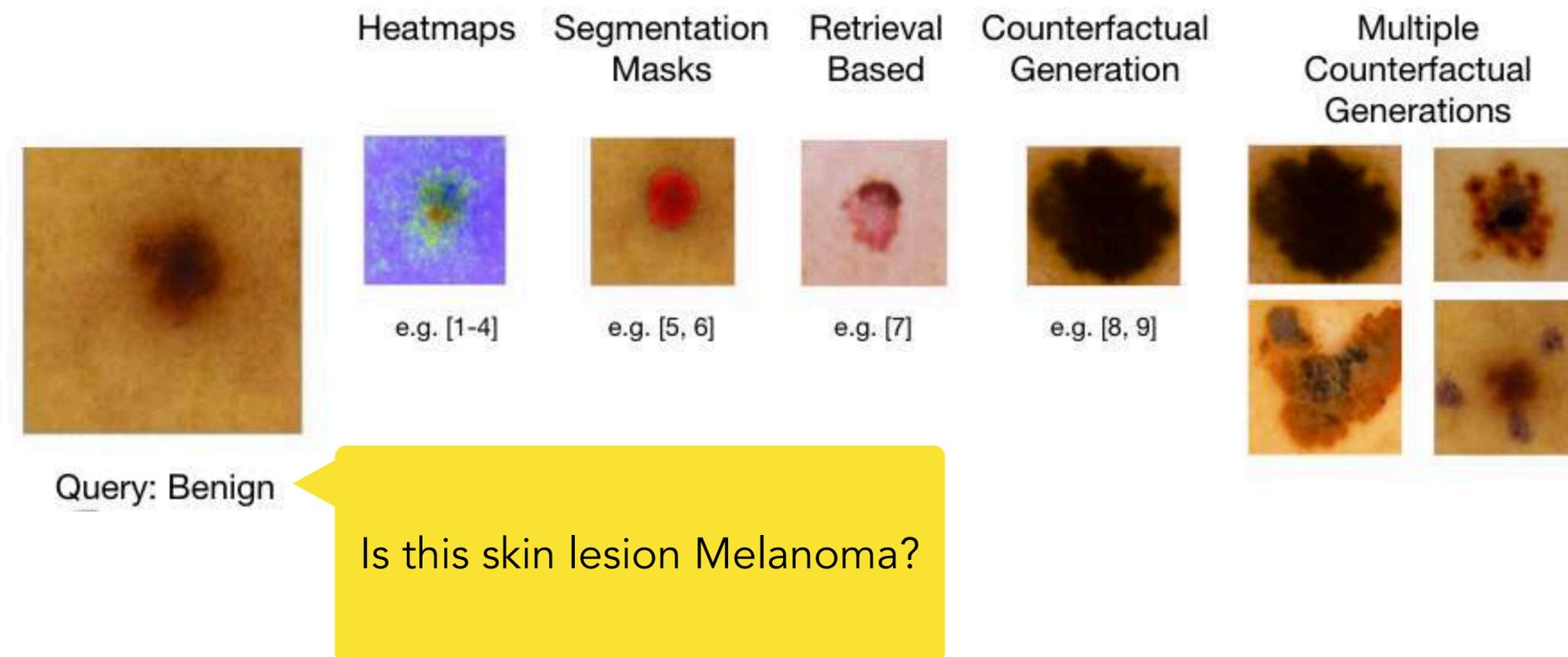
[Yeh, Arik, Ravikumar, Pfister, K. Neurips 20]



Ok, great but...

Haven't you heard about generative models?

Instead of looking for concepts **within training set**, can we just use **generate** concepts using generative models?



DISSECT: Disentangled Simultaneous Explanations via Concept Traversals

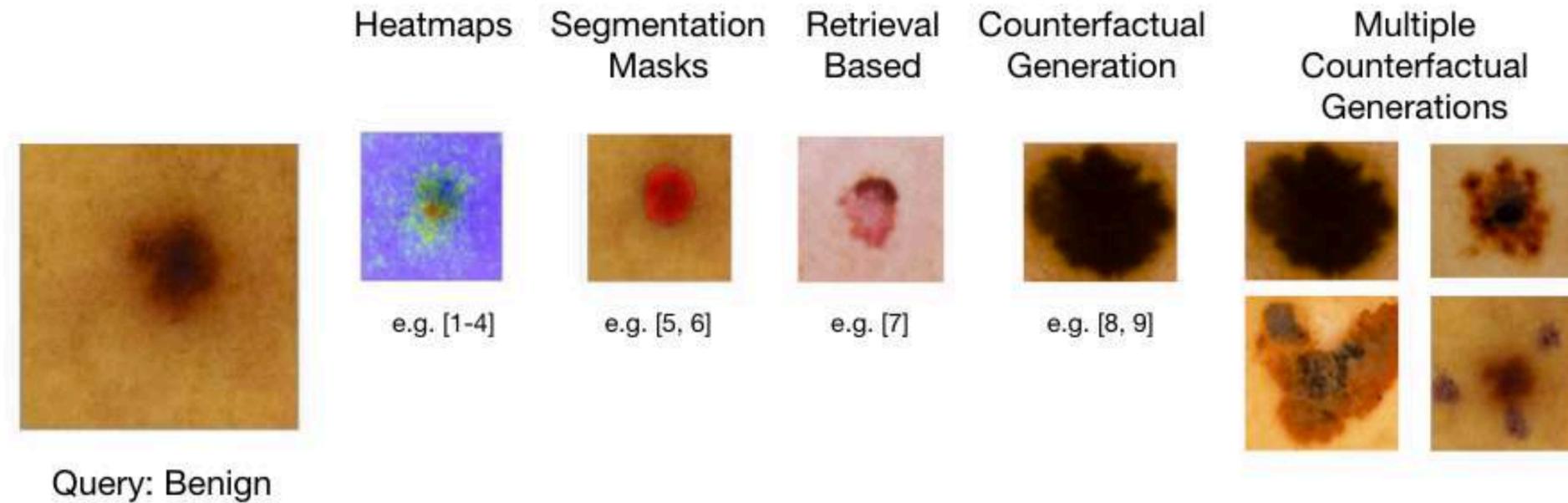
[Ghandeharioun, K., Li, Jou, Eoff, Picard, 2021]

Asma Ghandeharioun



DISSECT: Disentangled Simultaneous Explanations via Concept Traversals

[Ghandeharioun, K., Li, Jou, Eoff, Picard, 2021]

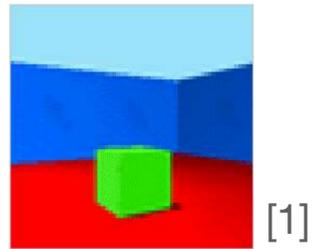


Is this skin lesion Melanoma?

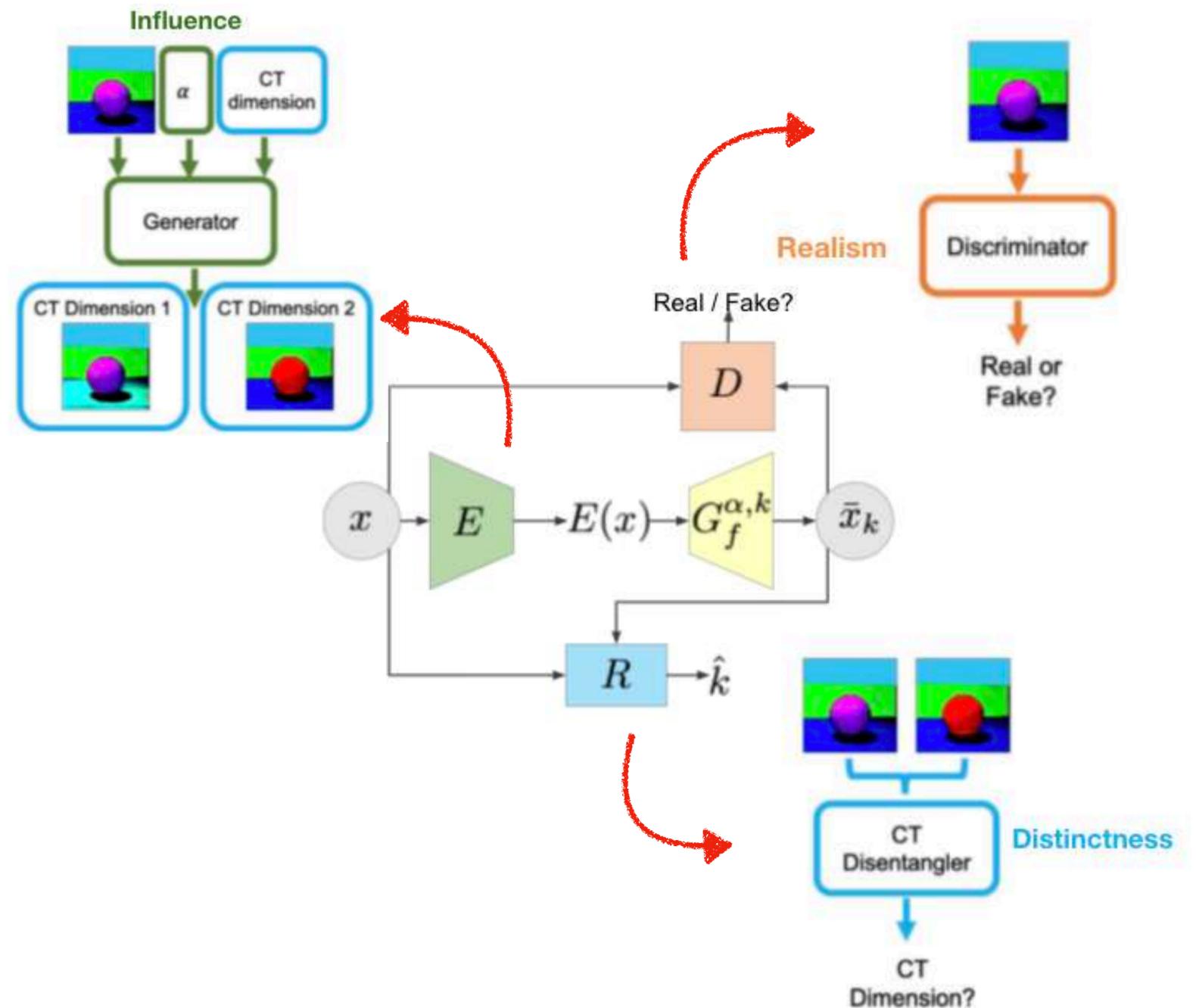
- [1] Erhan et al. "Visualizing higher-layer features of a deep network". University of Montreal, 2009.
- [2] Smilkov et al. "SmoothGrad: Removing noise by adding noise". ICMLW 2017.
- [3] Sundararajan et al. "Axiomatic attribution for deep networks". ICML 2017.
- [4] Lundberg et al. "A unified approach to interpreting model predictions". NeurIPS 2017.
- [5] Ghorbani et al. "Towards automatic concept-based explanations". NeurIPS 2019.
- [6] Santamaria-Pang, et al. "Towards Emergent Language Symbolic Semantic Segmentation and Model Interpretability". MICCAI 2020.
- [7] Silva et al. "Interpretability-guided content-based medical image retrieval". MICCAI 2020.
- [8] Samangouei et al. "ExplainGAN: Model explanation via decision boundary crossing transformations". ECCV 2018.
- [9] Singla et al. "Explanation by progressive exaggeration". ICLR 2020.

DISSECT: Disentangled Simultaneous Explanations via Concept Traversals

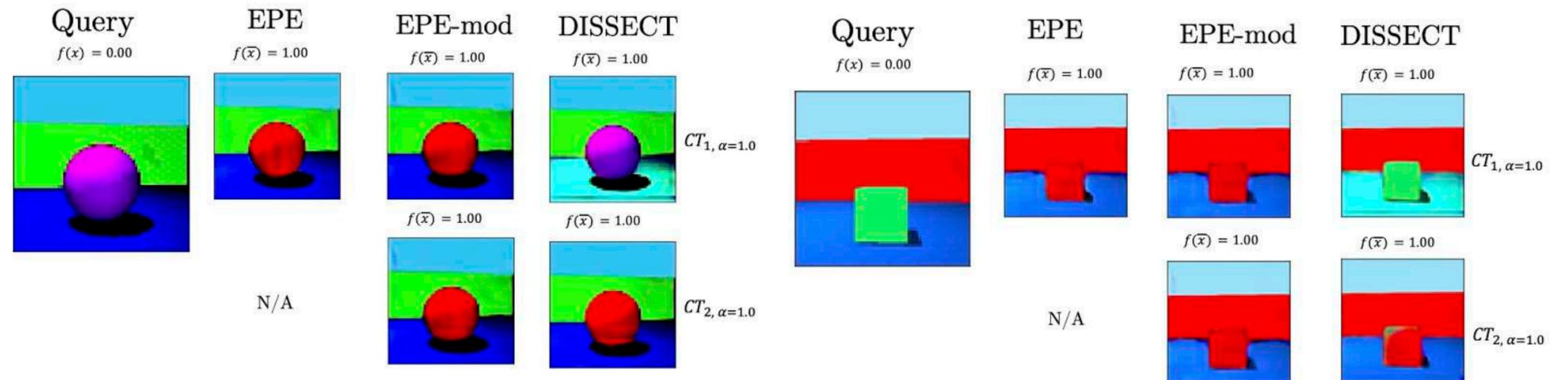
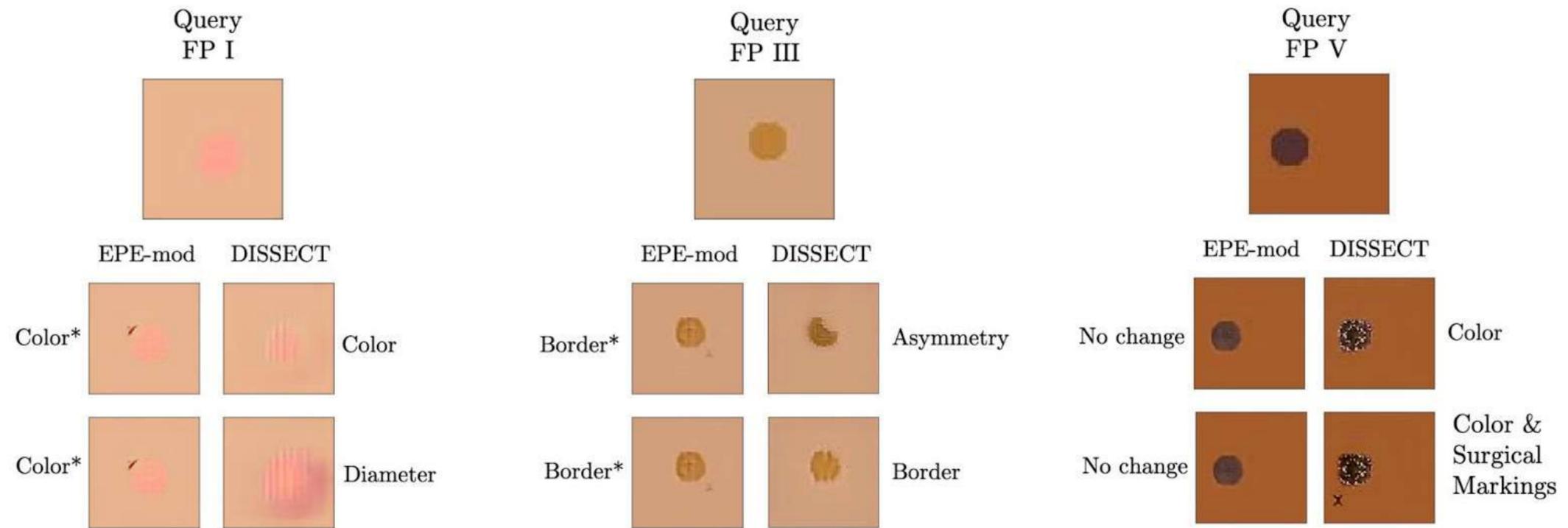
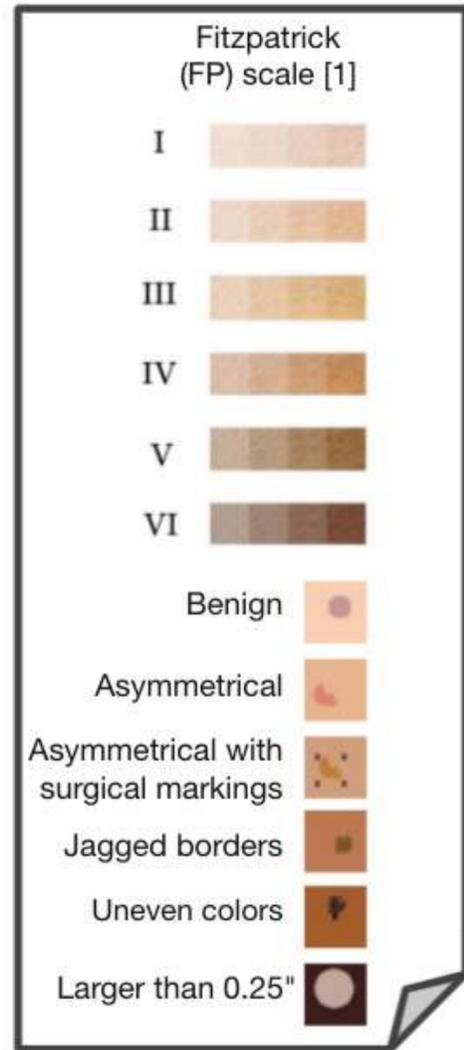
[Ghandeharioun, K., Li, Jou, Eoff, Picard, 2021]



- Desiderata
 - Influential (to classifier's decision)
 - Distinct concept traversals
 - Stable generation
 - High substitutability (can replace real data)
 - High realism (in data manifold)

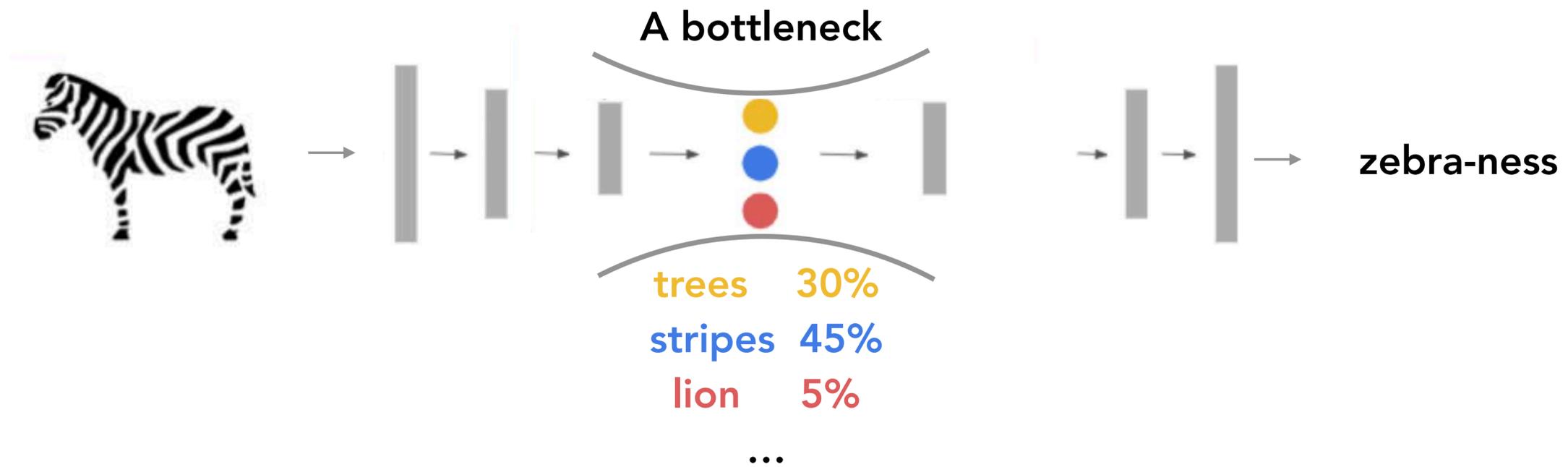


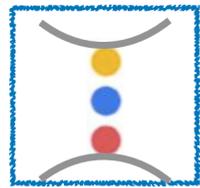
Concept traversals in dermatology and 3D shapes dataset



Ok, great but...

Can we flip this around and build a new model?





Concept bottleneck models

[Goh et al., ICML 20]

Pang Wei
Koh*

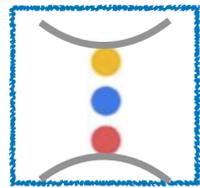


Thao
Nguyen*



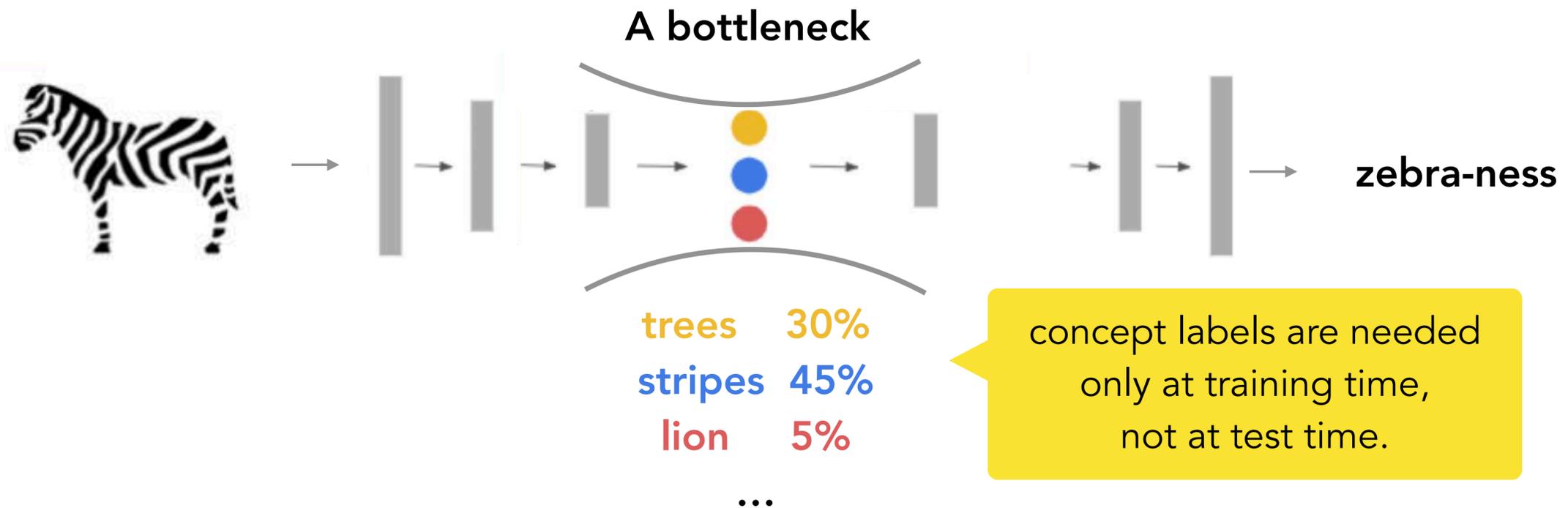
Yew Siang
Tang*

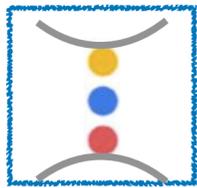




Concept bottleneck models

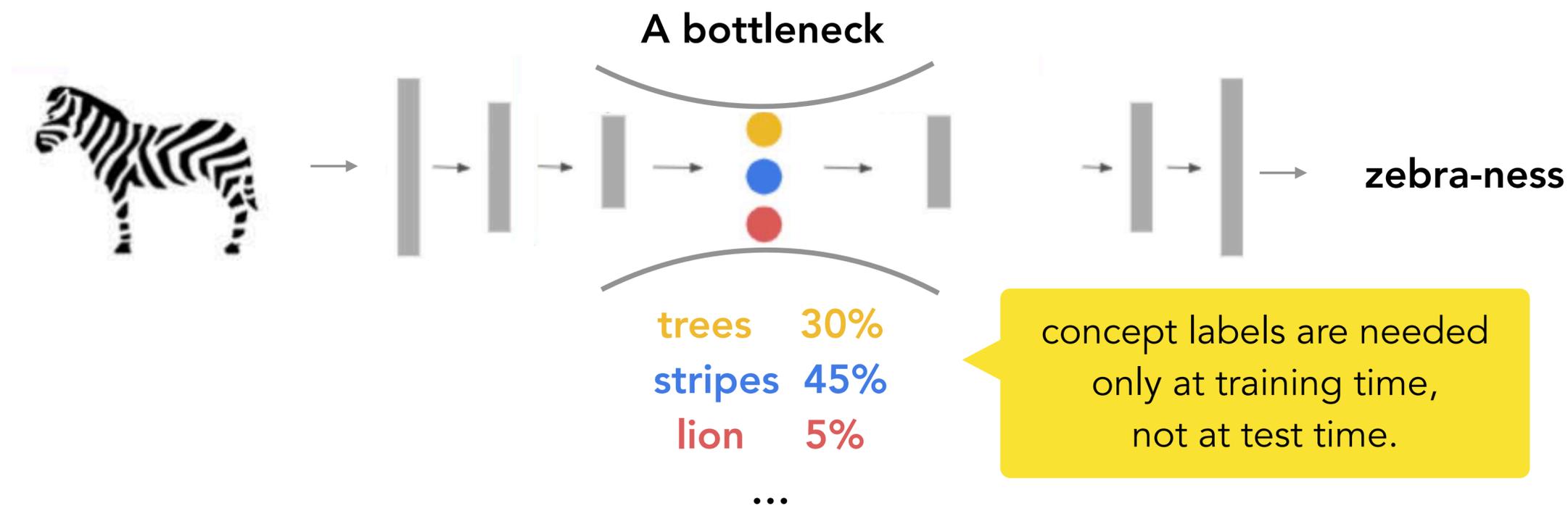
[Goh et al., ICML 20]





Concept bottleneck models

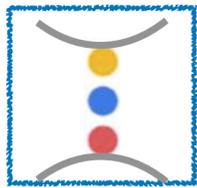
[Goh et al., ICML 20]



First thing to check: is the performance impacted? - No.

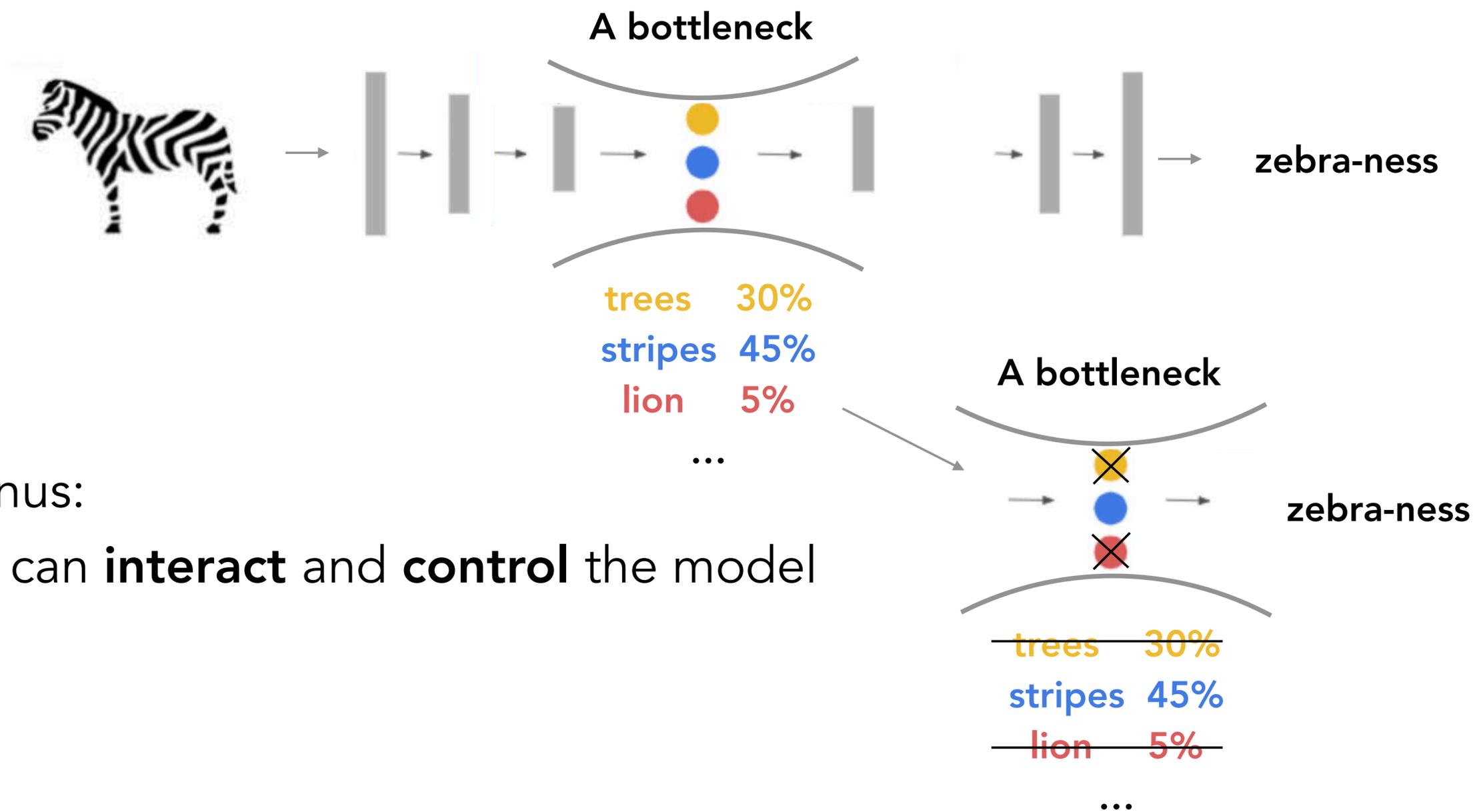
concept
bottleneck
models

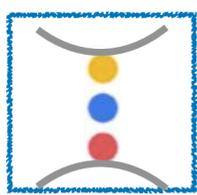
MODEL	y RMSE (OAI)	y ERROR (CUB)
INDEPENDENT	0.435 ± 0.024	0.240 ± 0.012
SEQUENTIAL	0.418 ± 0.004	0.243 ± 0.006
JOINT	0.418 ± 0.004	0.199 ± 0.006
STANDARD	0.441 ± 0.006	0.175 ± 0.008
NO BOTTLENECK	0.443 ± 0.008	0.173 ± 0.003



Concept bottleneck models

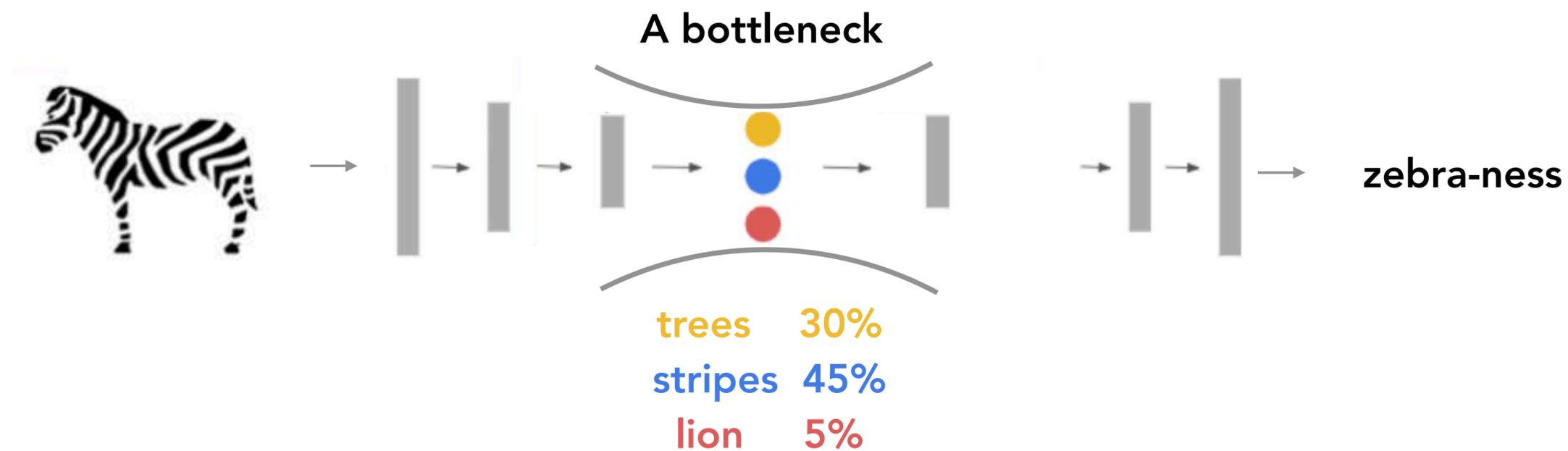
[Goh et al., ICML 20]





Concept bottleneck models

[Goh et al., ICML 20]

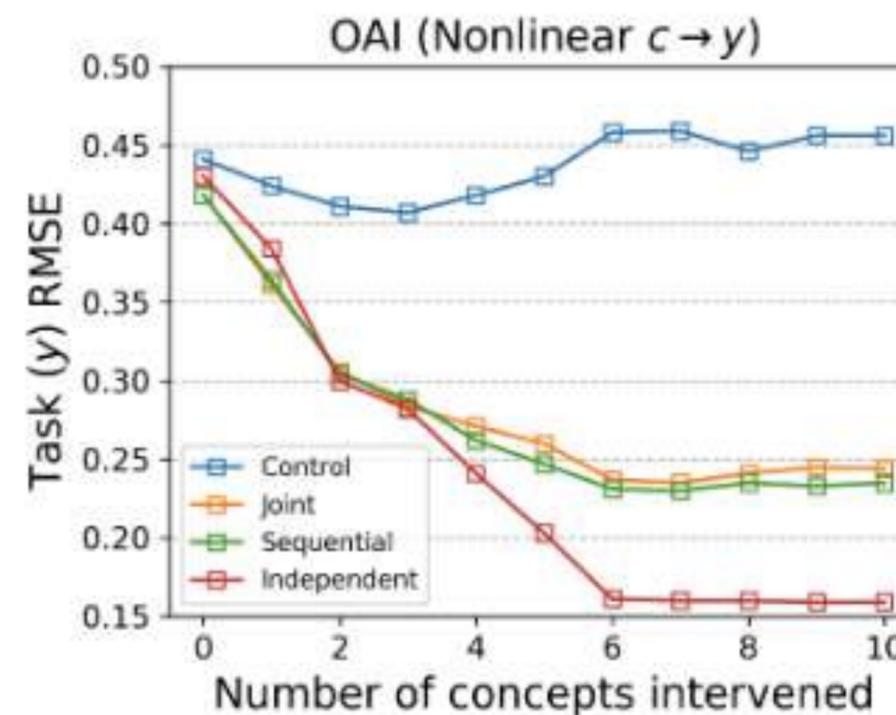


Bonus:

we can **interact** and **control** the model

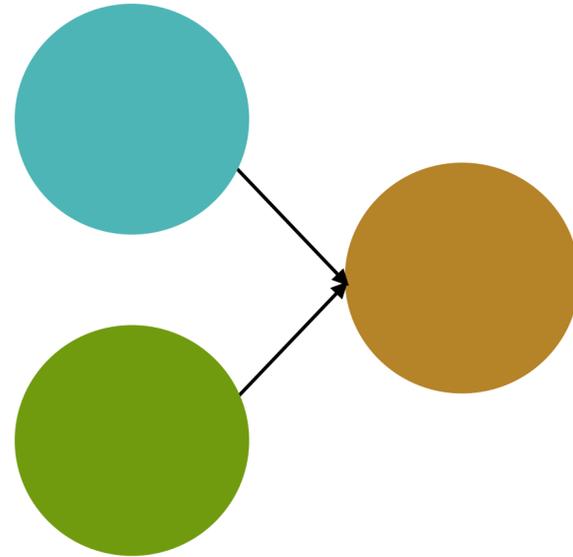


Based on my expertise,
symptom X should not
contribute to the diagnosis.

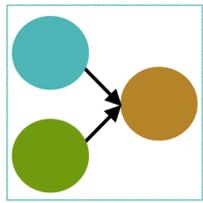


Ok, great but...

what about causality?



Based on my expertise,
symptom X should not
contribute to the diagnosis.



CaCE: Causal TCAV score.

[Goyal et al., 20]

Yash Goyal

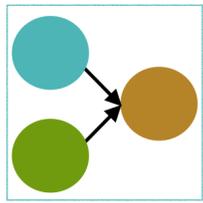


Amir Feder



Uri Salit





CaCE: Causal TCAV score.

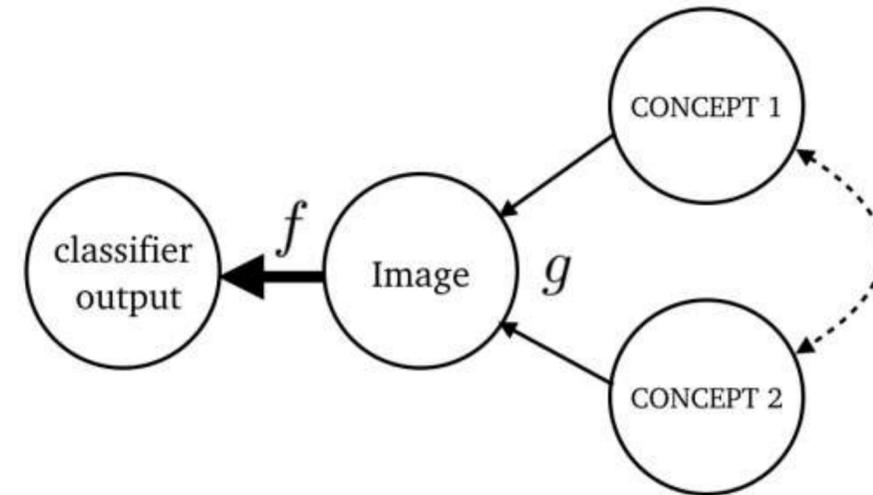
[Goyal et al., 20]

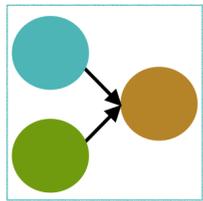
- Basic idea: Do operations on concepts using a generative model to produce $do(C_0 = 1)$ and $do(C_0 = 0)$. Calculate ATE.

Definition 1 (Causal Concept Effect, CaCE).

The causal effect of a binary concept C_0 on the output of the classifier f under the generative process g is:

$$CaCE(C_0, f) = \mathbb{E}_g [f(I)|do(C_0 = 1)] - \mathbb{E}_g [f(I)|do(C_0 = 0)].$$





CaCE: Causal TCAV score.

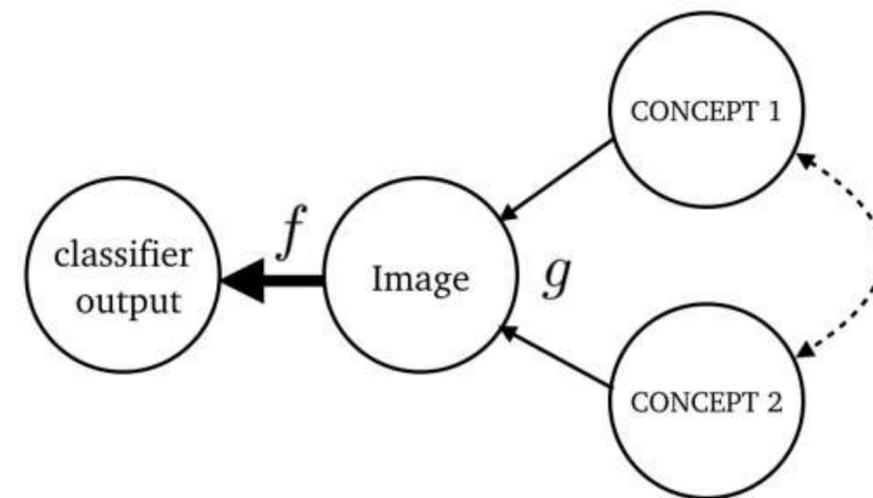
[Goyal et al., 20]

- Basic idea: Do operations on concepts using a generative model to produce $do(C_0 = 1)$ and $do(C_0 = 0)$. Calculate ATE.

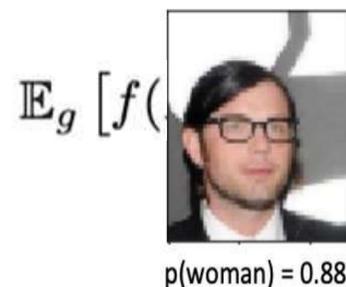
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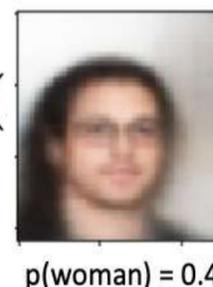
e.g., gender classifier f , ATE with glasses concept?



$\mathbb{E}_g [f(I)$

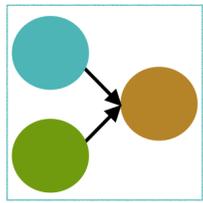
$|do(C_0 = 1)] - \mathbb{E}_g [f(I)$

glasses



$|do(C_0 = 0)]$

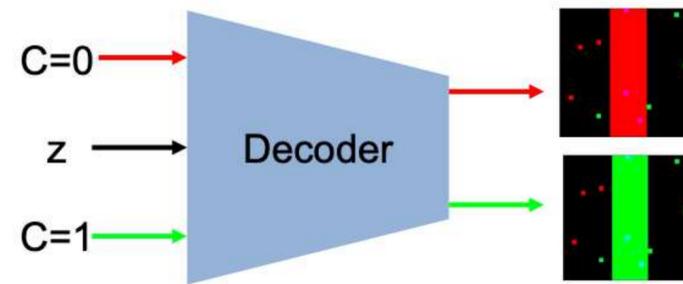
no glasses



CaCE: Causal TCAV score.

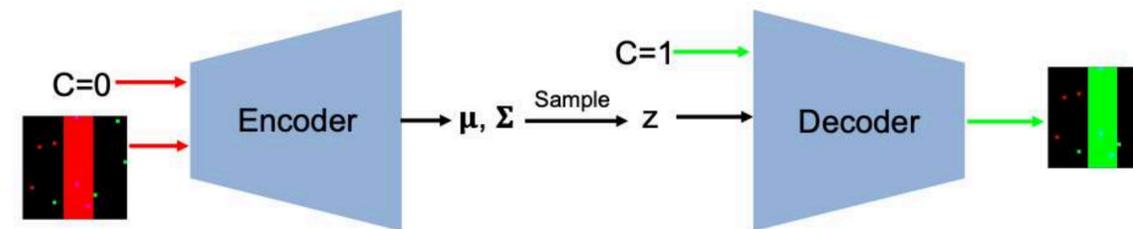
[Goyal et al., 20]

- Can we train a generative model 'good enough' to make this work?



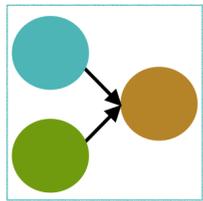
Dec-CaCE

Use sampled z
testing general distributions



EncDec-CaCE

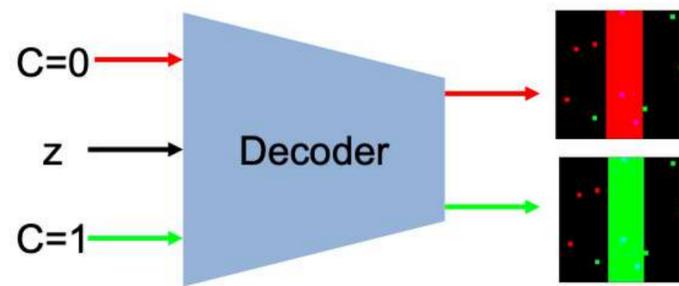
Use a particular instance
testing particular population



CaCE: Causal TCAV score.

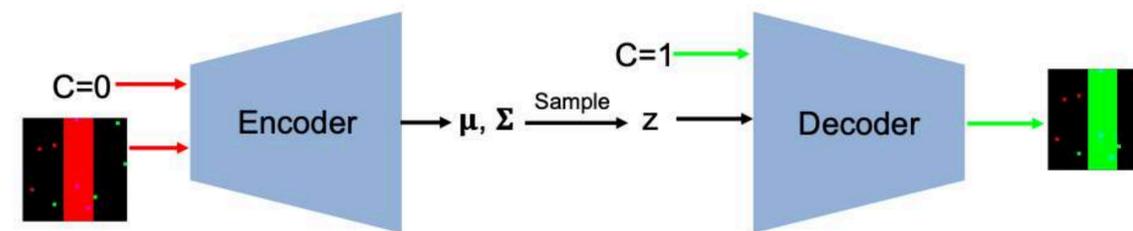
[Goyal et al., 20]

- Can we train a generative model 'good enough' to make this work?



Dec-CaCE

Use sampled z
testing general distributions

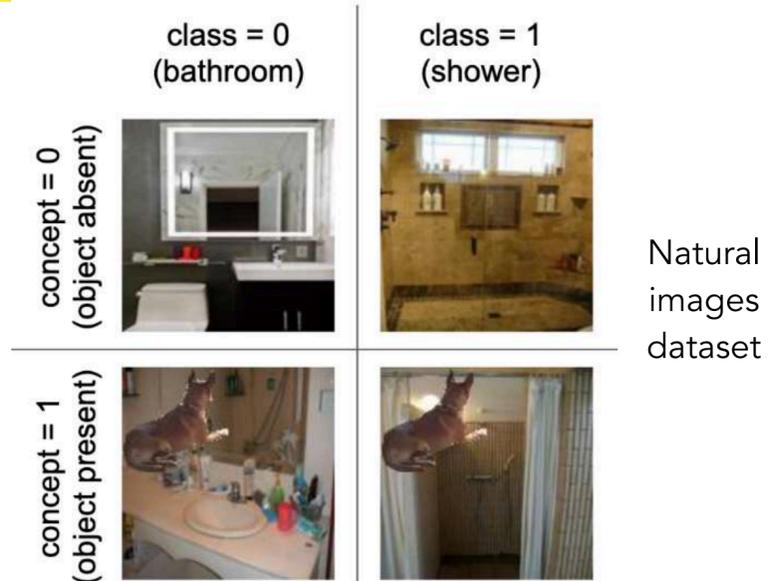


EncDec-CaCE

Use a particular instance
testing particular population

Table 3. CaCE scores for natural images dataset

% of obj in 'bathroom'	% of obj in 'shower'	GT-CaCE	Dec-CaCE	EncDec-CaCE	ConExp (baseline)	TCAV
60	40	0.13	0.154	0.078	0.23	0.723
99	01	0.694	0.651	0.345	0.841	1.000
95	05	0.604	0.543	0.262	0.791	0.988
99	50	0.328	0.31	0.291	0.49	0.944

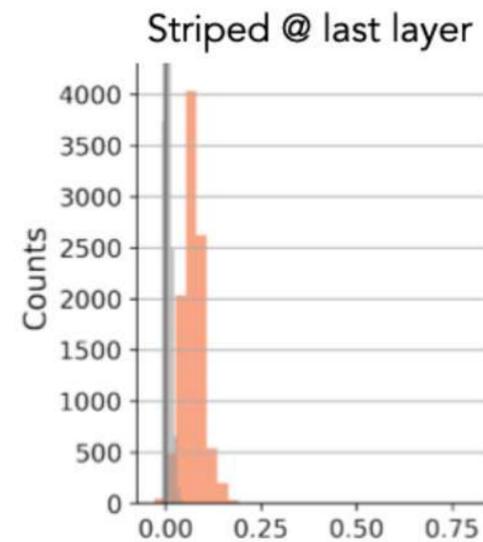


Natural images dataset

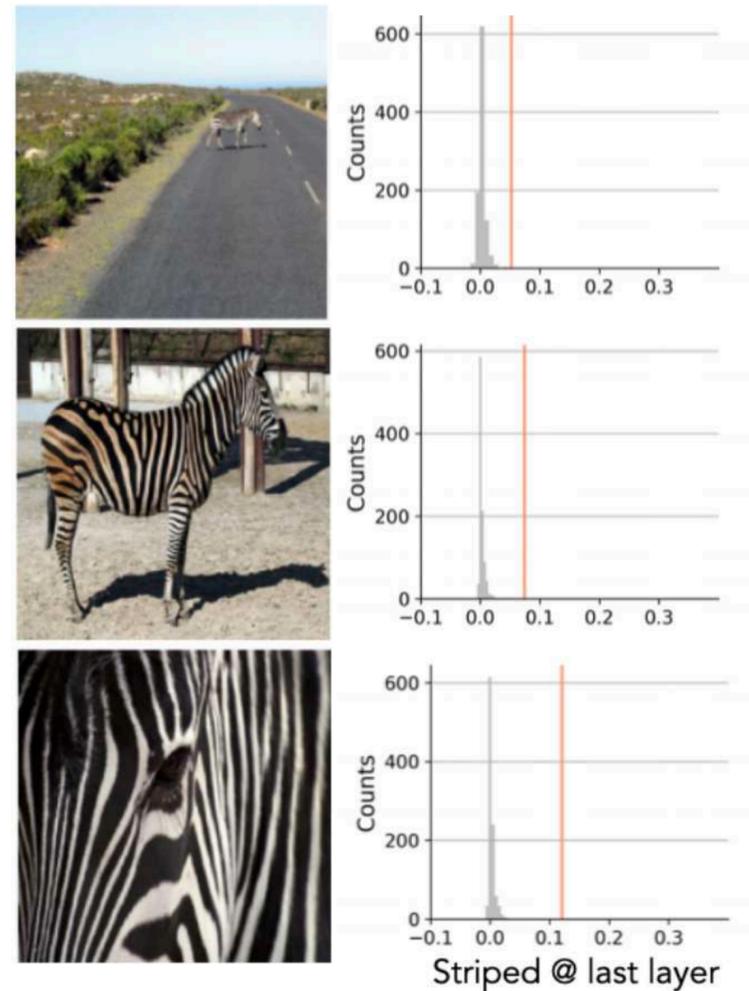
But

These are all global explanations only.
what about local?
[ongoing work]

All the zebras



My zebras!



Combine TCAV + IG to provide both global and local explanations

Jessica Schrouff

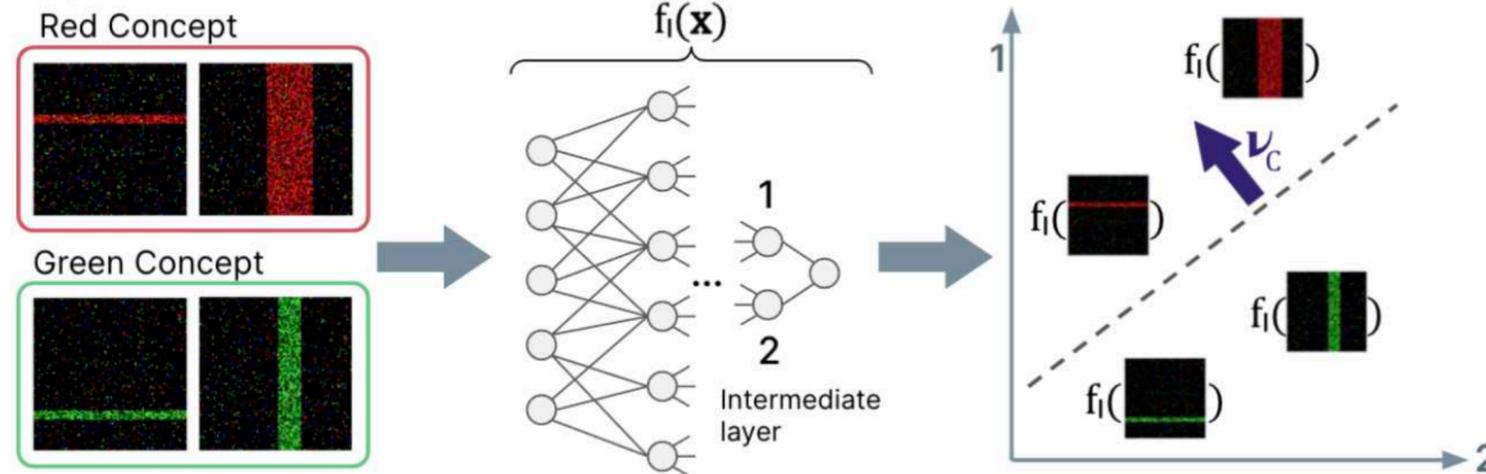


Sebastien Baur

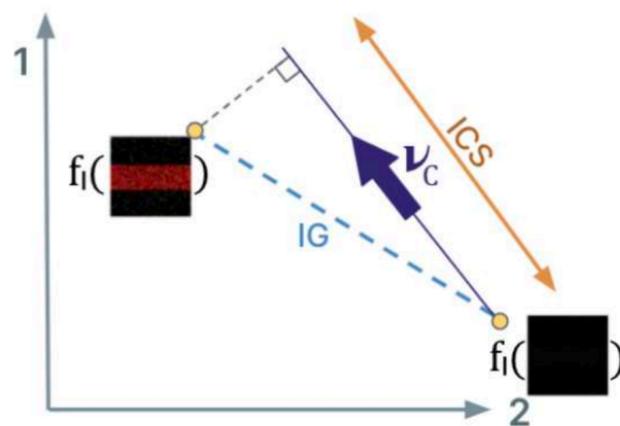


Combine TCAV + IG to provide both global and local explanations

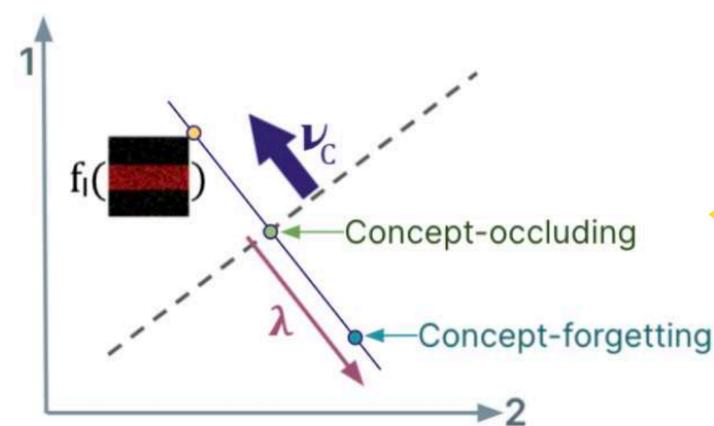
A. Training CAV



B. ICS vs IG



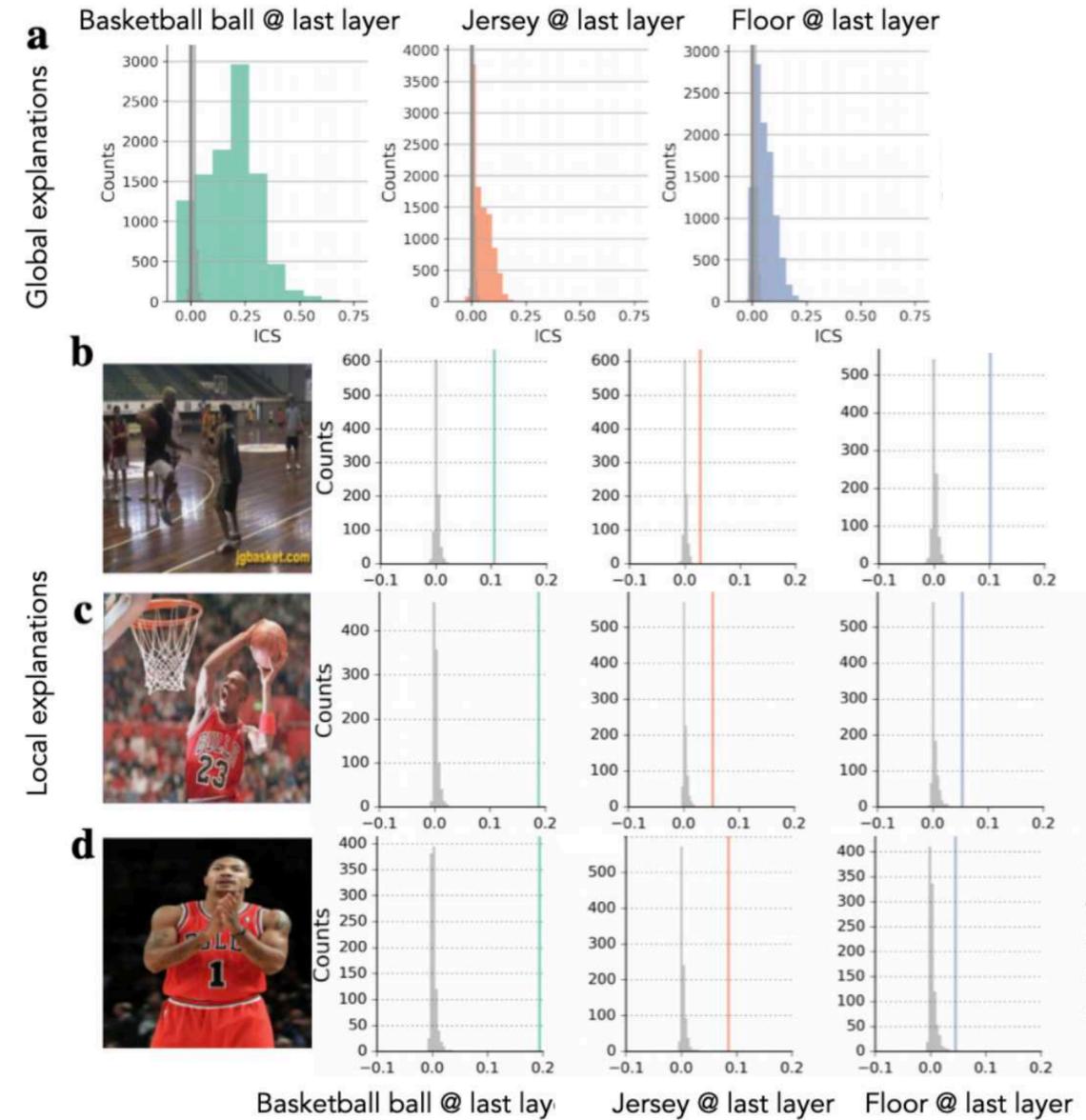
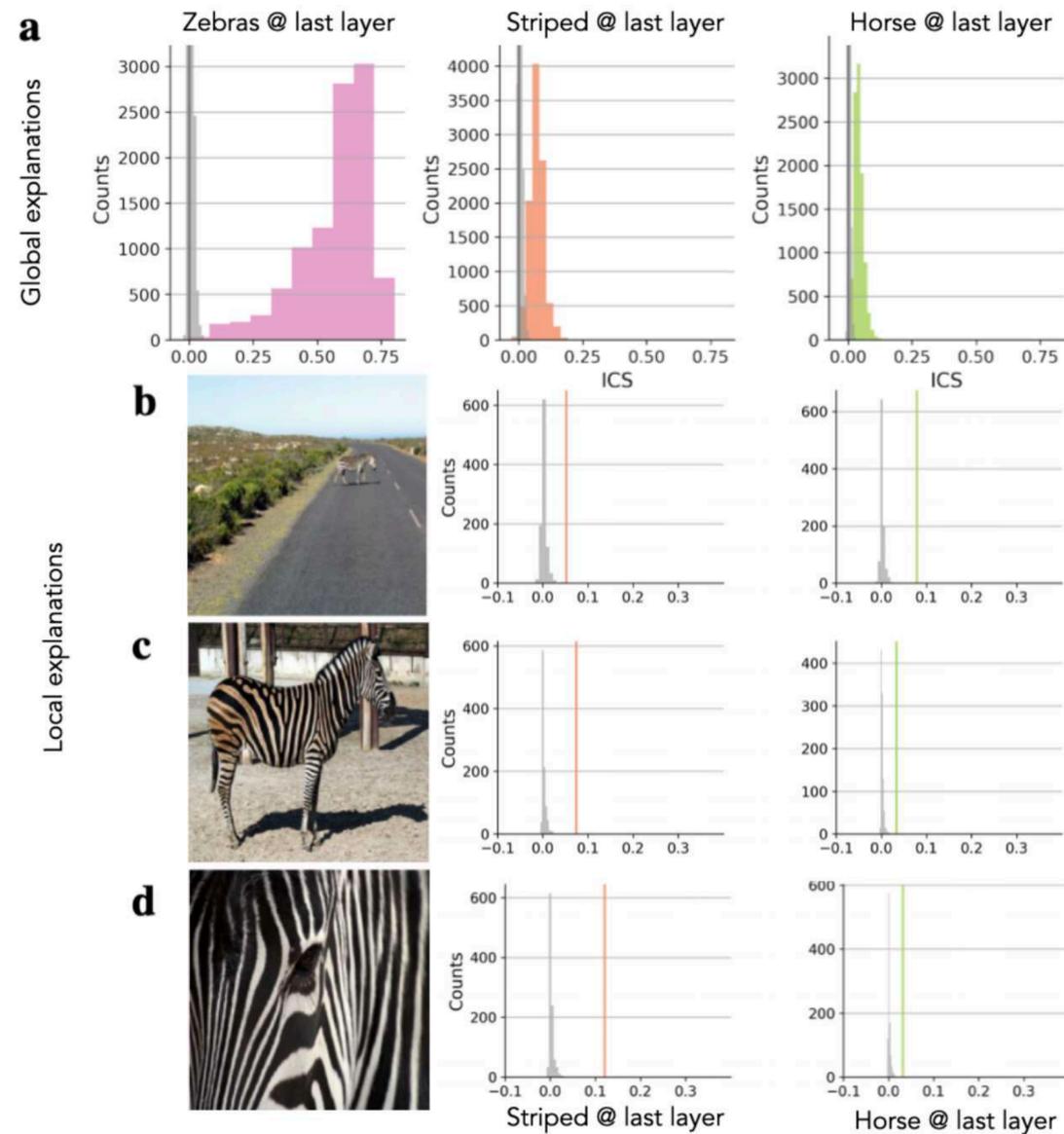
C. Baselines



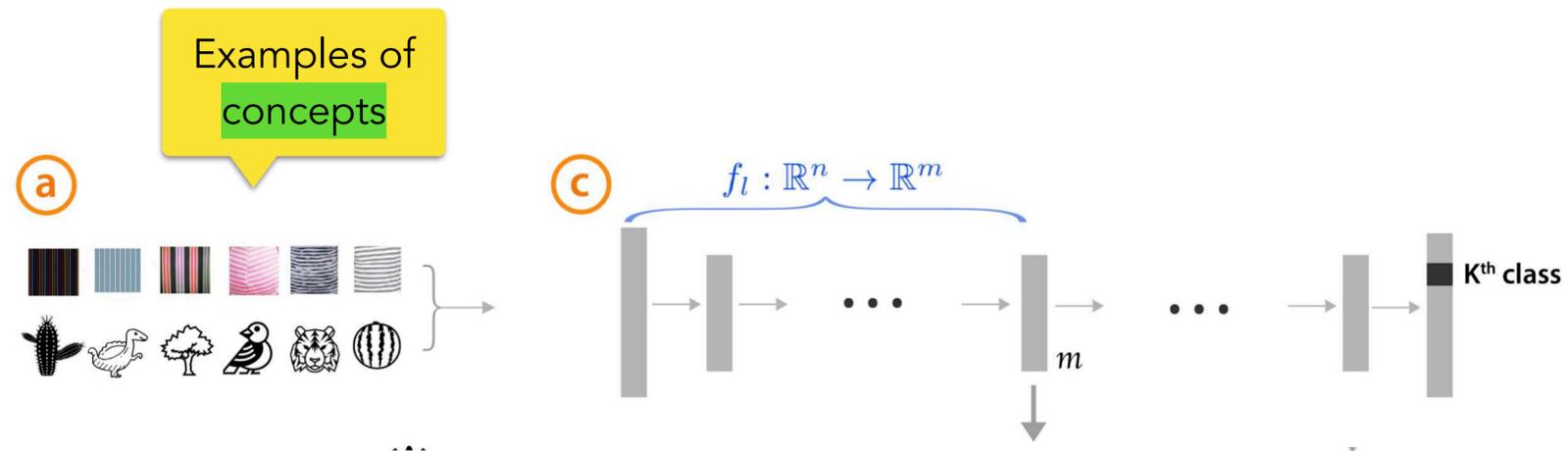
New baselines for concepts

Integrate on the path of a CAV
 \leftrightarrow
 A projection of path integration

Combine TCAV + IG to provide both global and local explanations

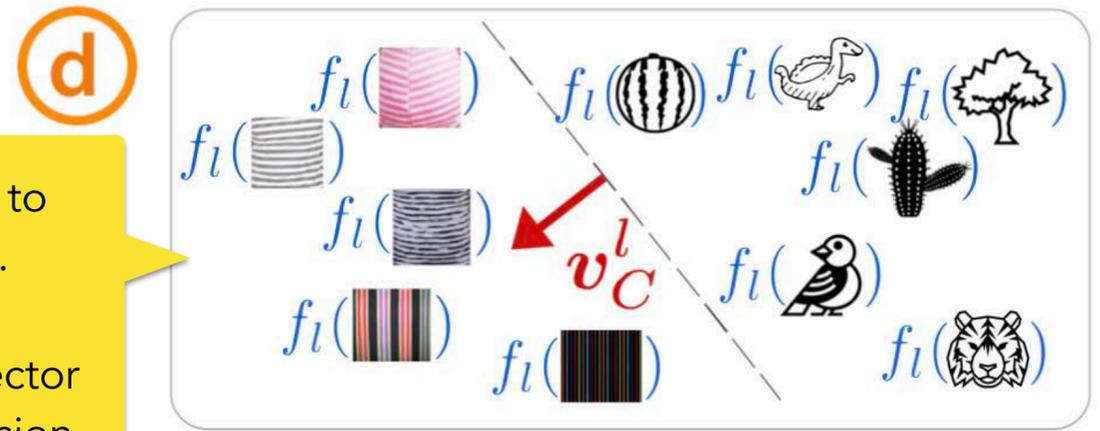


1: Test hypothesis that should be true by craft a ground-truth dataset



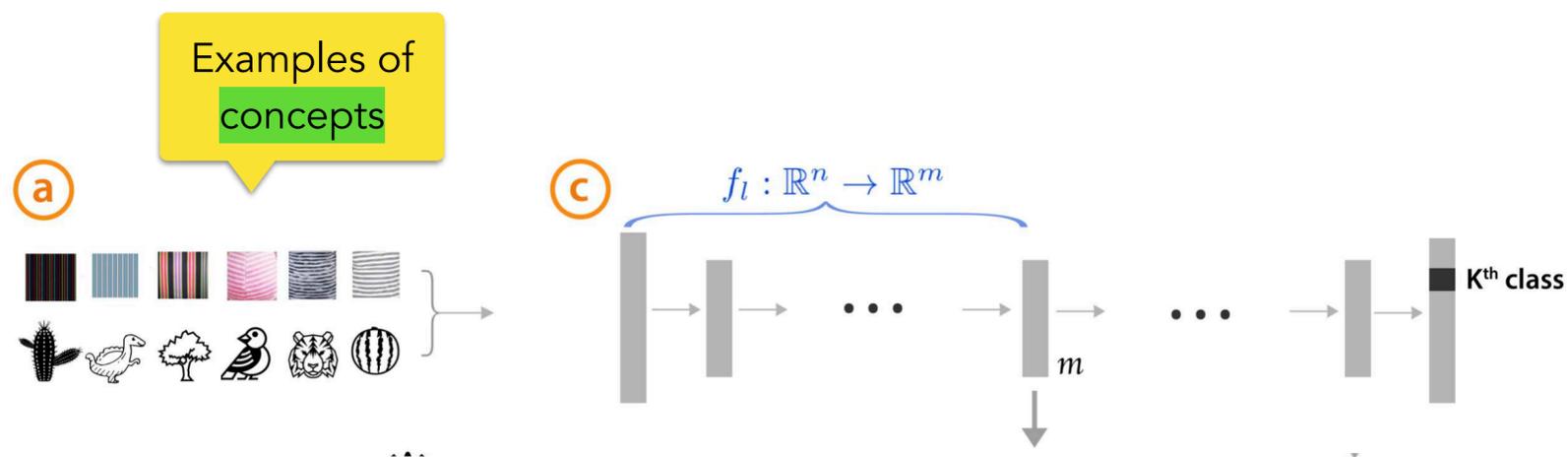
Train a linear classifier to separate activations.

CAV (v_C^l) is the vector **orthogonal** to the decision boundary.



How important was the **striped concept** to this **zebra** image classifier?

1: Test hypothesis that should be true by craft a ground-truth dataset

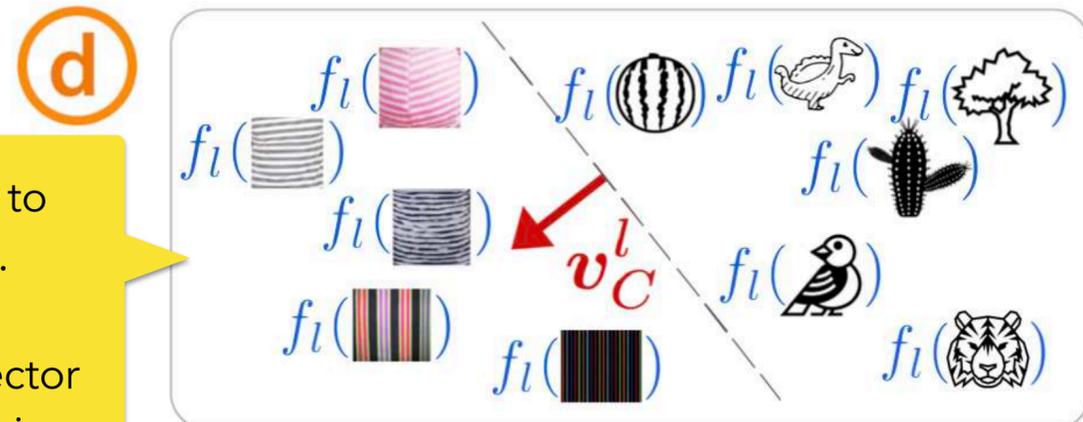


$$S_{C,k,l}(\mathbf{x}) = \begin{matrix} \text{zebra-ness} \rightarrow \frac{\partial p(z)}{\partial v_C^l} \\ \text{striped CAV} \rightarrow \end{matrix}$$

$$\text{TCAV}_{Q_{C,k,l}} = \frac{|\{\mathbf{x} \in X_k : S_{C,k,l}(\mathbf{x}) > 0\}|}{|X_k|}$$

Train a linear classifier to separate activations.

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1: Test hypothesis that should be true by craft a ground-truth dataset

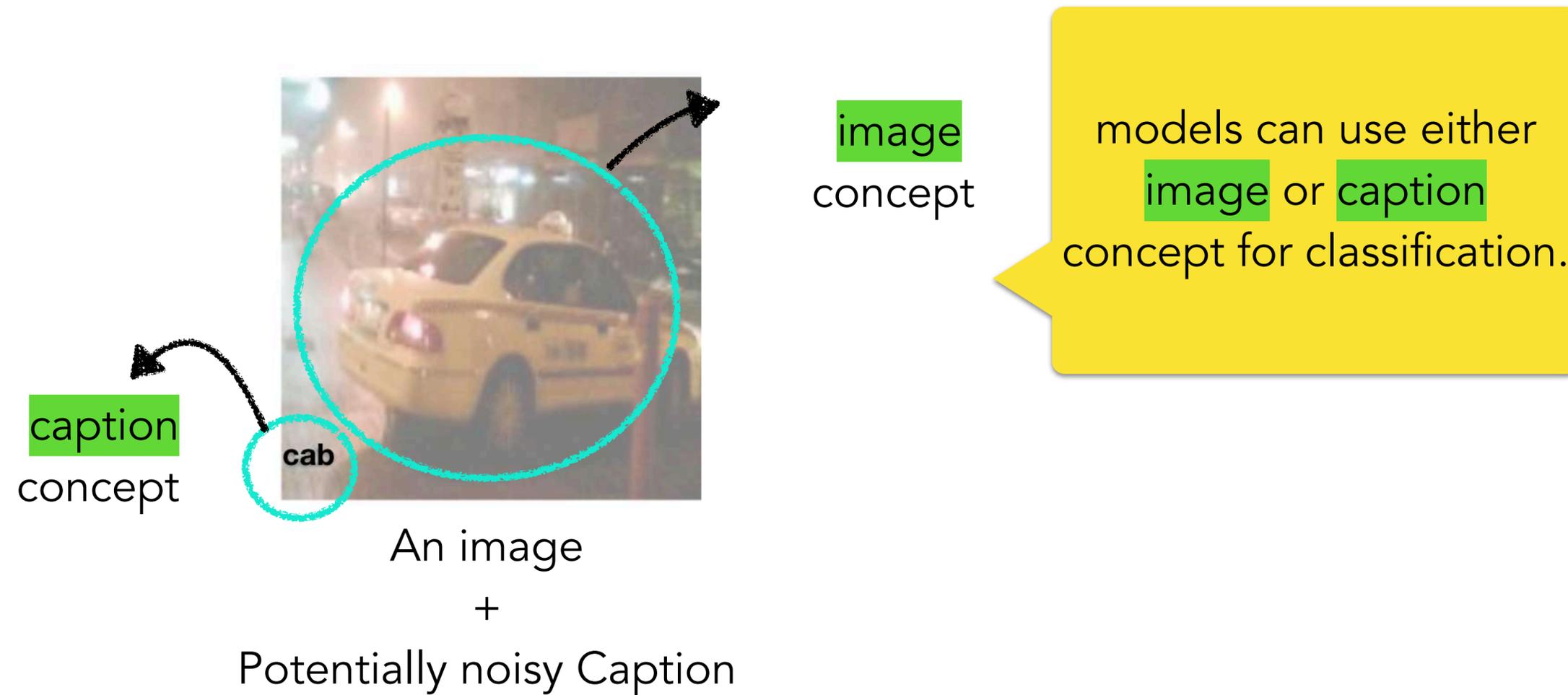


An image

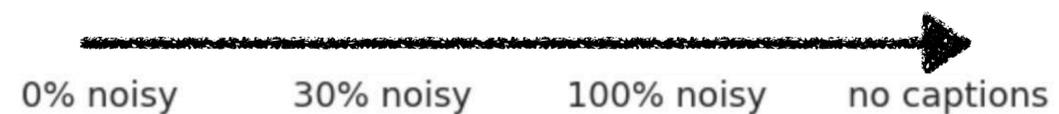
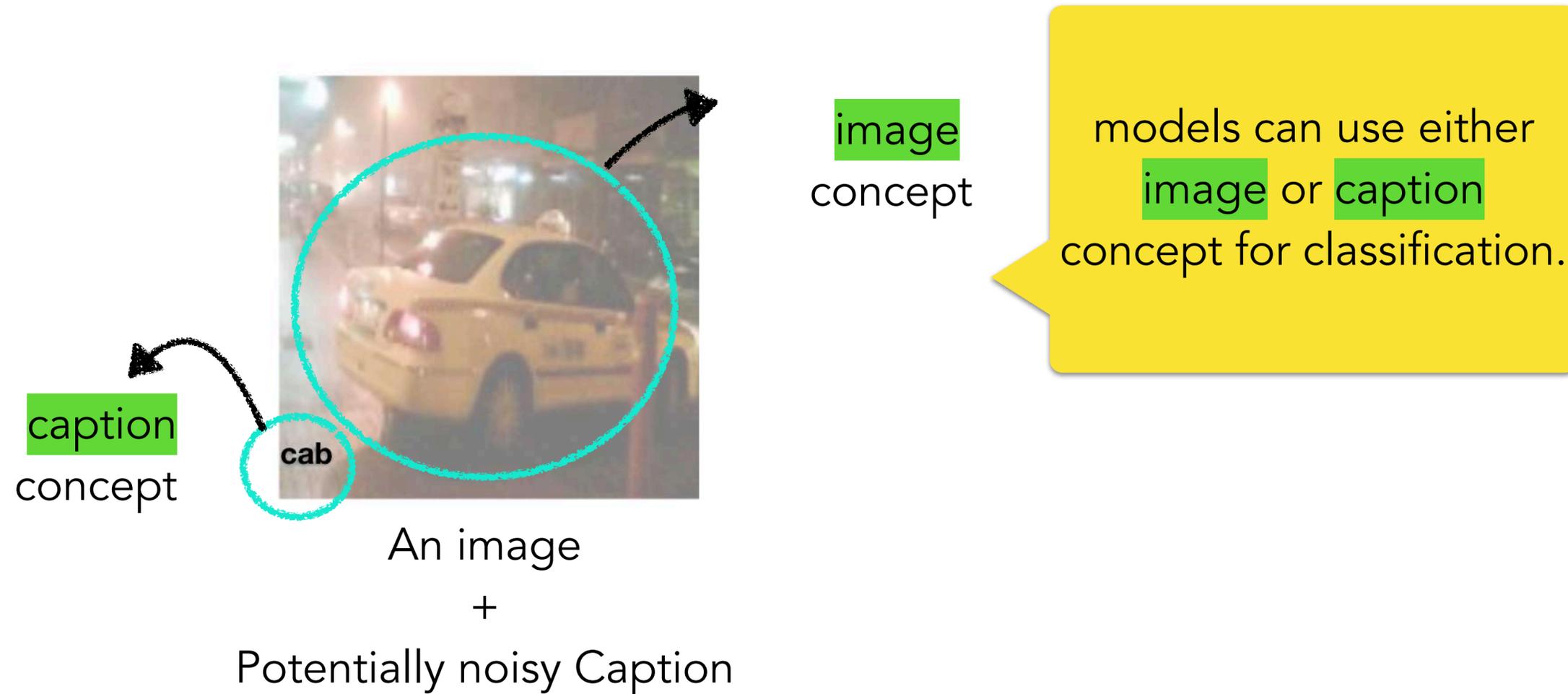
+

Potentially noisy Caption

1: Test hypothesis that should be true by craft a ground-truth dataset



1: Test hypothesis that should be true by craft a ground-truth dataset



Four models trained with different caption noise levels

1: Test hypothesis that should be true by craft a ground-truth dataset

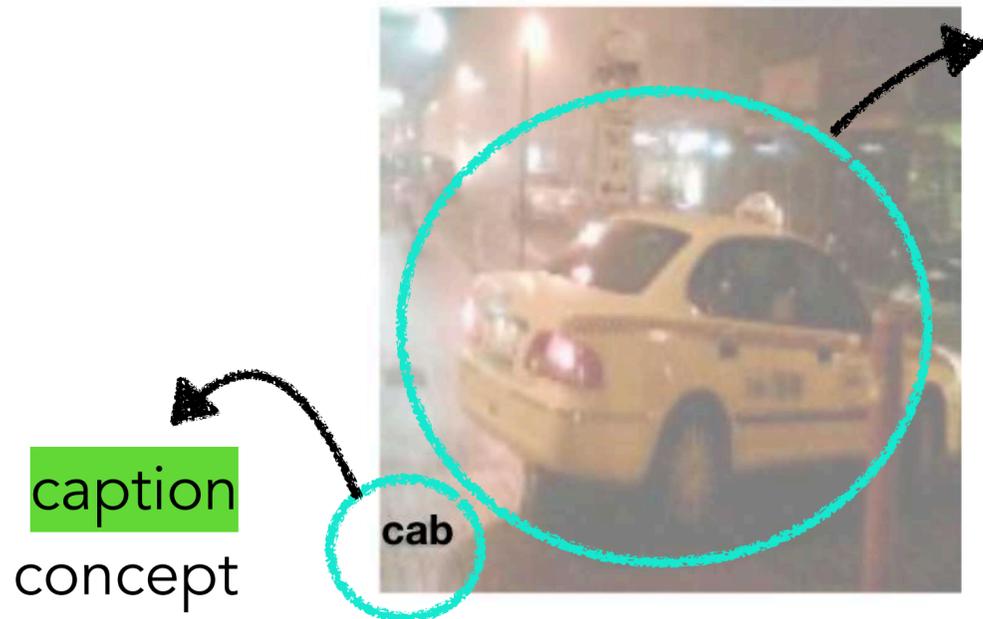


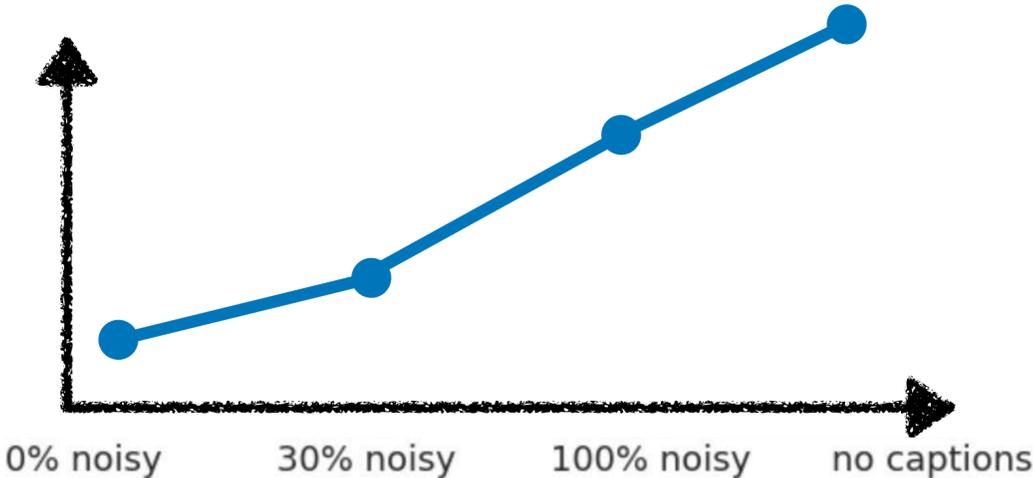
image concept

models can use either image or caption concept for classification.



Test models with no caption image.

Test accuracy = Importance of image concept



Four models trained with different caption noise levels

1: Test hypothesis that should be true by craft a ground-truth dataset

Test accuracy
with
no caption image

