

Introduction to Interpretable Machine Learning

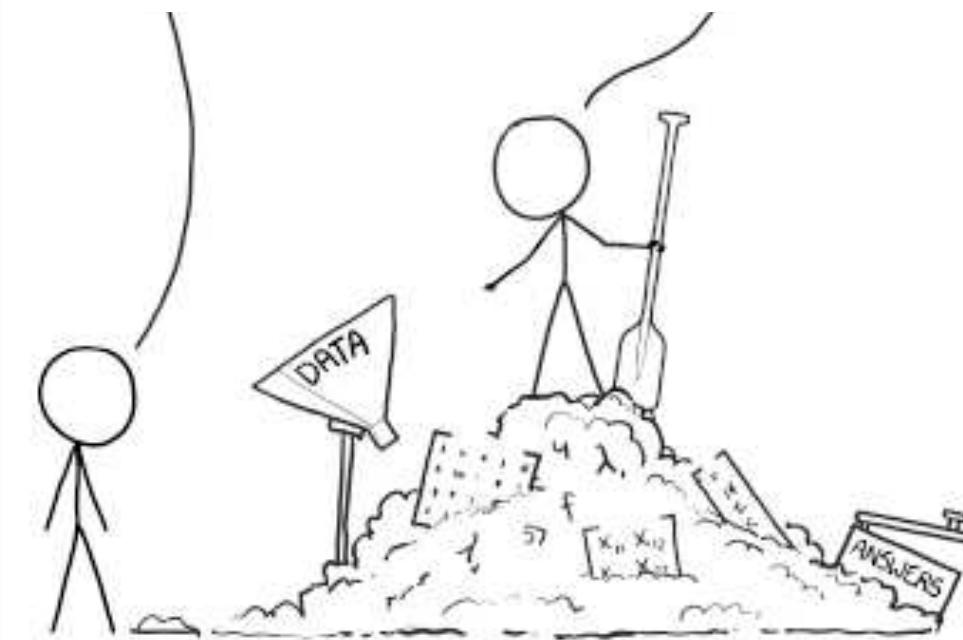


credit:<https://s-media-cache-ak0.pinimg.com>

Been Kim
Google Brain
Deep Learning Summer School 2018
@Vector institute



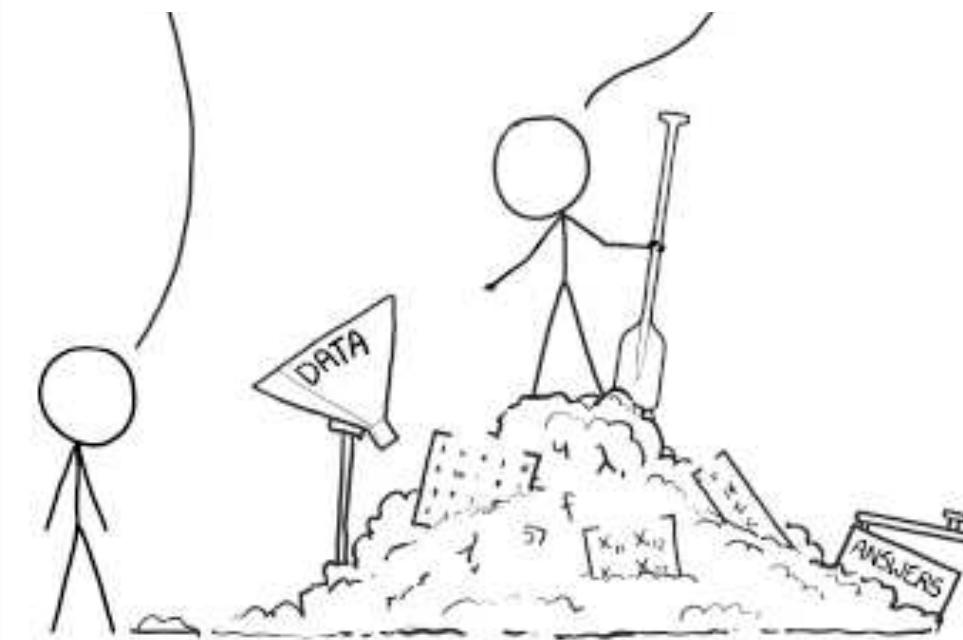
THIS IS YOUR MACHINE LEARNING SYSTEM?



<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.

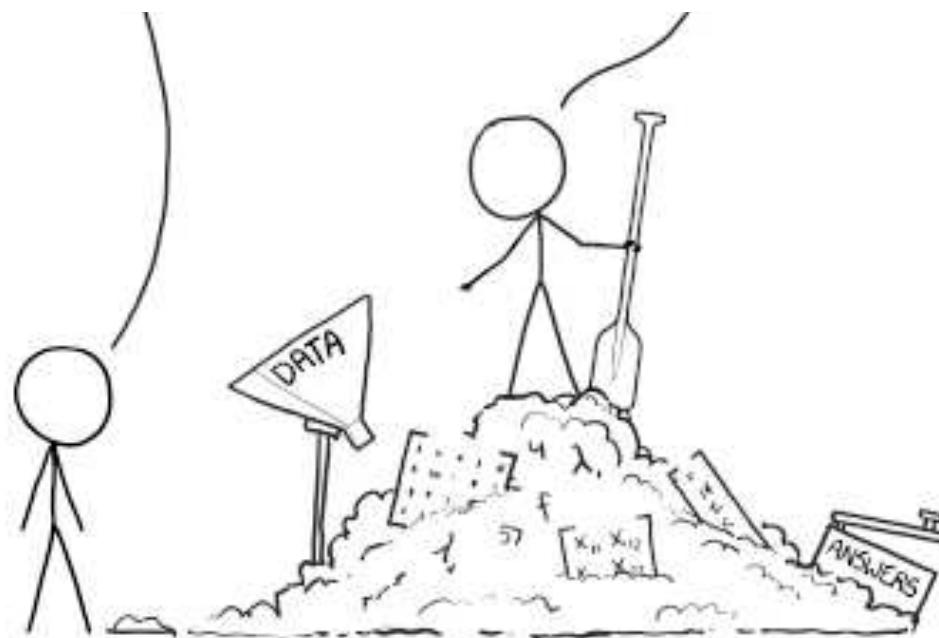


<https://xkcd.com/>

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.

WHAT IF THE ANSWERS ARE WRONG? |



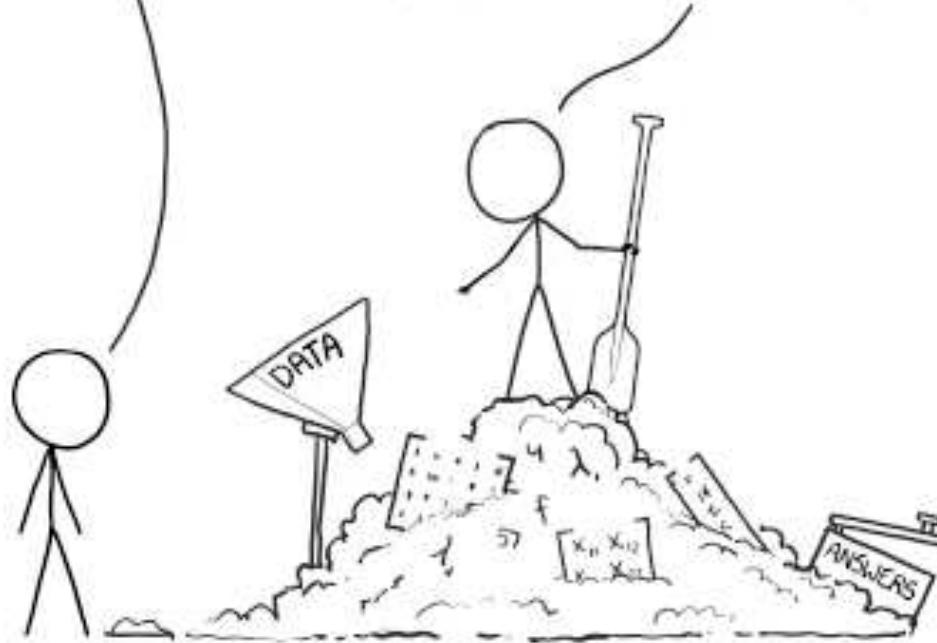
<https://xkcd.com/>

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.

WHAT IF THE ANSWERS ARE WRONG?

JUST STIR THE PILE UNTIL
THEY START LOOKING RIGHT.



<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.

WHAT IF THE ANSWERS ARE WRONG?

JUST STIR THE PILE UNTIL
THEY START LOOKING RIGHT.

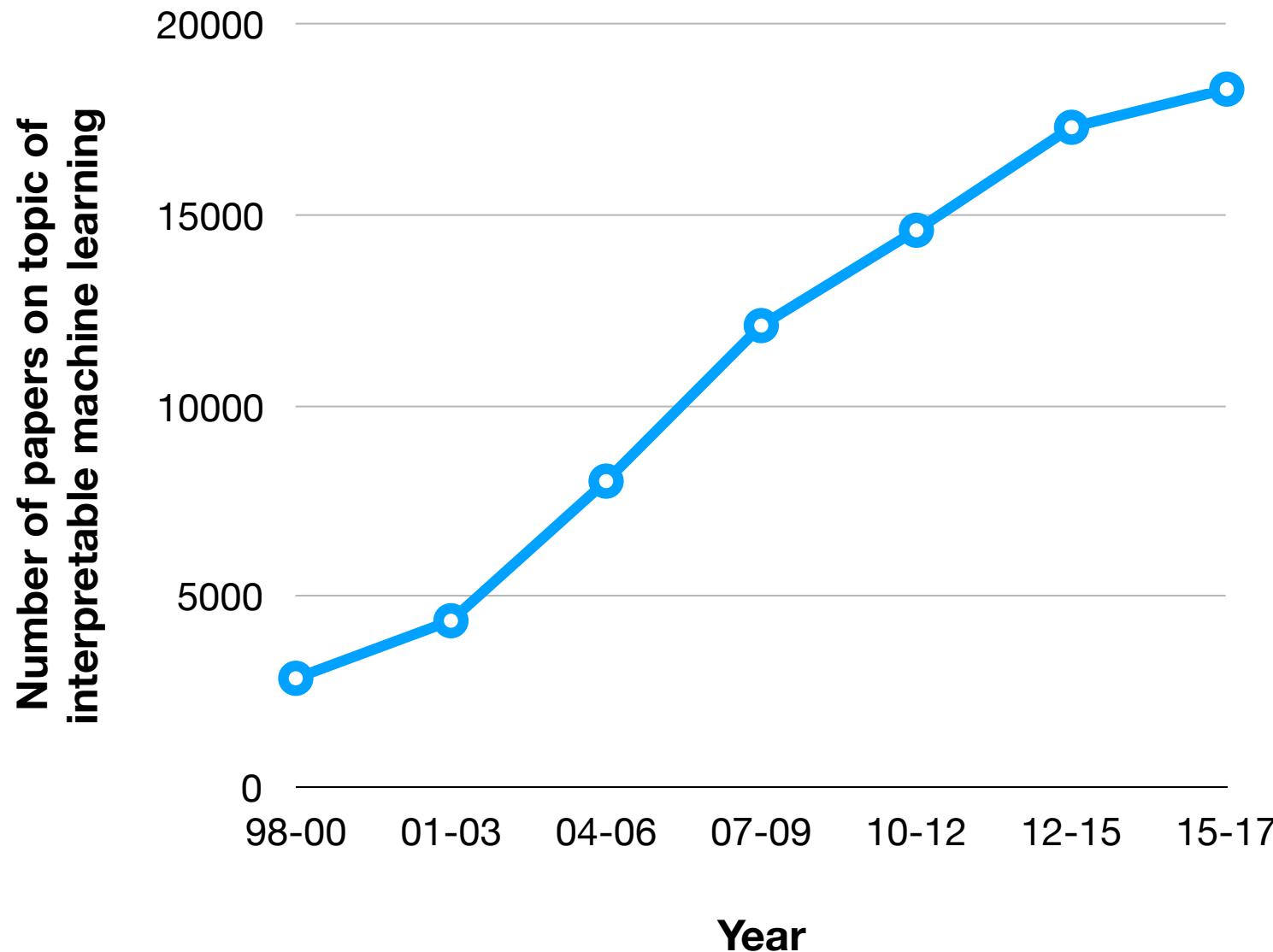


<https://www.youtube.com/watch?v=icqDxNab3Do>



<https://xkcd.com/>

ML community is responding



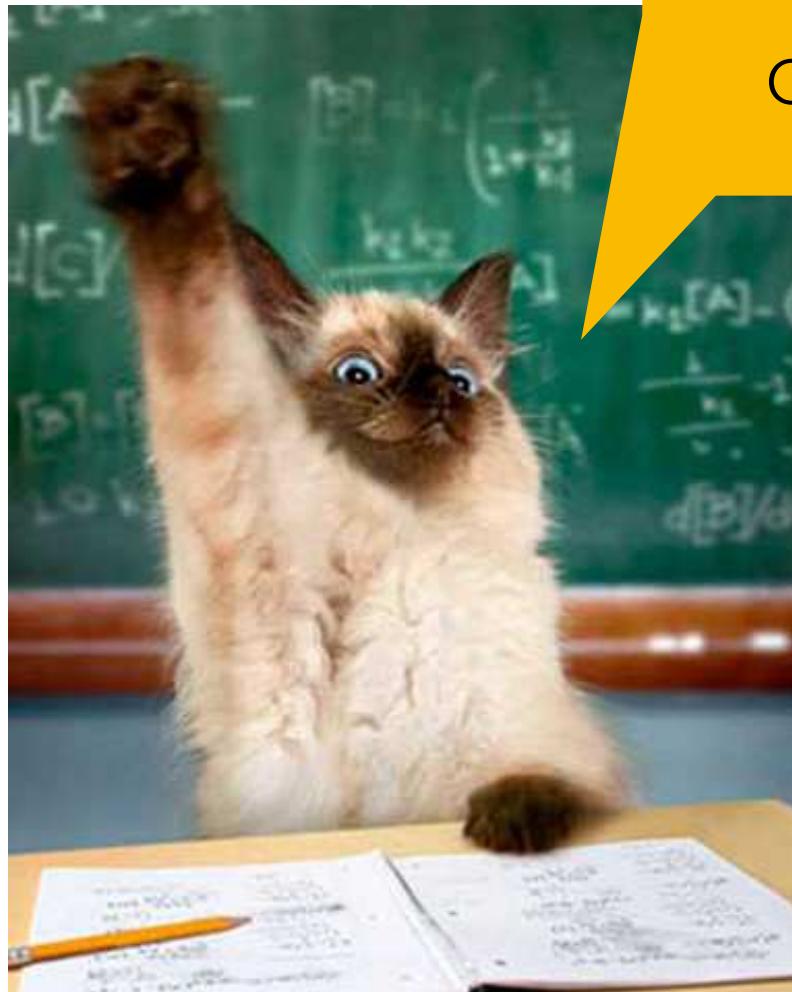
This is not a new problem.
Why now?

Complexity and prevalence!



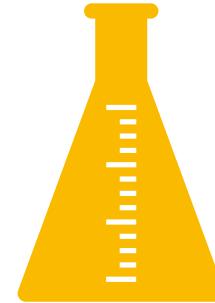
I heard you can just use
decision trees...

Can we go home now?

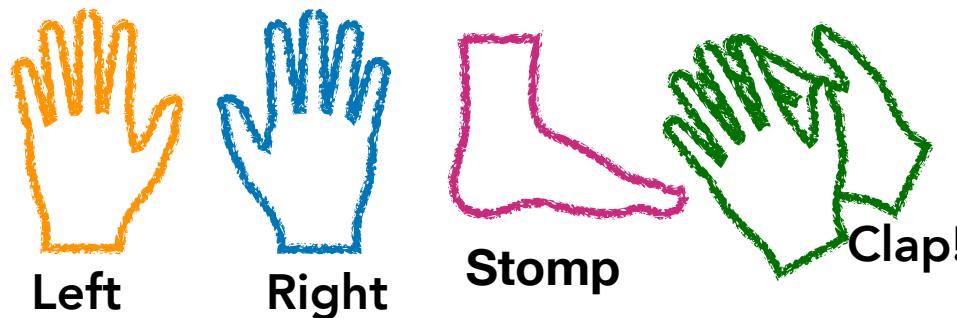


<http://www.ogroup.com.au/raise-your-hand-when-you-should-and-why-you-should/>

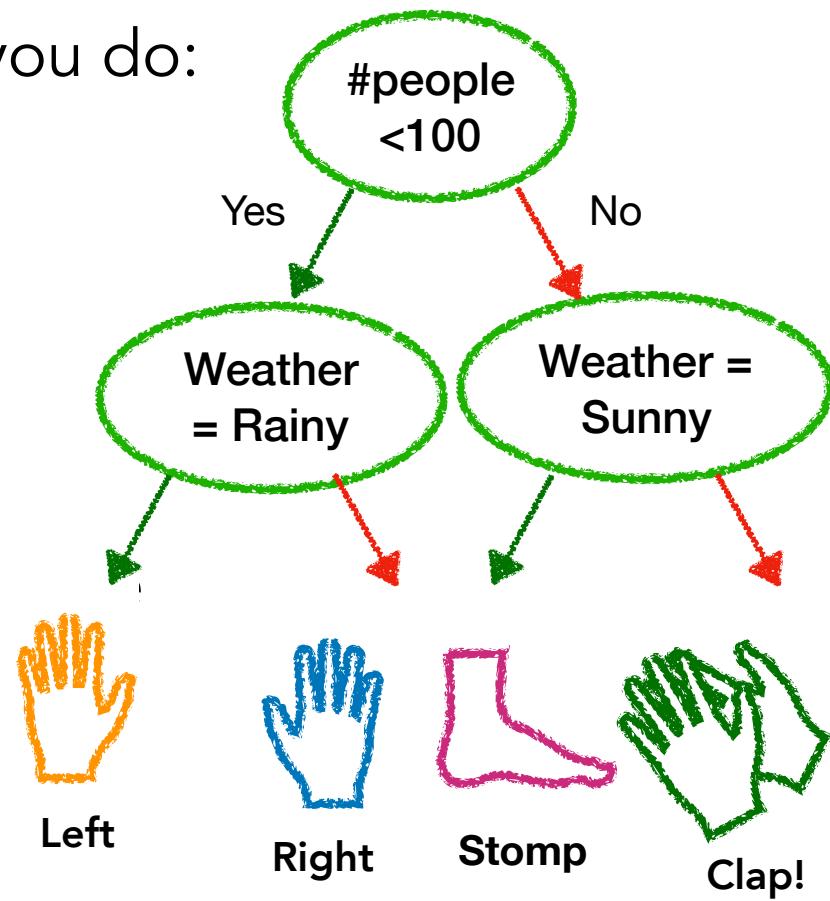
Experiment.



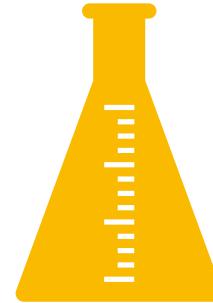
- I will show you a decision tree. Follow the right path given a data point, and you do:



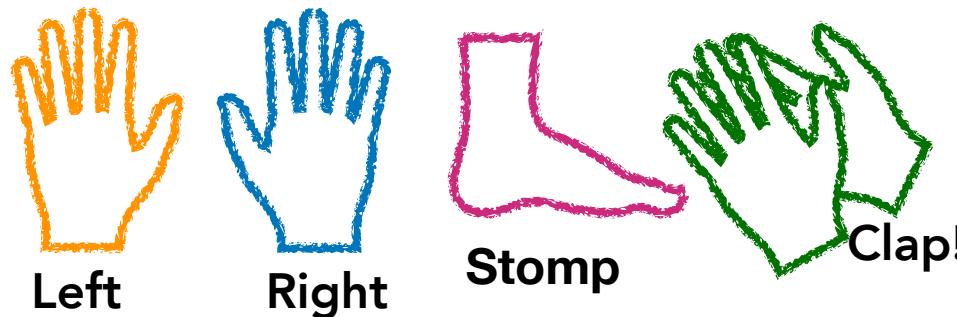
Data = [Sunny, 200]



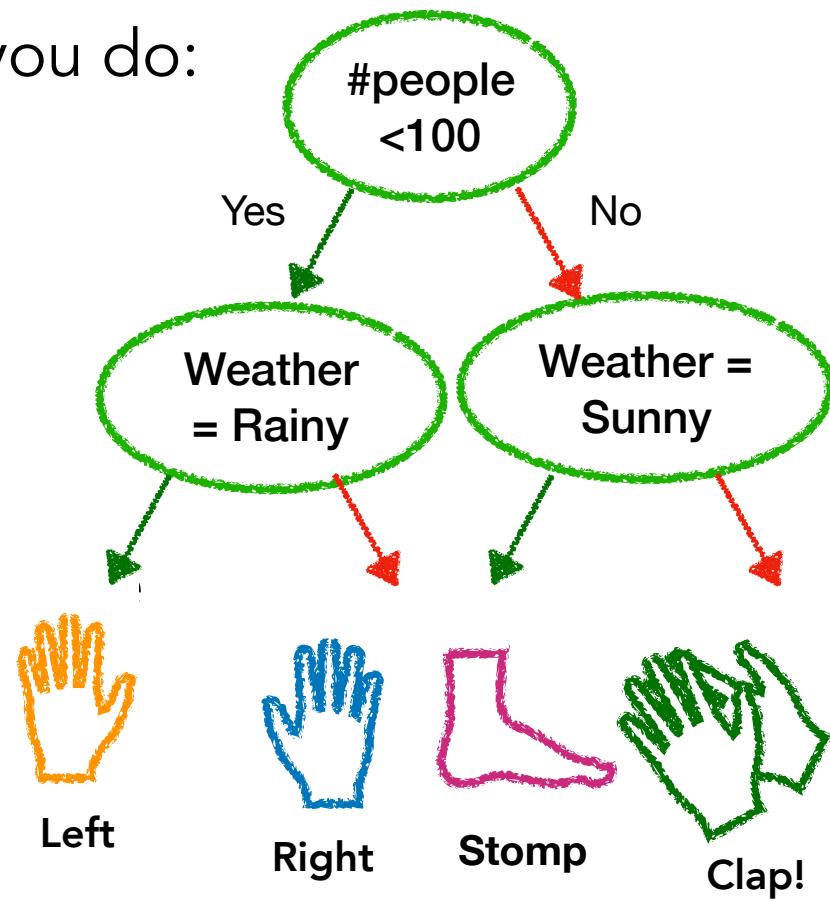
Experiment.



- I will show you a decision tree. Follow the right path given a data point, and you do:

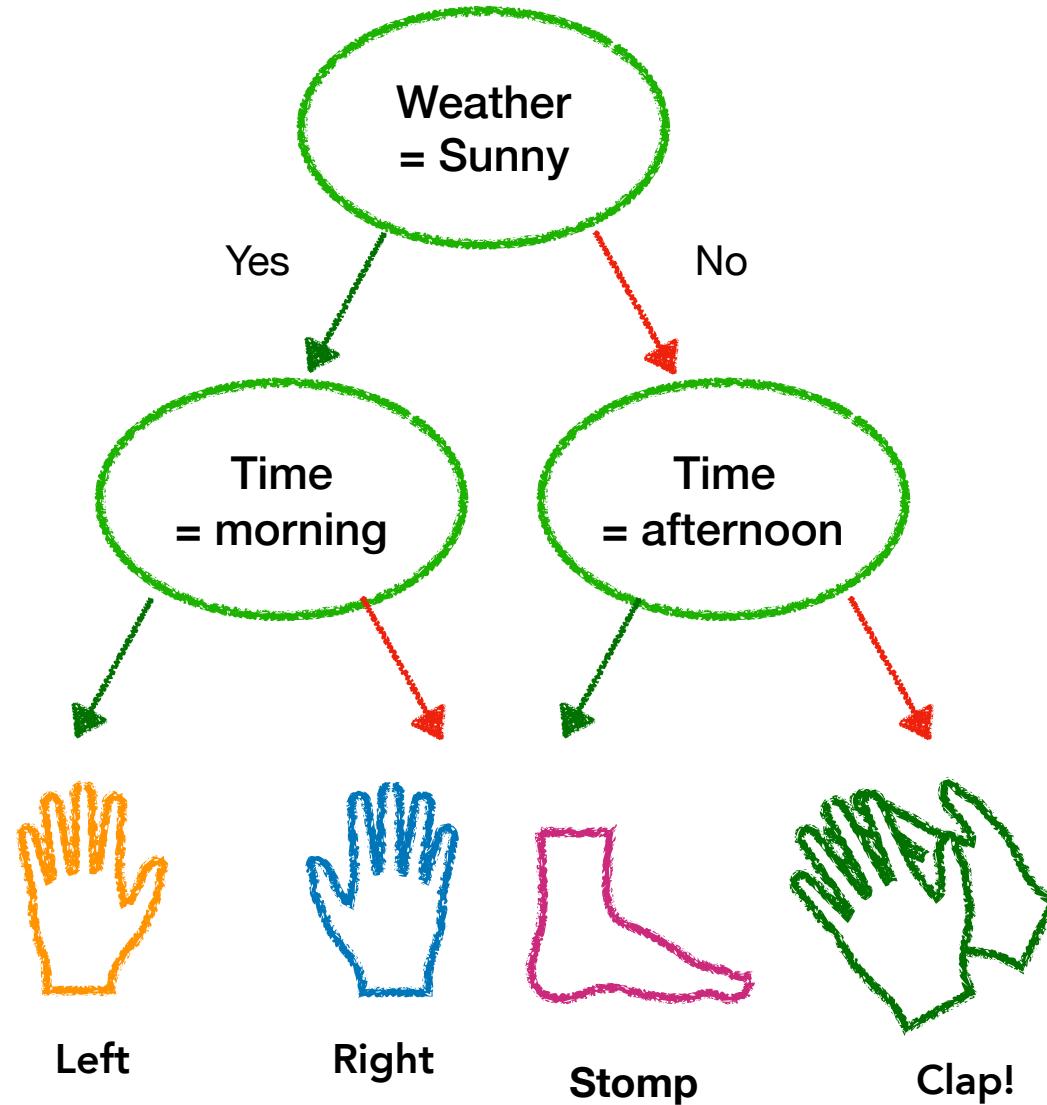


Data = [Sunny, 200]

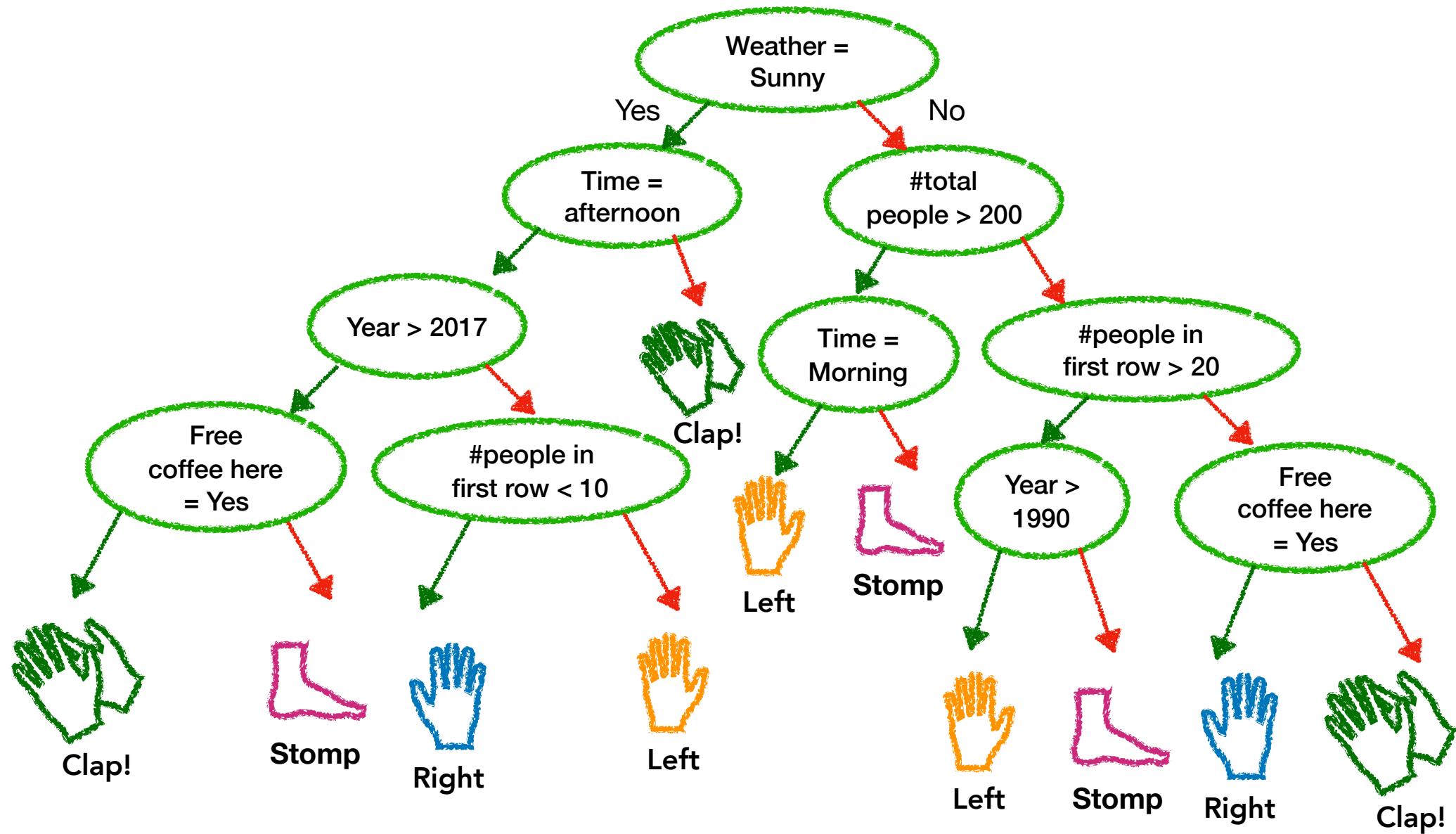


- As soon as you know the answer, do the action!

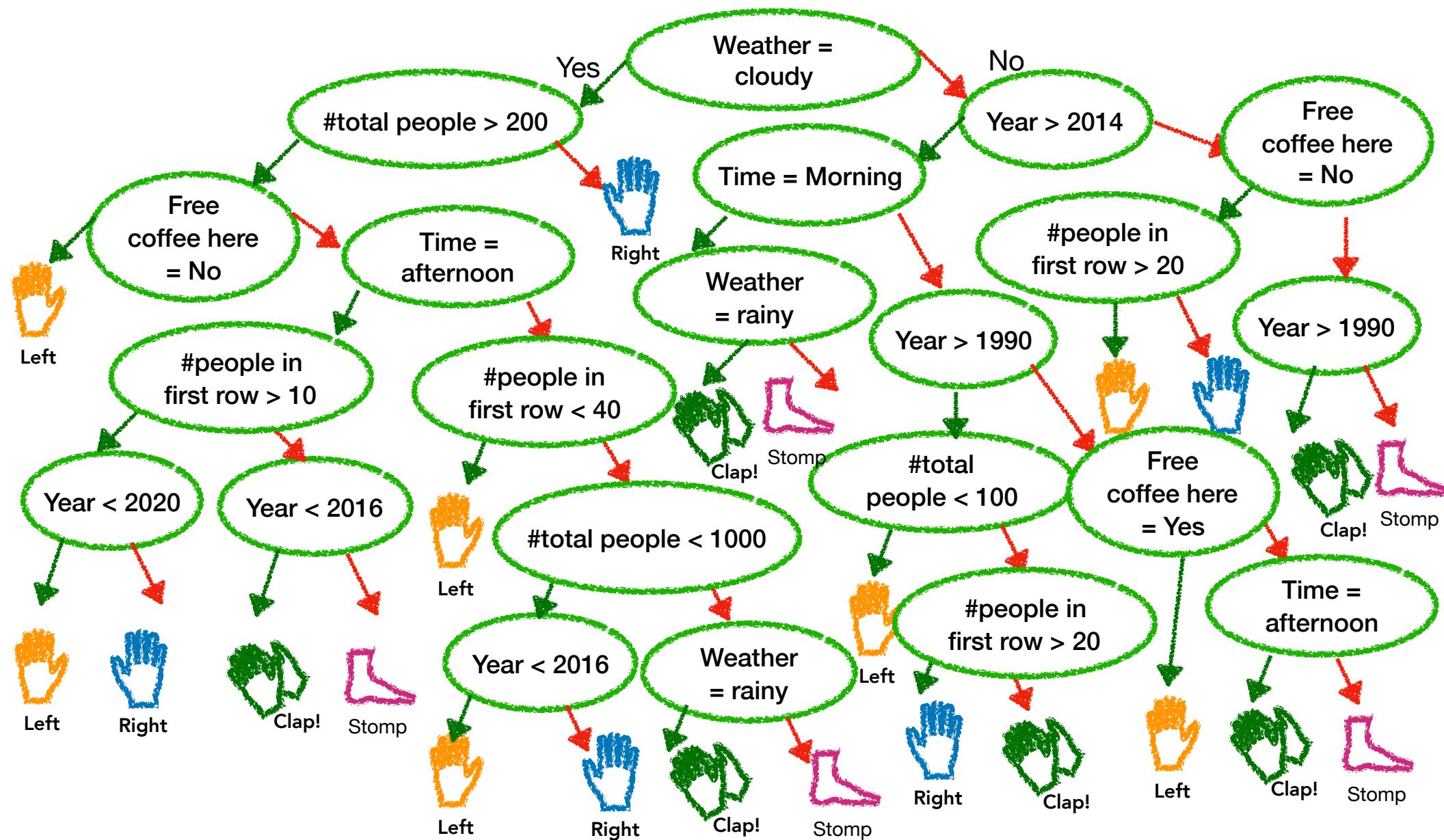
Sample decision tree #1



Sample decision tree #2



Sample decision tree #3



Sample decision tree #3

And can you explain
what the overall logic of the system was?

If I give you a lot of data points,
can you guess which feature was most
'important' (i.e., used in more number of examples)?



 Common misunderstanding:
Decision trees and linear models are
always interpretable.

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 (thirty 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

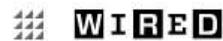


**Are you saying decision
trees, rule lists and rule
sets don't work?!**

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

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

Is interpretability possible at all?



Our Machines Now Have Knowledge We'll Never Understand

SUBSCRIBE

DAVID WEINBERGER BACKCHANNEL 04.18.17 08:22 PM

OUR MACHINES NOW HAVE KNOWLEDGE WE'LL NEVER UNDERSTAND

SHARE



SHARE
176



TWEET



COMMENT

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?



Our Machines Now Have Knowledge We'll Never Understand

SUBSCRIBE

DAVID WEINBERGER BACKCHANNEL 04.18.17 08:22 PM

OUR MACHINES NOW HAVE KNOWLEDGE WE'LL



Common misunderstanding:
We 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
theories, or really any mechanistic explanation at all.



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.

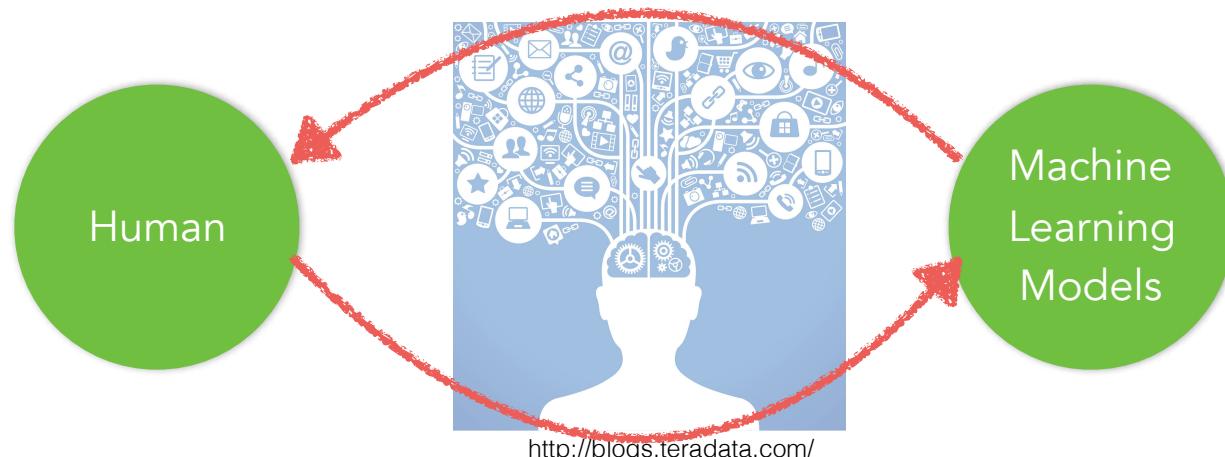
<https://>

My goal

interpretability

To use machine learning **responsibly**
we need to ensure that

1. our **values** are aligned
2. our **knowledge** is reflected

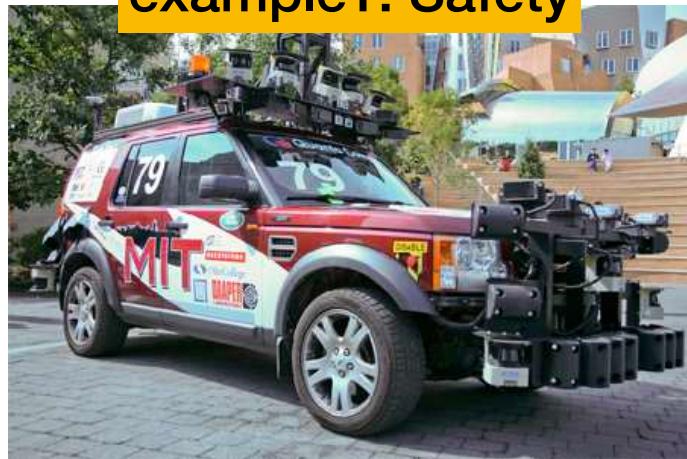


Why interpretability?

Fundamental **underspecification** in the problem

Why interpretability?

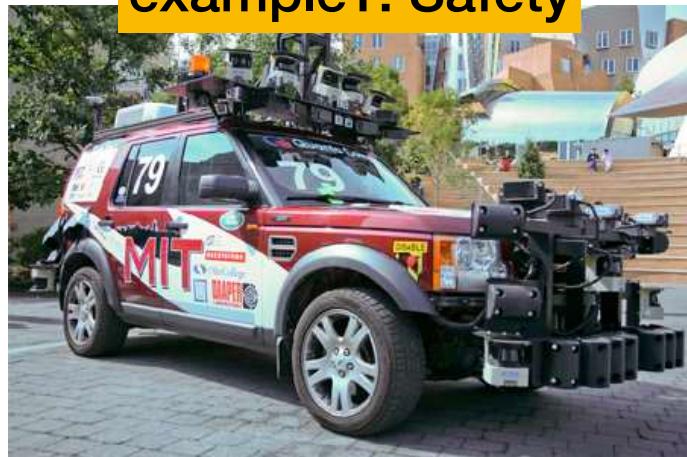
example1: Safety



Fundamental **underspecification** in the problem

Why interpretability?

example1: Safety



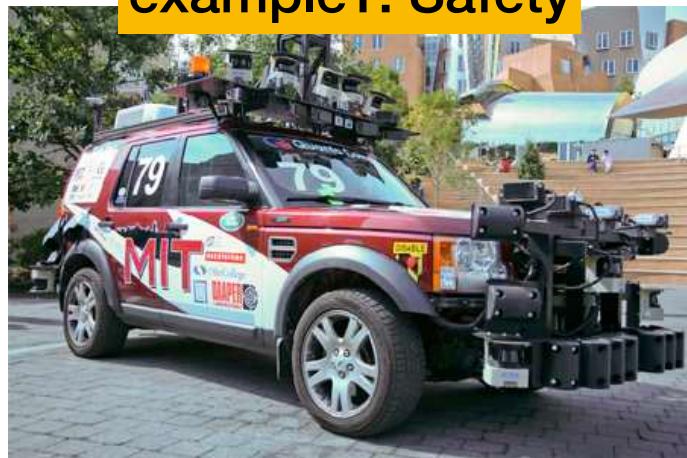
example 2: Science



Fundamental **underspecification** in the problem

Why interpretability?

example1: Safety



example 2: Science



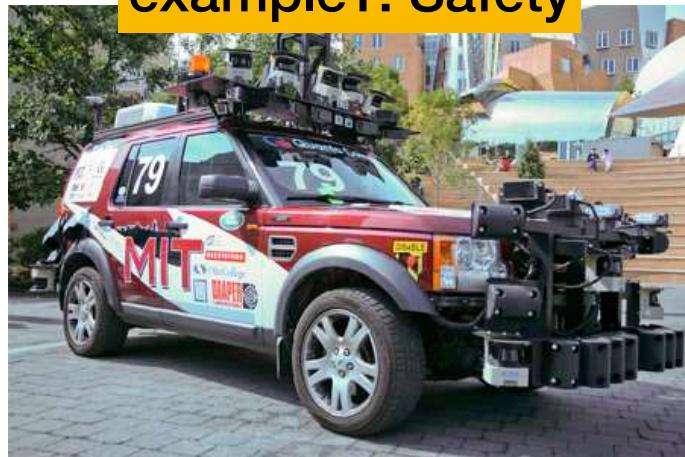
Fundamental **underspecification** in the problem

example3: mismatched objectives



Why interpretability?

example1: Safety



example 2: Science



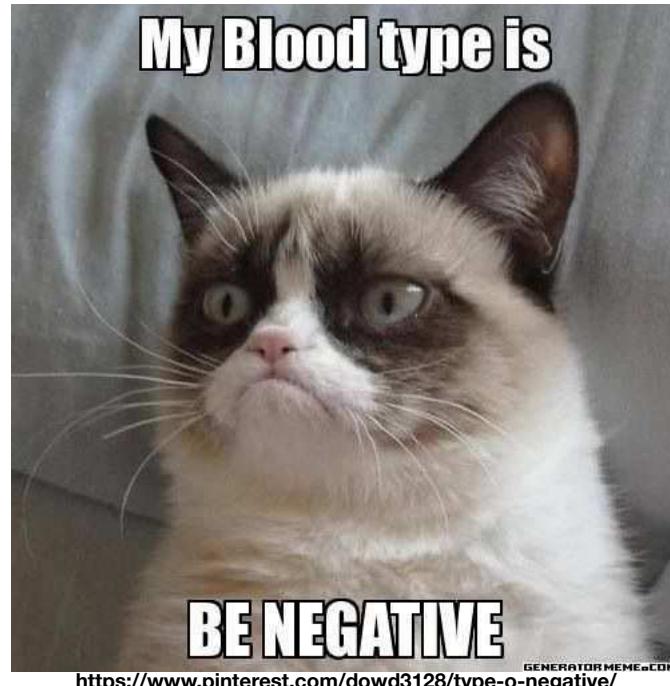
Fundamental **underspecification** in the problem



Common misunderstanding:

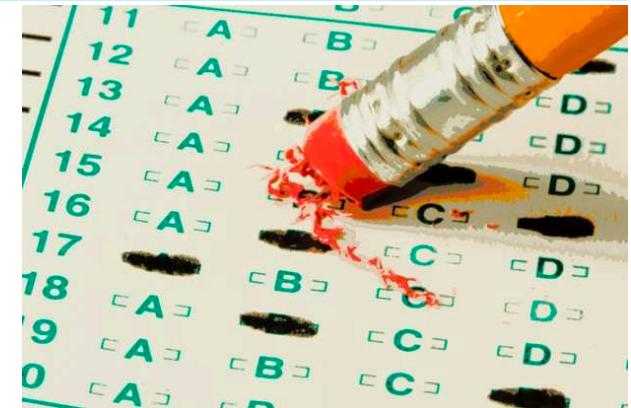
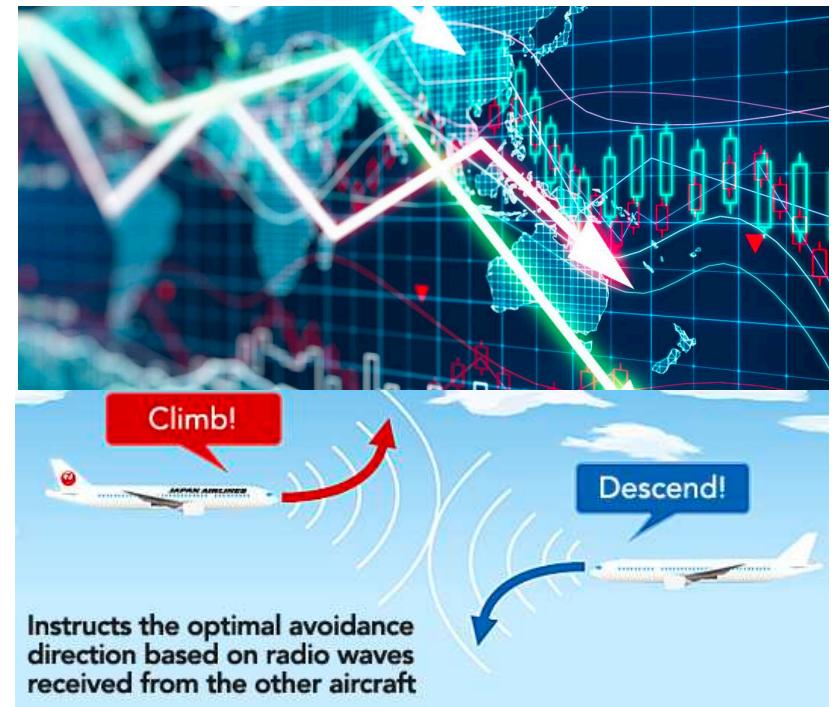
More data or more clever algorithm will solve interpretability.

What is NOT underspecification?



When we may **not** want interpretability

- No significant consequences or when predictions are all you need.
- Sufficiently well-studied problem
- Prevent gaming the system - mismatched objectives.



https://cdn.theatlantic.com/assets/media/img/mt/2015/04/shutterstock_11926084/lead_large.jpg
https://www.jal.com/assets/img/flight/safety/equipment/pic_tcas_001_en.jpg

<http://www.cinemablend.com/pop/Netflix-Using-Amazon-Cloud-Explore-Artificial-Intelligence-Movie-Recommendations-62248.html>

When we may **not** want interpretability

- No significant consequences or when predictions are all you need.
- Sufficiently well-studied problem
- Prevent gaming the mismatched objectives.



https://cdn.theatlantic.com/assets/media/img/mt/2015/04/shutterstock_11926084/lead_large.jpg
https://www.jal.com/assets/img/flight/safety/equipment/pic_tcas_001_en.jpg

<http://www.cinemablend.com/pop/Netflix-Using-Amazon-Cloud-Explore-Artificial-Intelligence-Movie-Recommendations-62248.html>

Interpretability

?

**fairness
accountability
trust
causality etc.**

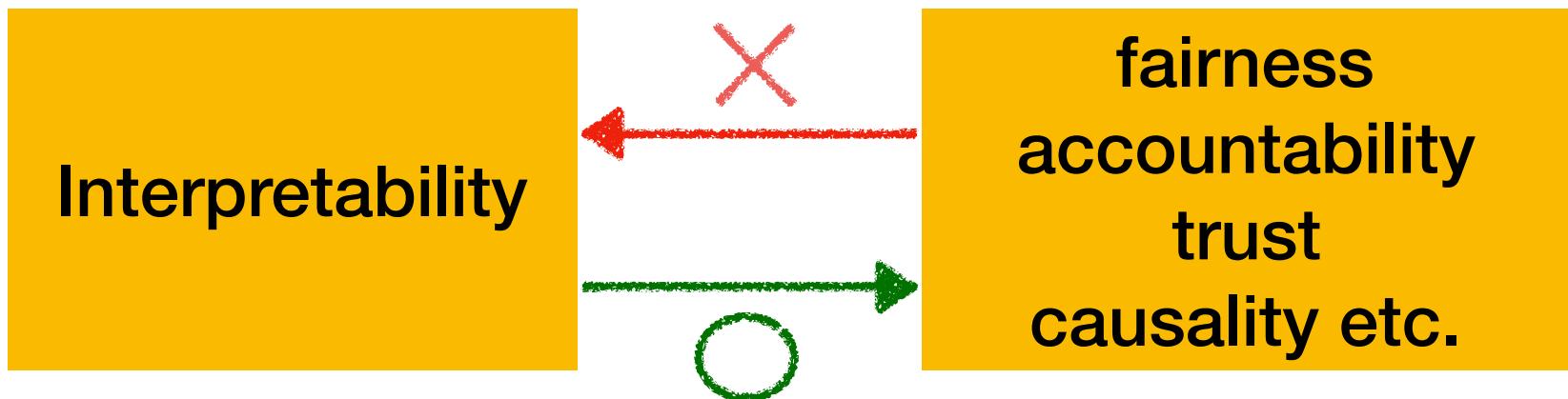
Interpretability

fairness
accountability
trust
causality etc.



Common misunderstanding:
Trust, fairness and interpretability
are all the same thing.

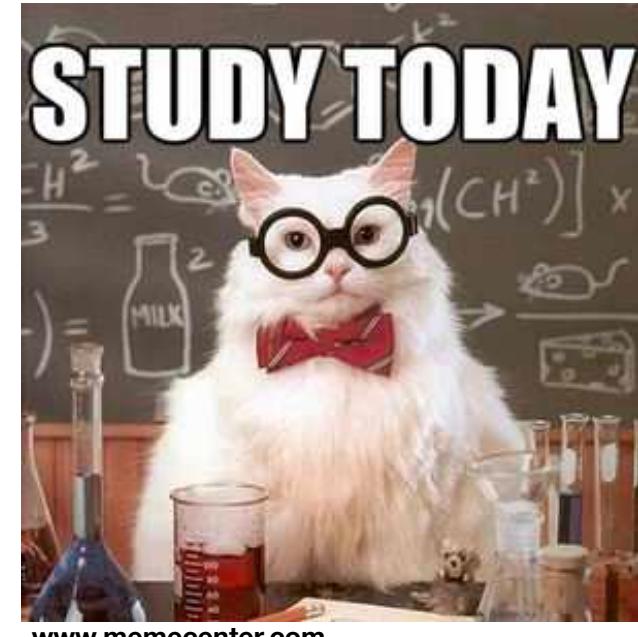
Our cousins are not us



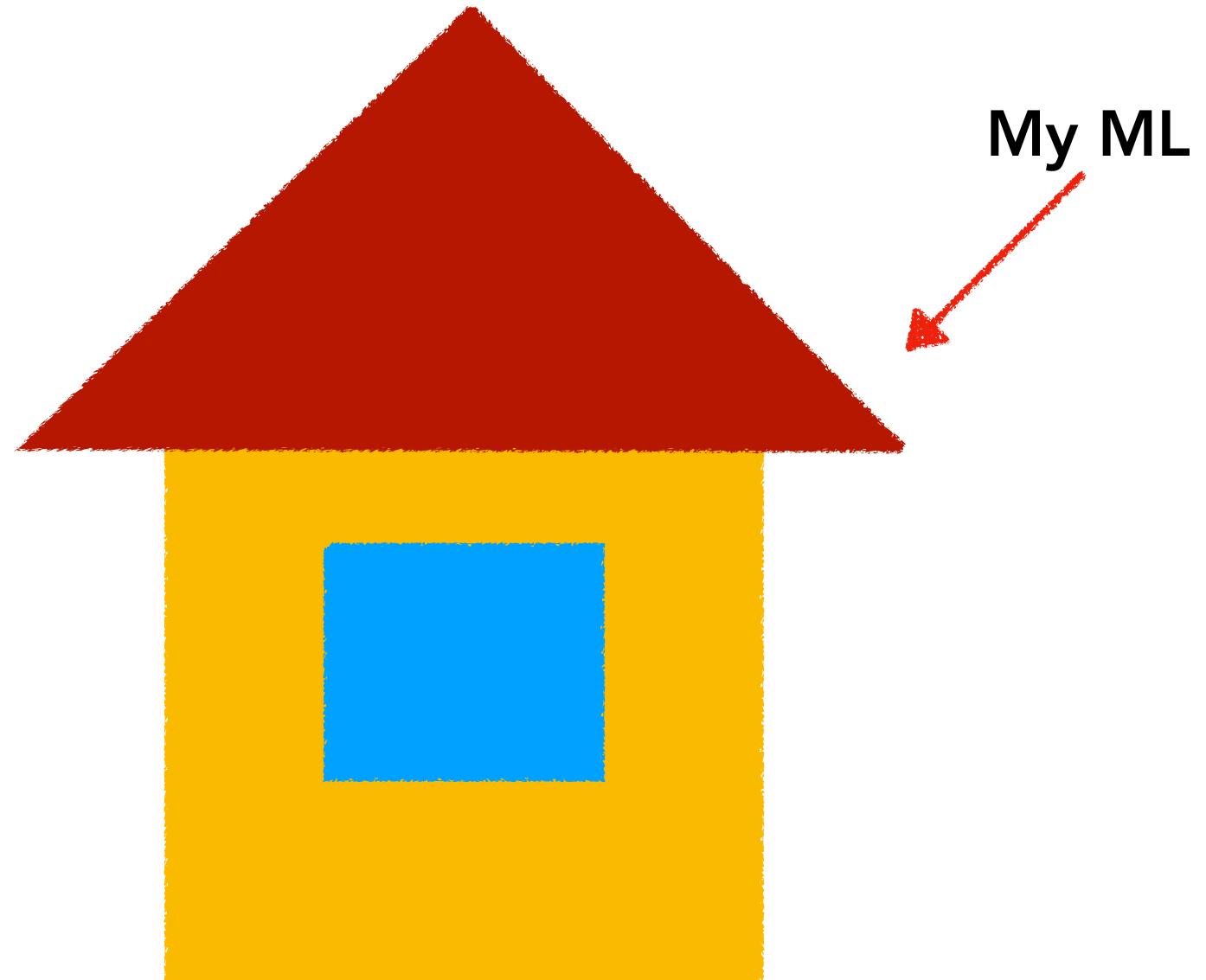
- Interpretability can help with them **when we cannot formalize these ideas**
- But once formalized, you may not need interpretability.

Agenda

- **When** and **why** interpretability
- **Overview** of interpretability methods.
- How to **Evaluate** interpretability methods.

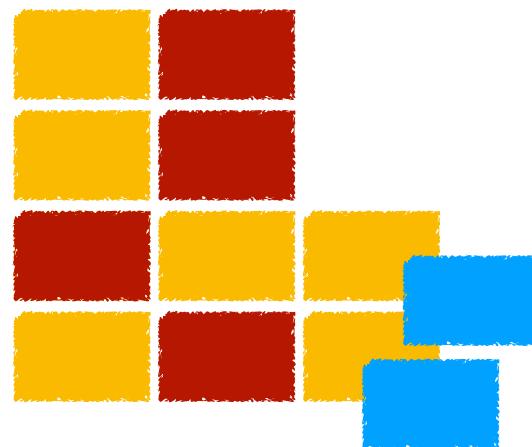


Types of interpretable methods



Types of interpretable methods

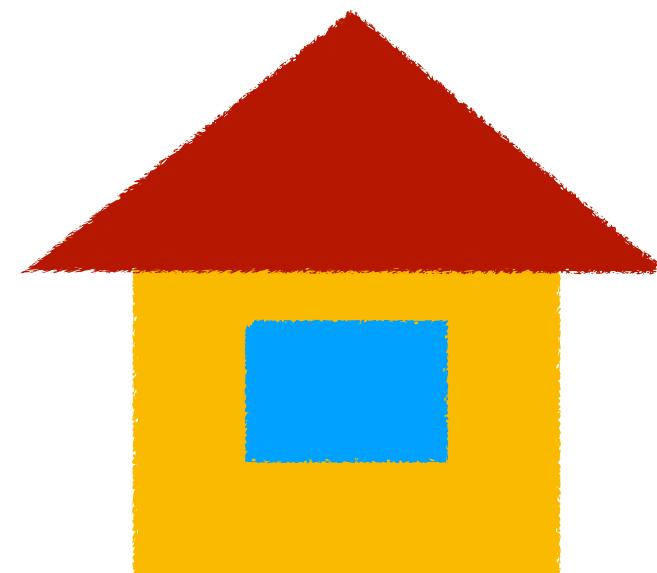
**Before building
any model**



**Building
a new model**

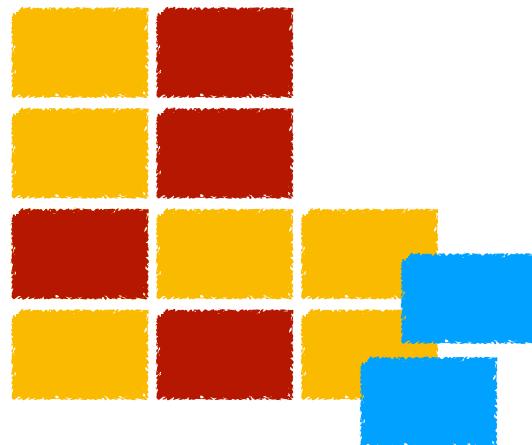


**After
building a model**



Types of interpretable methods

**Before building
any model**



**Building
a new model**

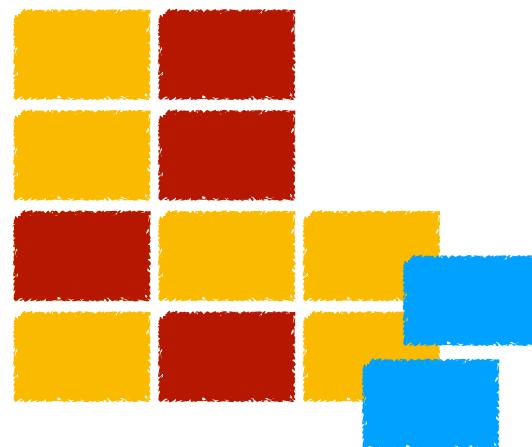


**After
building a model**

Common misunderstanding:
Interpretability is always about
machine learning models.

Types of interpretable methods

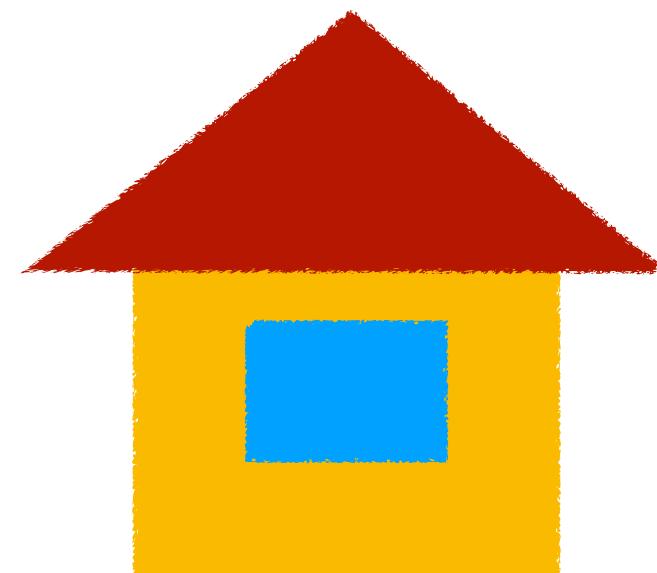
**Before building
any model**



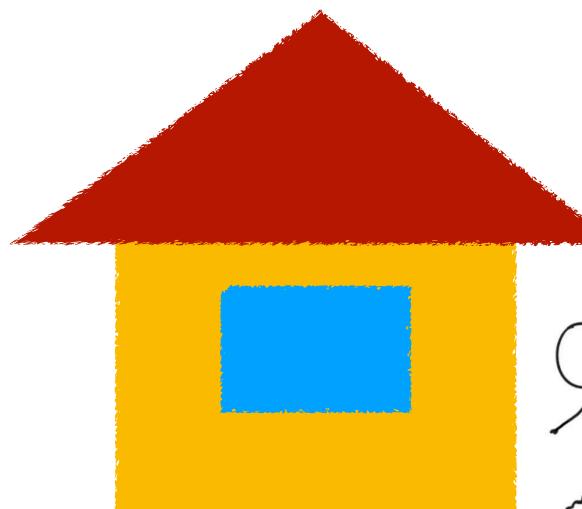
**Building
a new model**



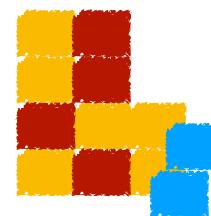
**After
building a model**



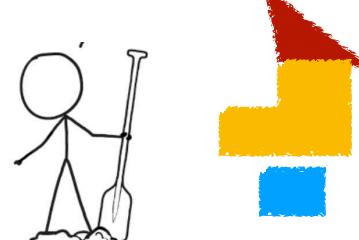
Types of interpretability methods



My ML



Before building
any model

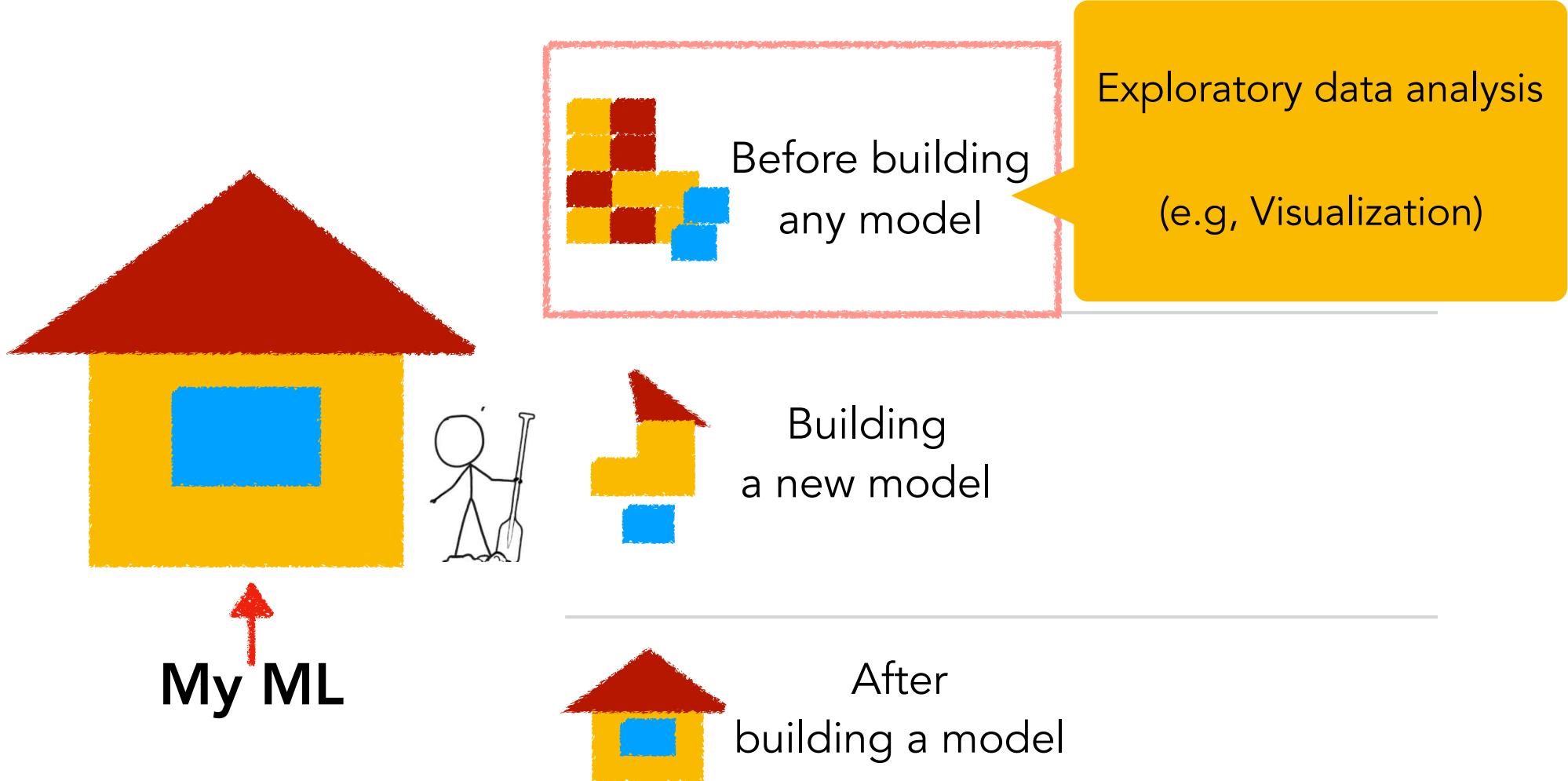


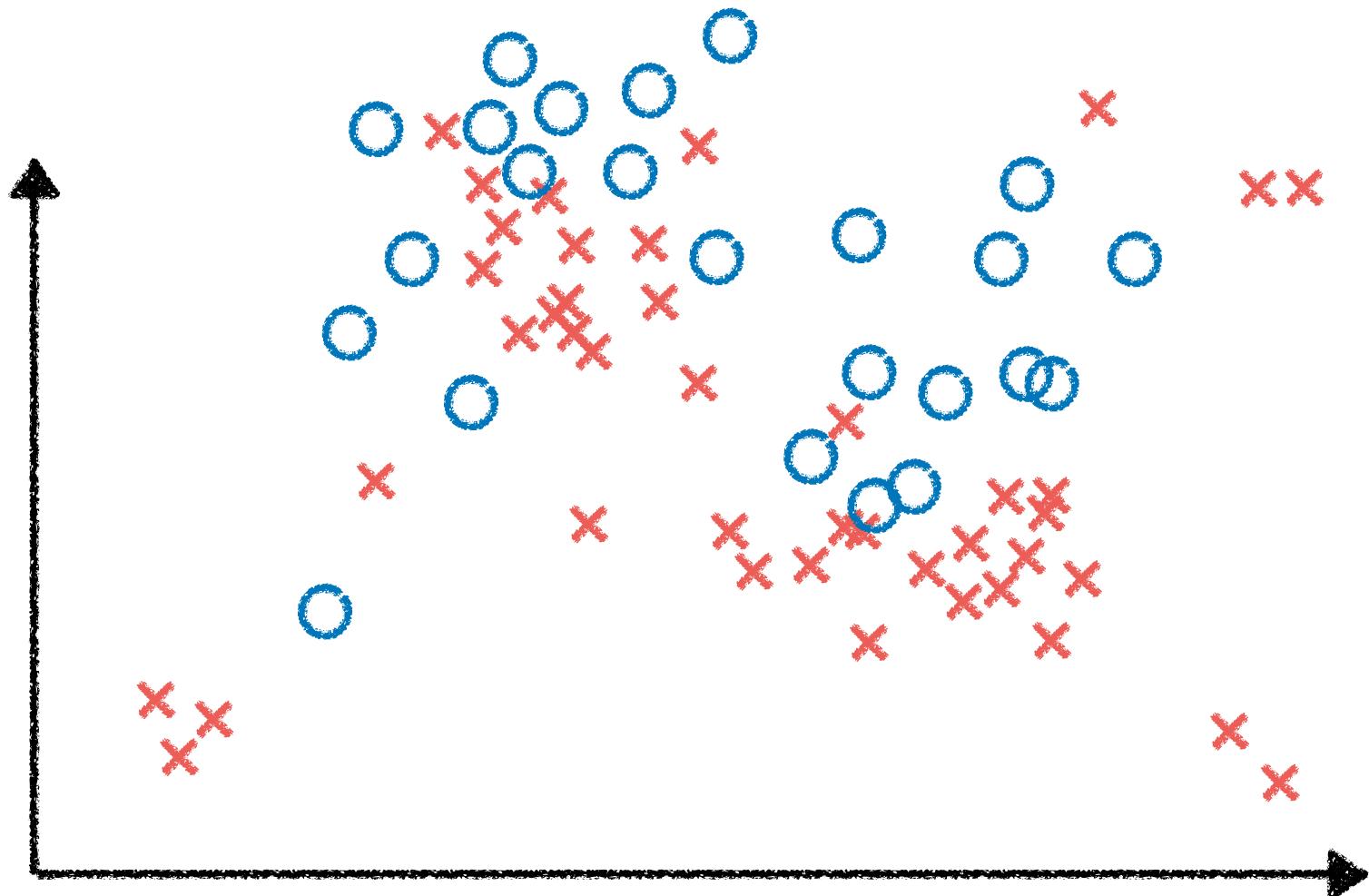
Building
a new model



After
building a model

Types of interpretability methods



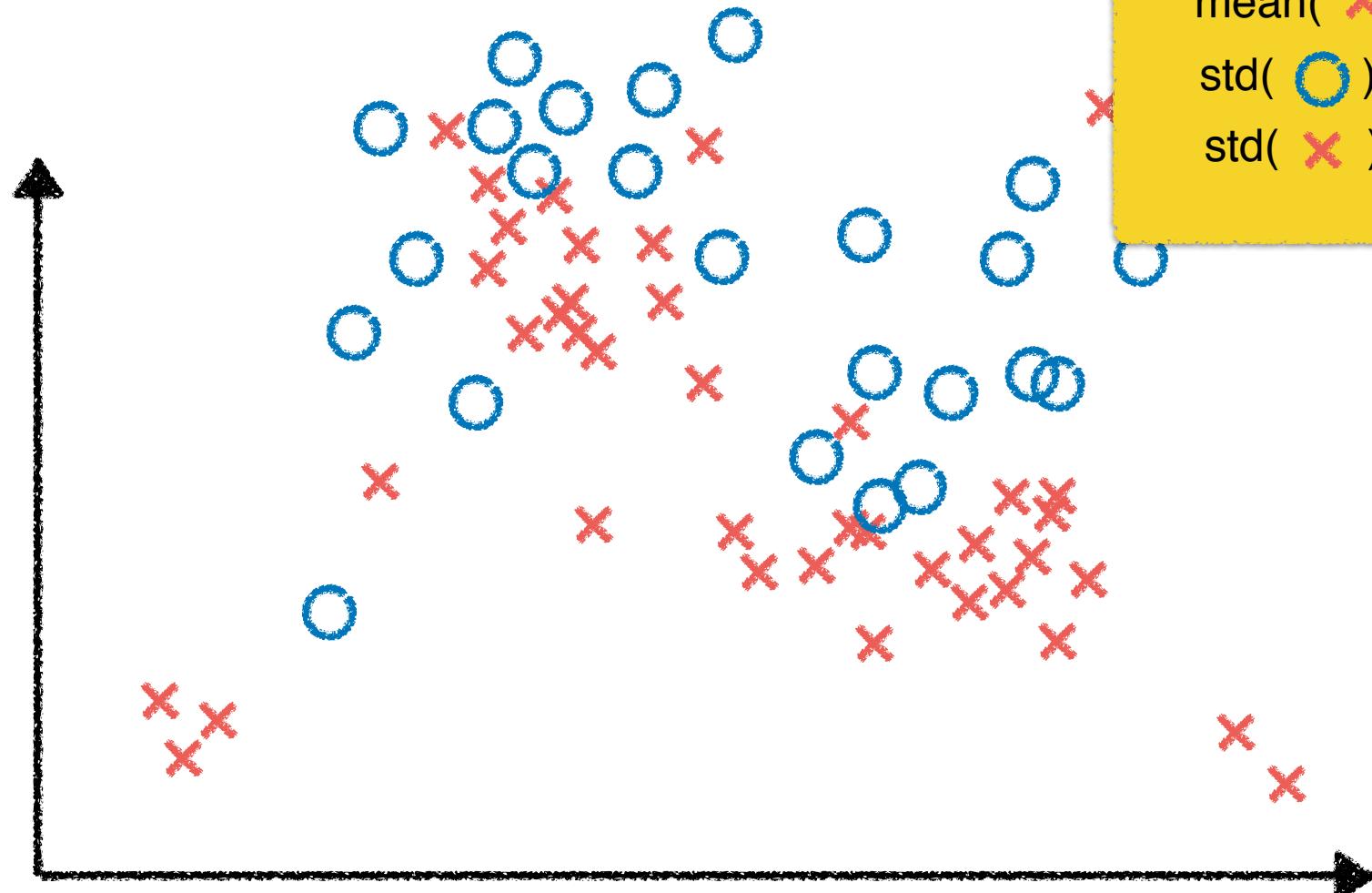


○ Class0

✗ Class1



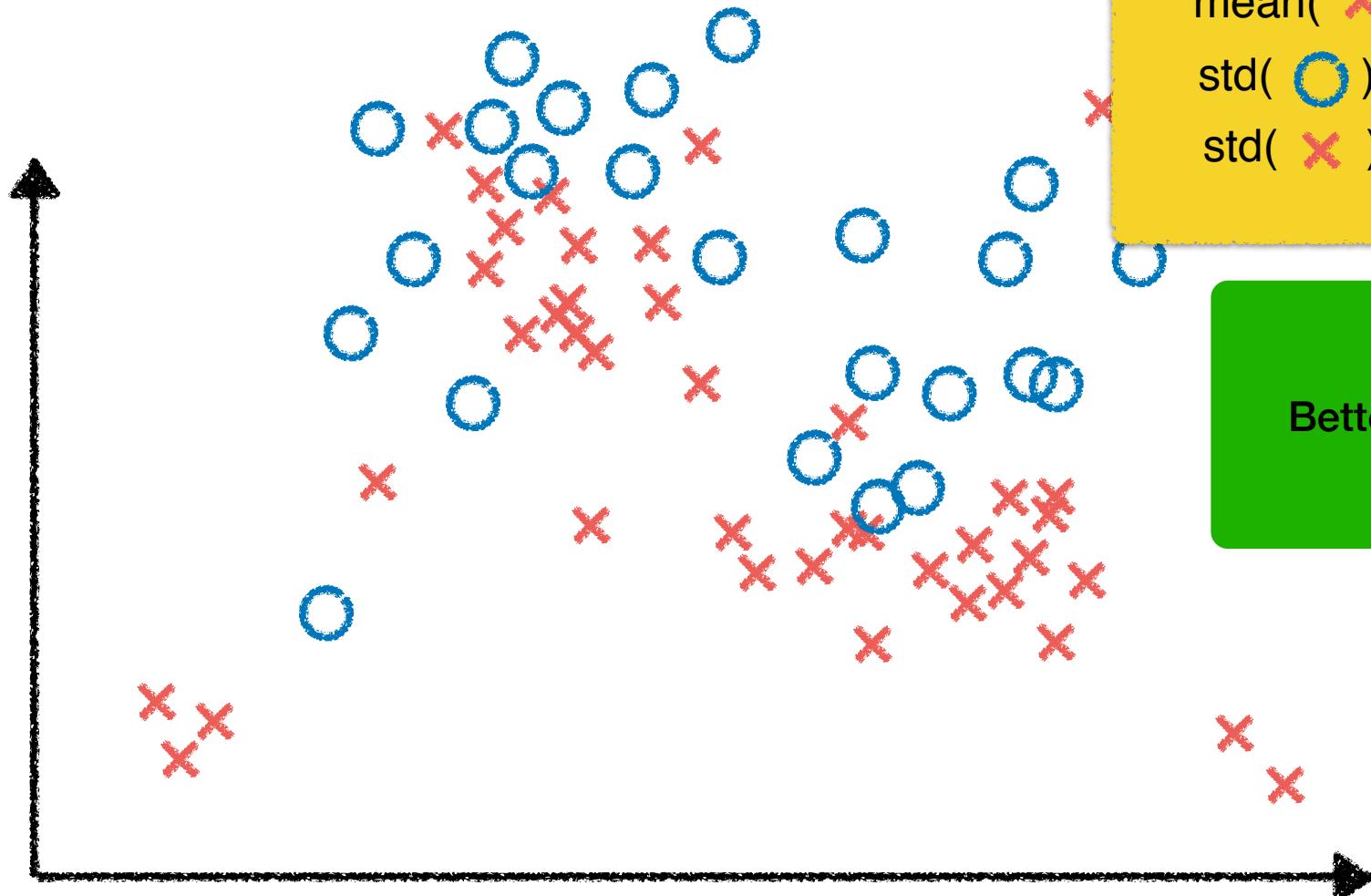
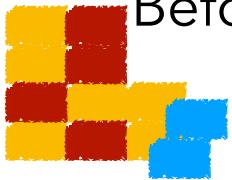
Before building any model



○ Class0

✗ Class1

Before building any model



○ Class0

✗ Class1

Descriptive statistics

mean(○)

mean(✗)

std(○)

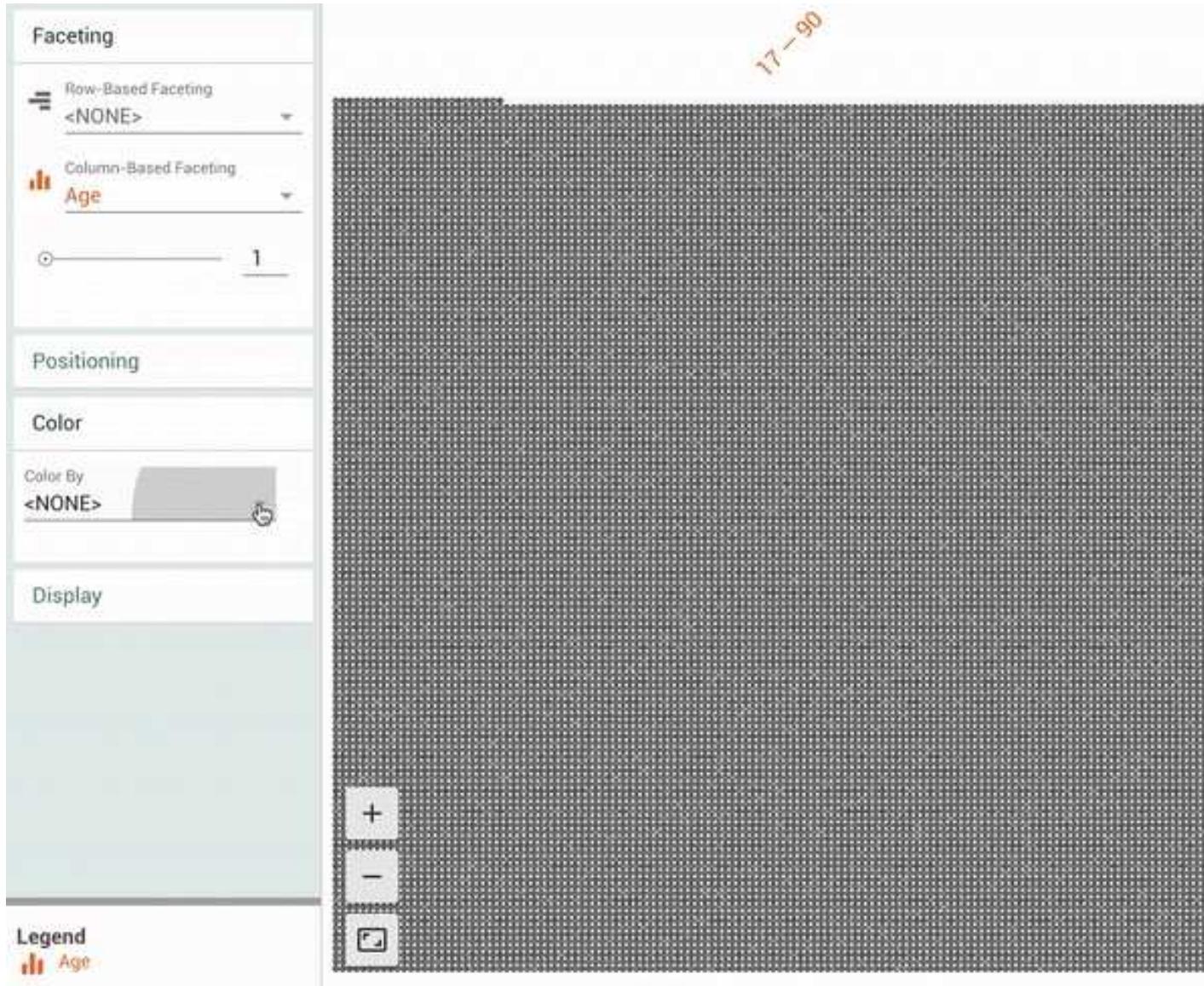
std(✗)

Better way?



Before building any model

Visualization for data exploration



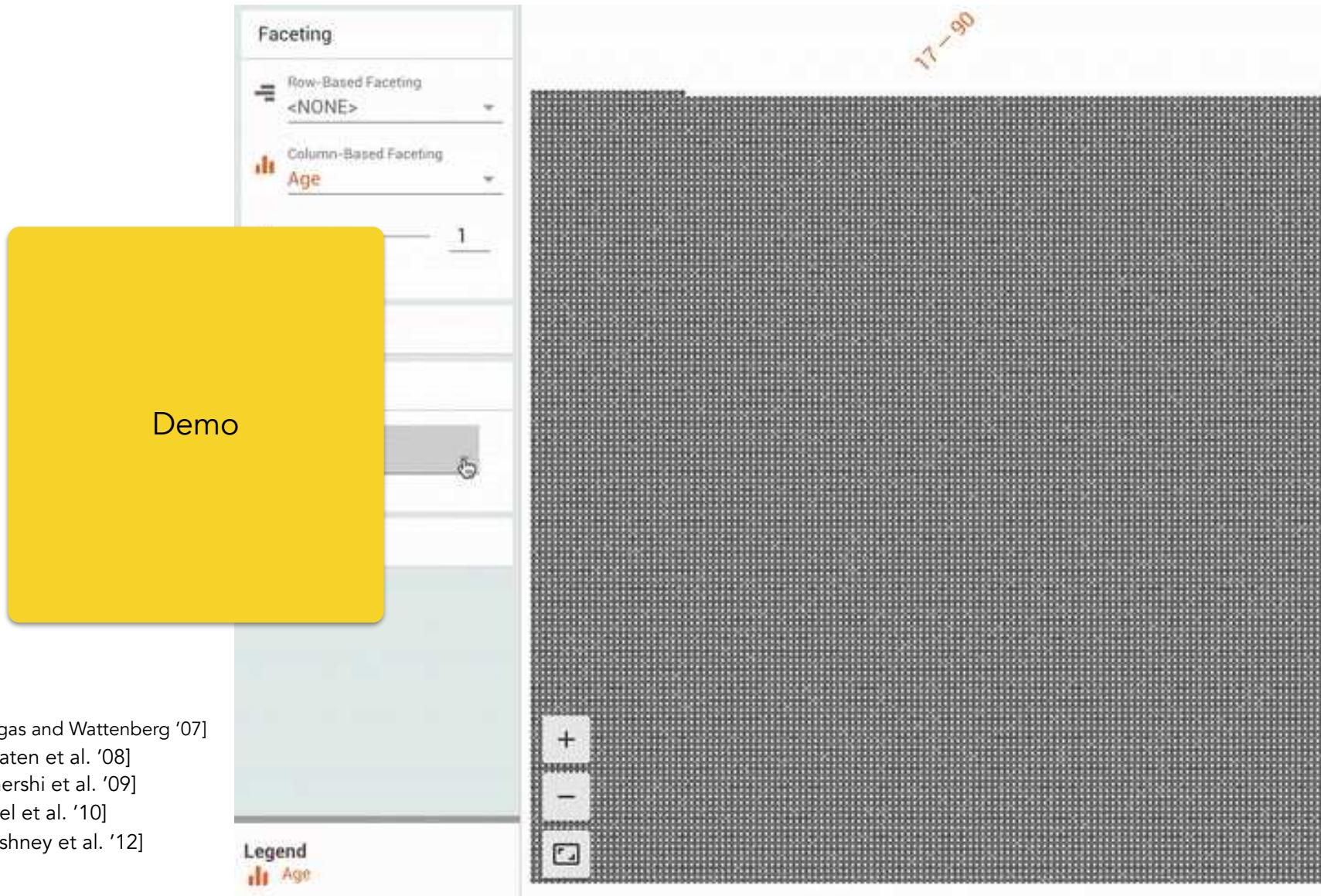
[Viégas and Wattenberg '07]
[Maaten et al. '08]
[Amershi et al. '09]
[Patel et al. '10]
[Varshney et al. '12]

<https://pair-code.github.io/tacets/quickdraw.html>



Before building any model

Visualization for data exploration

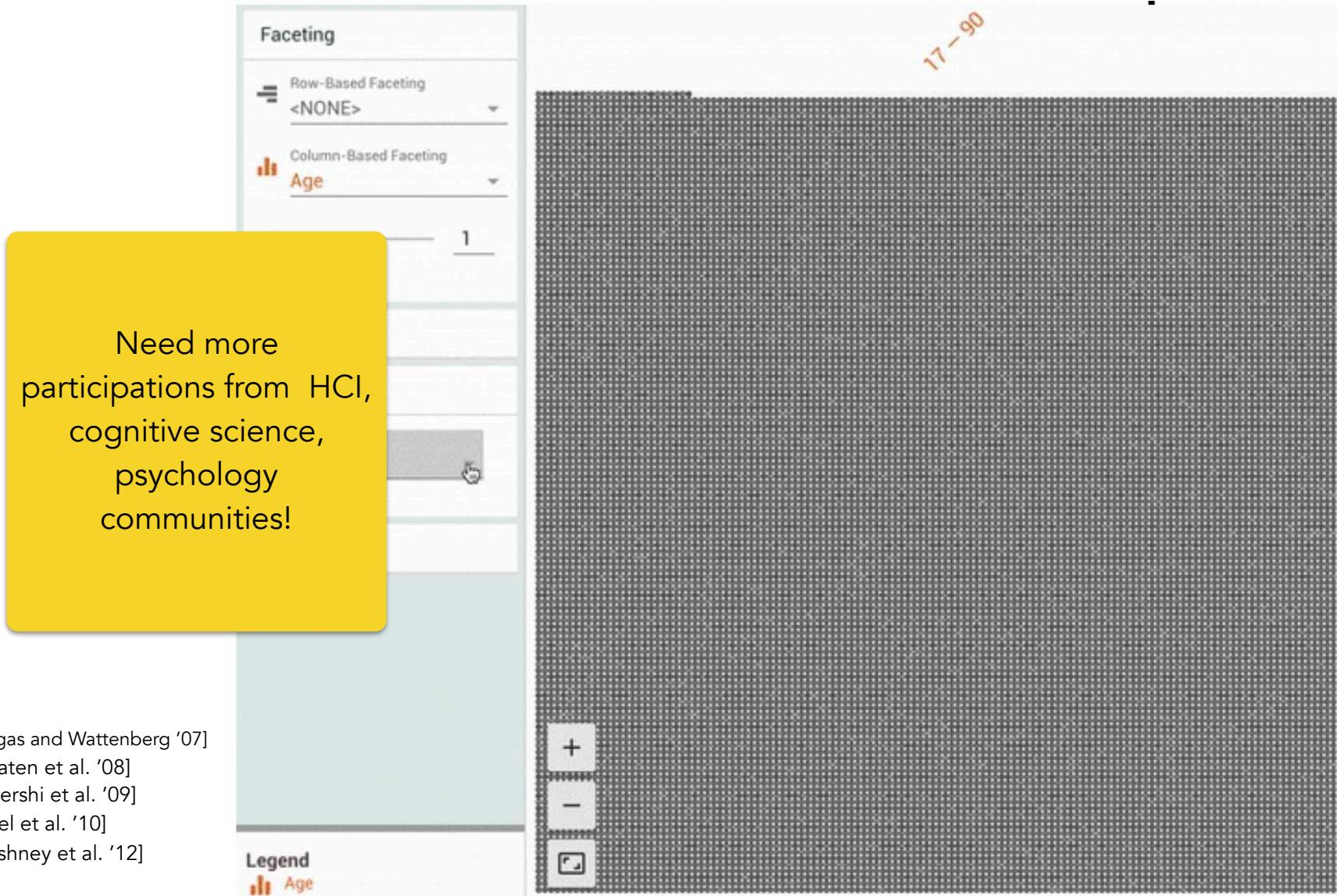


<https://pair-code.github.io/tacets/quickdraw.html>



Before building any model

Visualization for data exploration

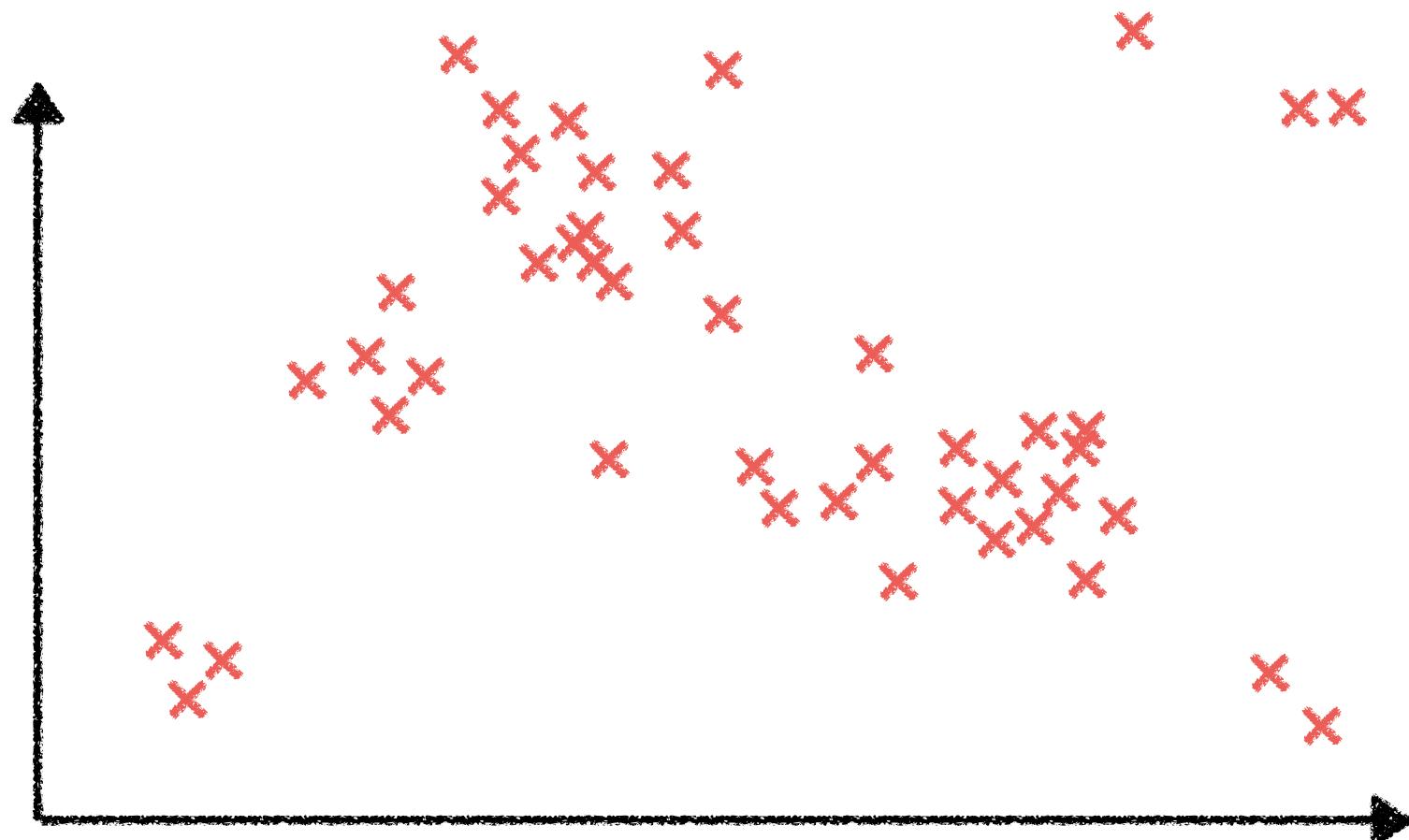


<https://pair-code.github.io/facets/quickdraw.html>



Before building any model

Exploratory data analysis

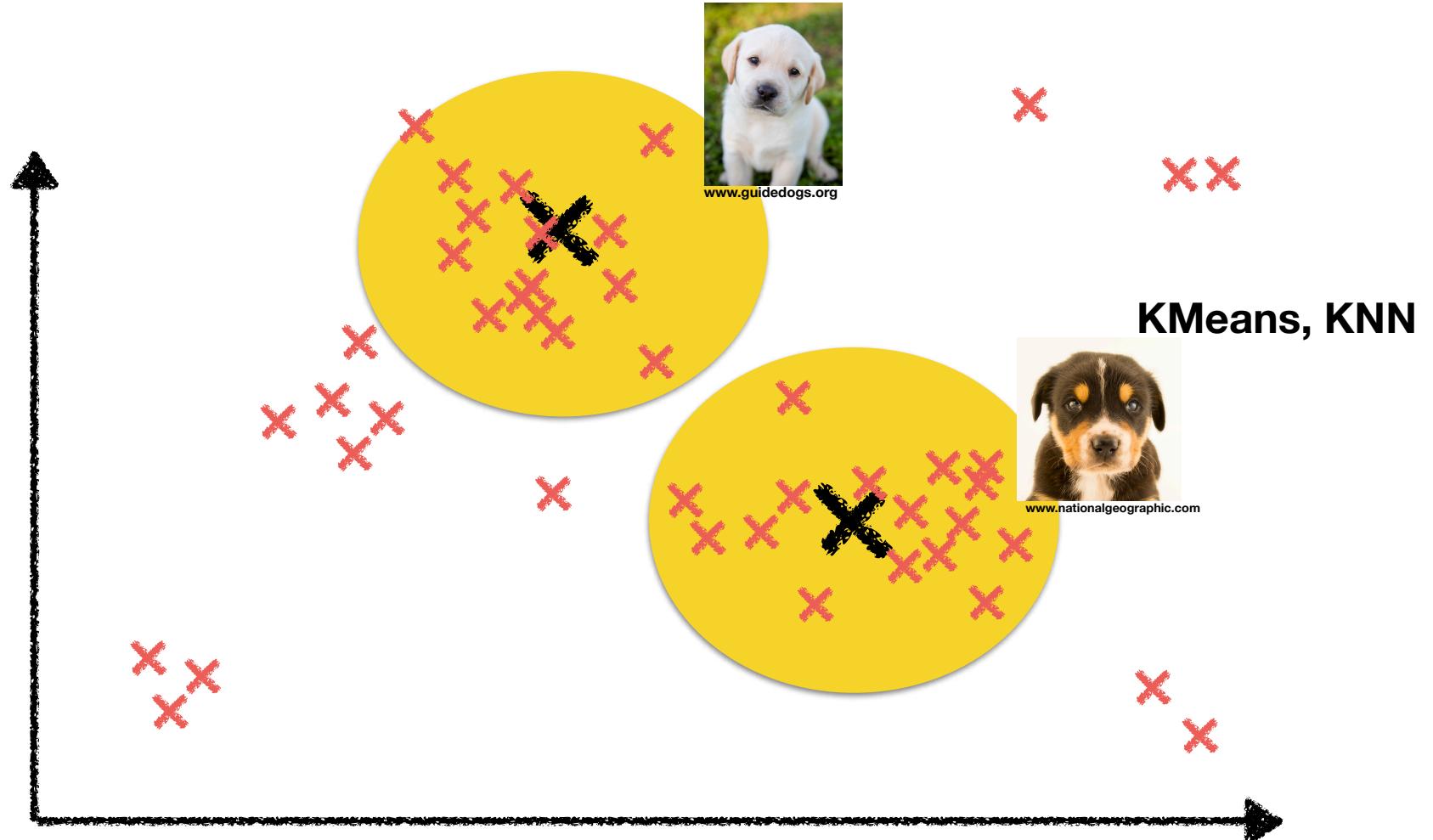


✖ Observed
data



Before building any model

Exploratory data analysis



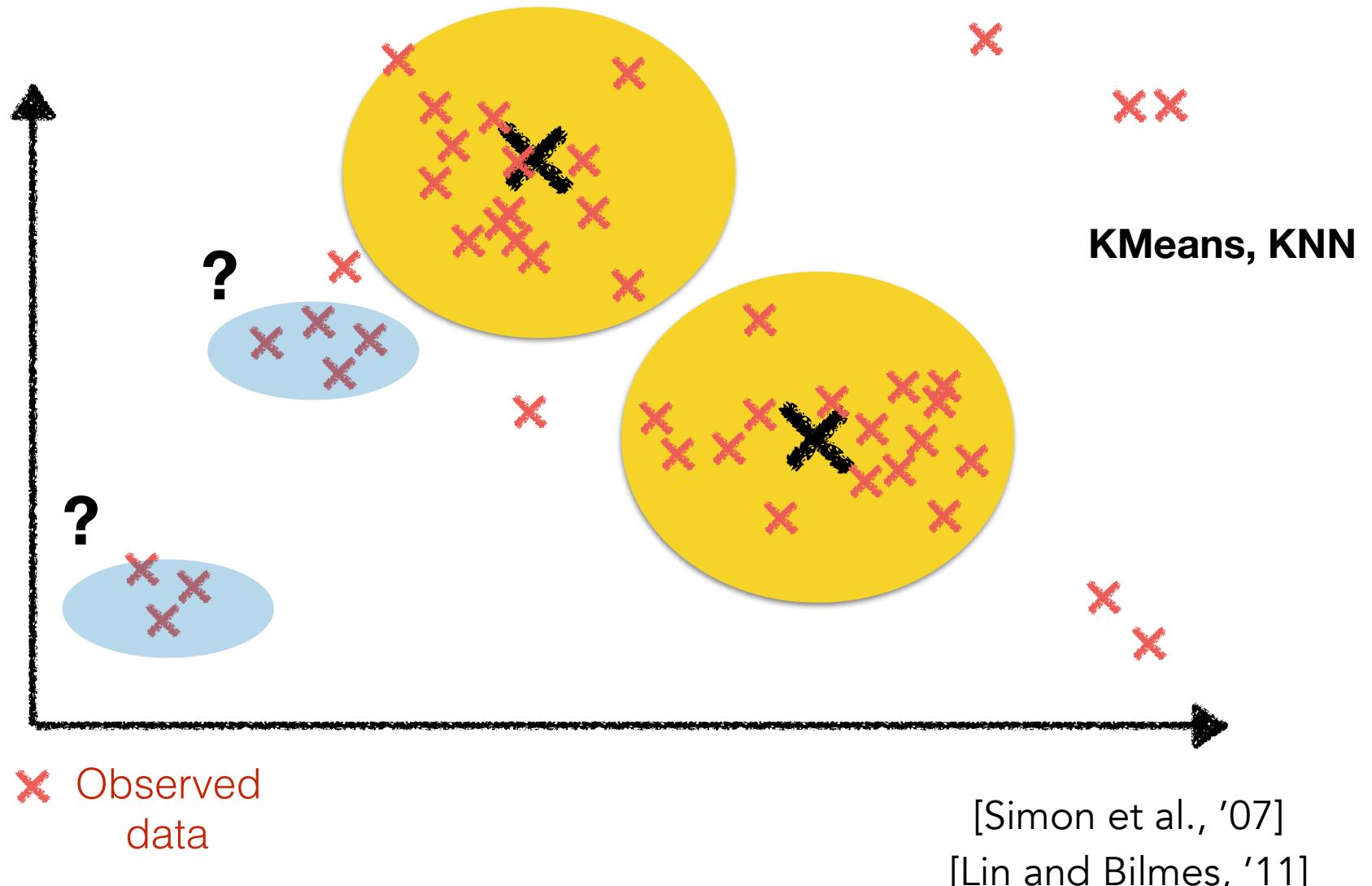
✖ Observed
data

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



Before building any model

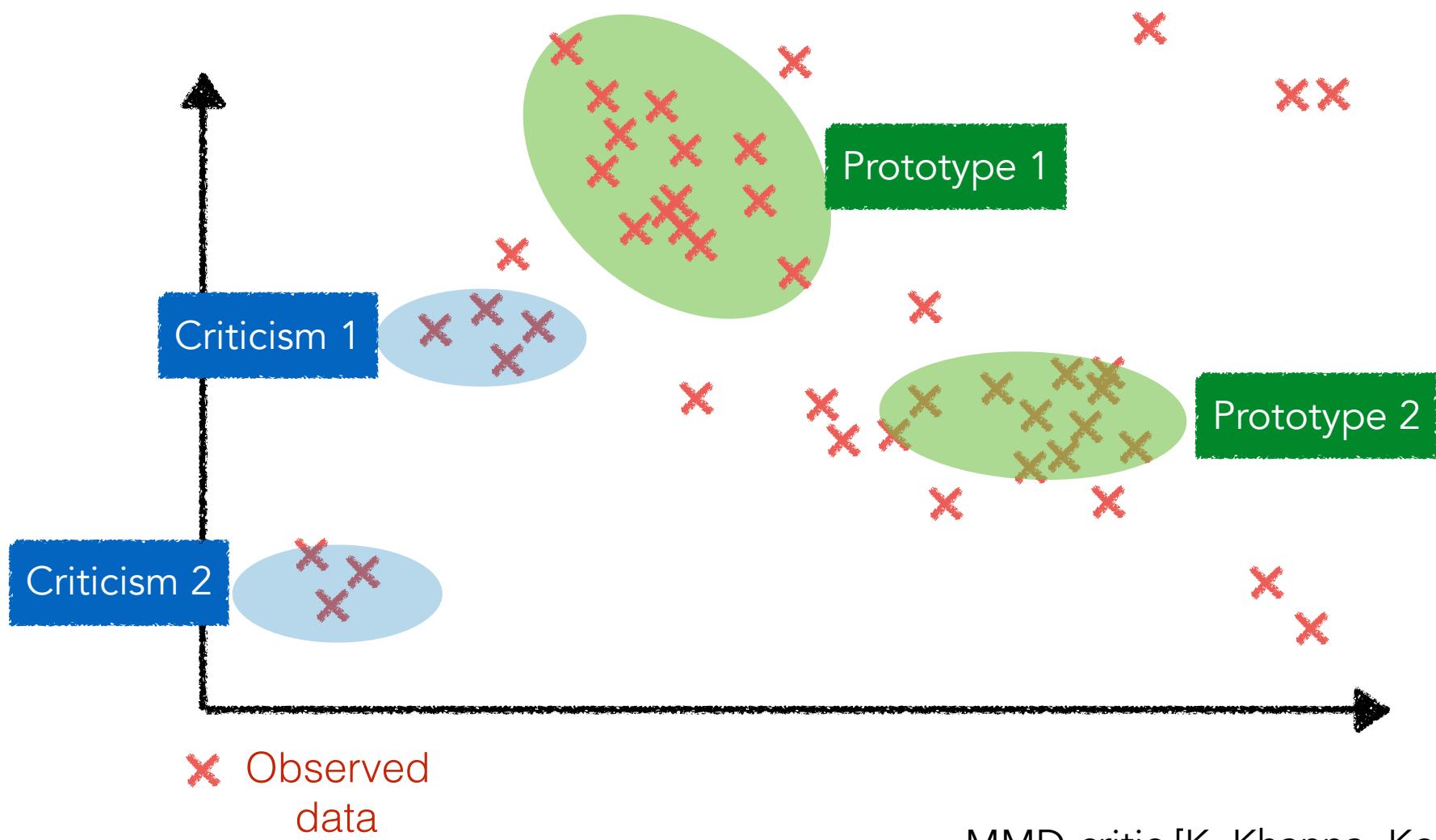
Exploratory data analysis





Before building any model

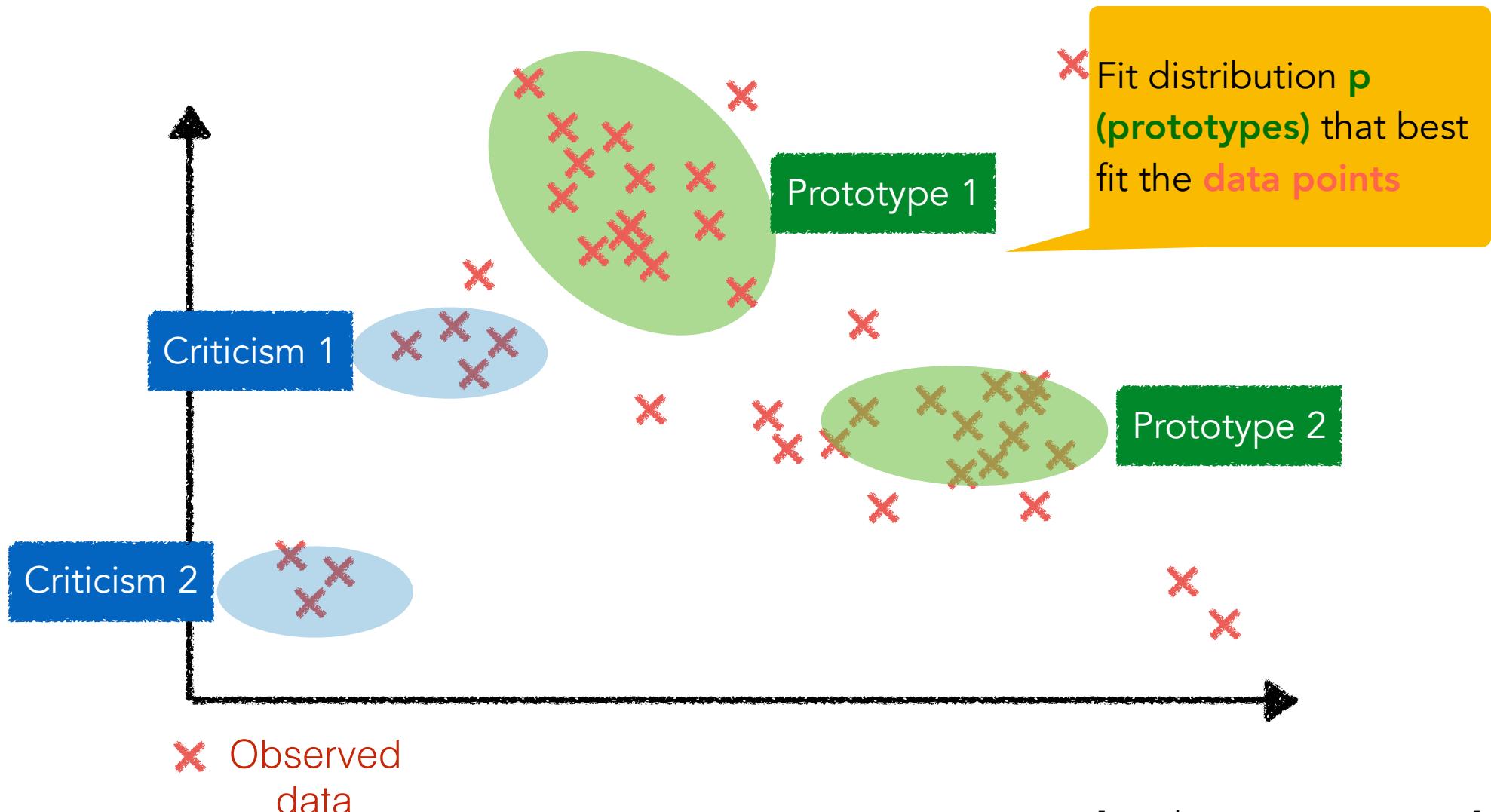
Exploratory data analysis





Before building any model

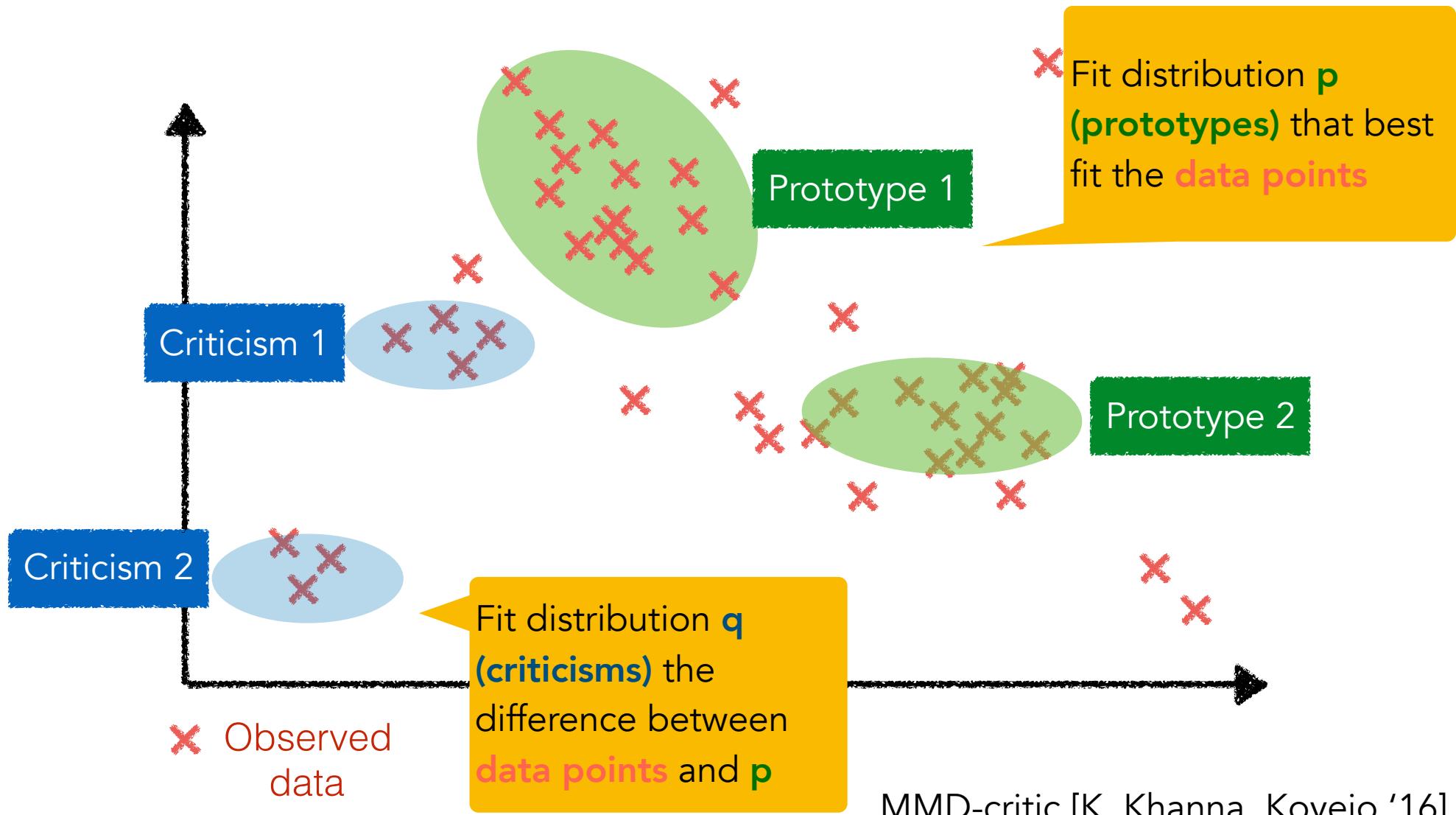
Exploratory data analysis





Before building any model

Exploratory data analysis

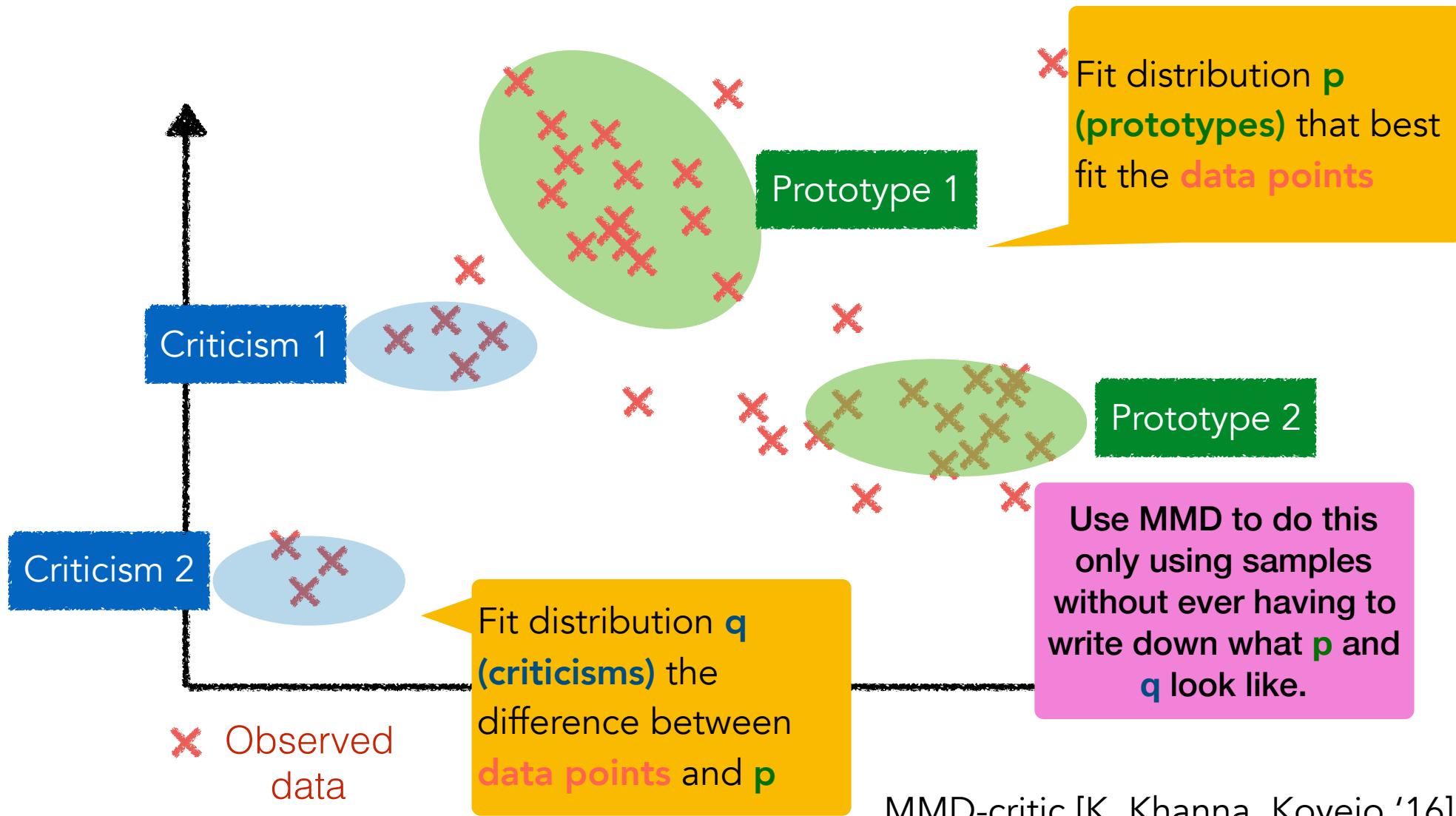


MMD-critic [K. Khanna, Koyejo '16]



Before building any model

Exploratory data analysis



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



Before building any model

Exploratory data analysis

Prototypes



Criticisms



Prototypes

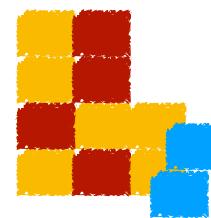
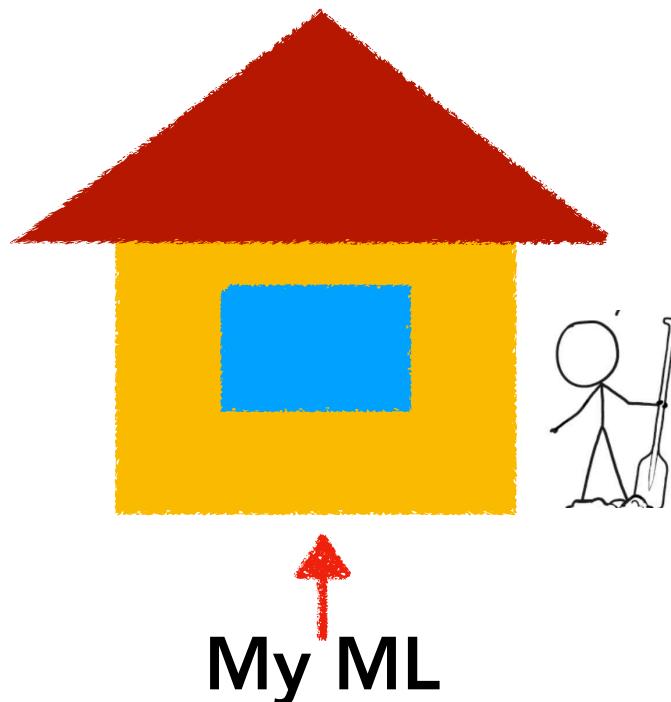


Criticisms



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

Types of interpretability methods



Before building
any model

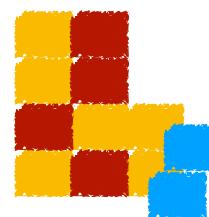
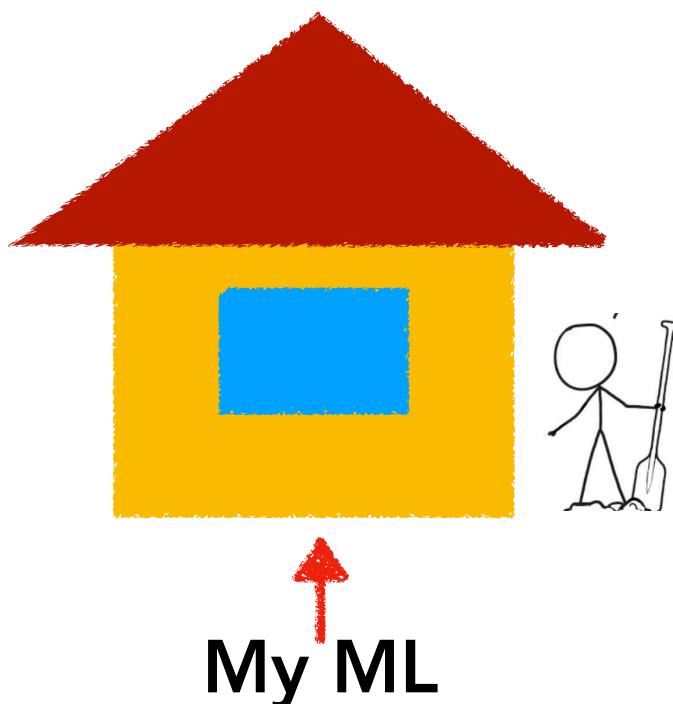


Building
a new model

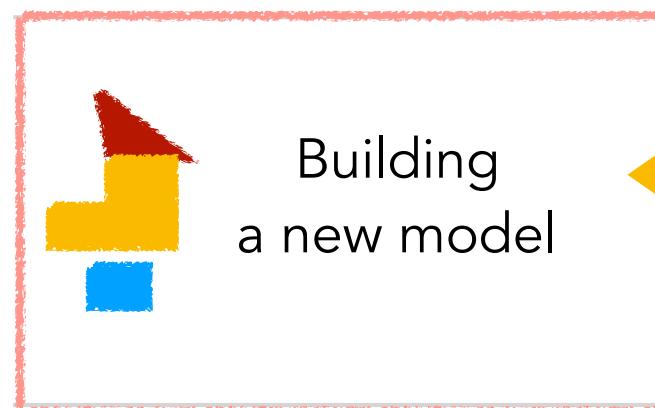


After
building a model

Types of interpretability methods



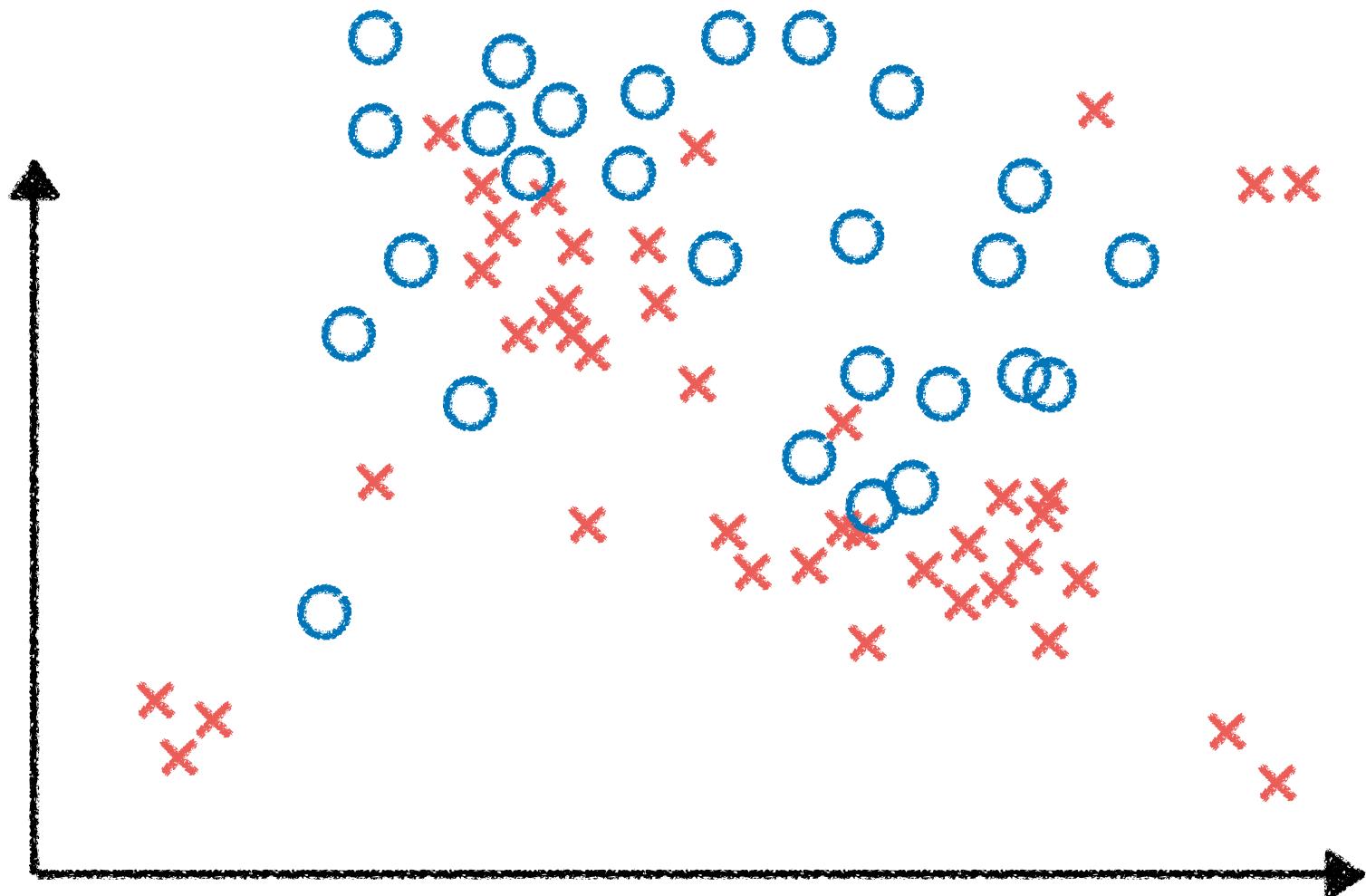
Before building
any model



After
building a model

What is the medium and
constraints we use to
explain?

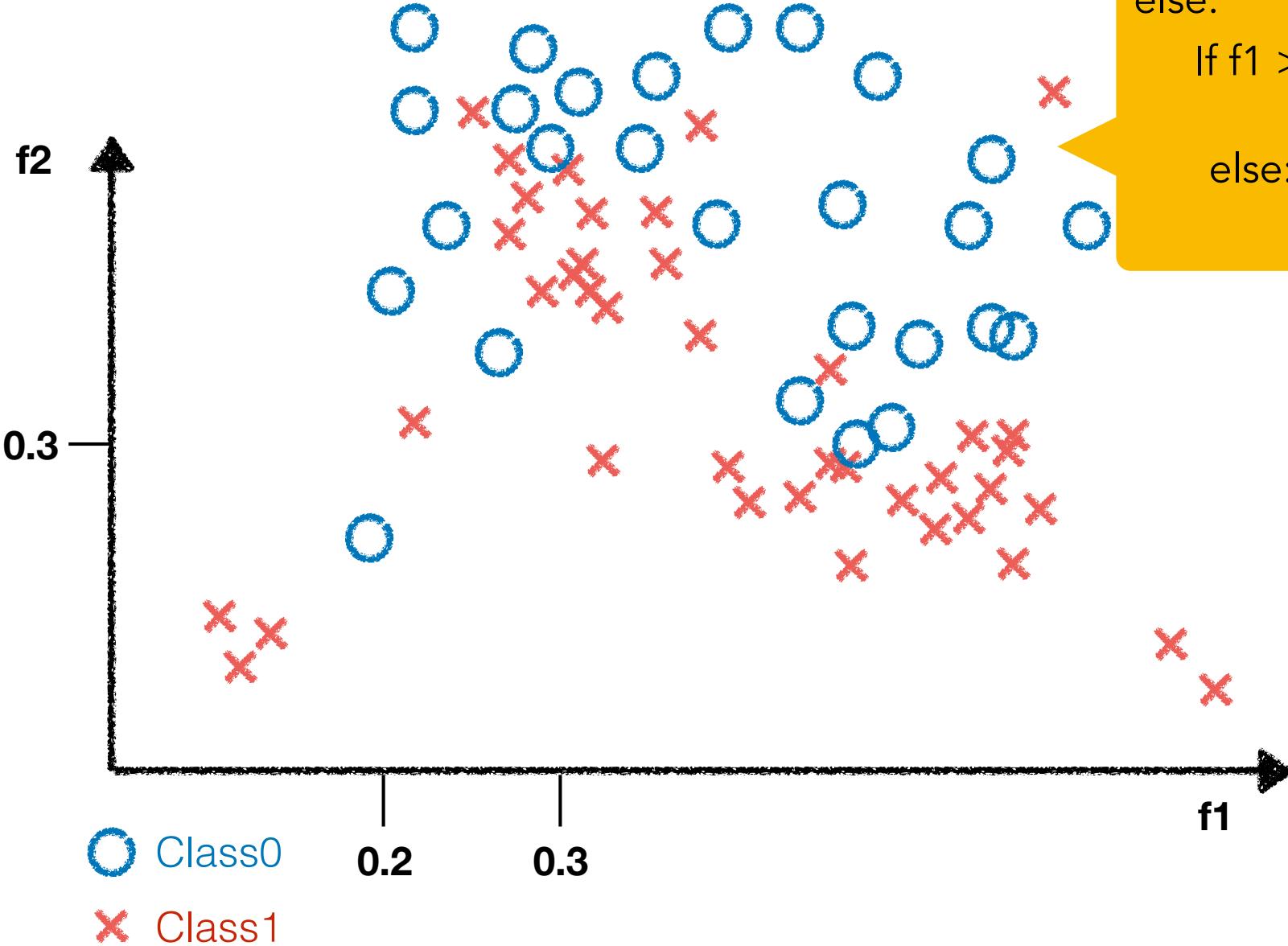
Rules, Examples, Sparsity
and Monotonicity



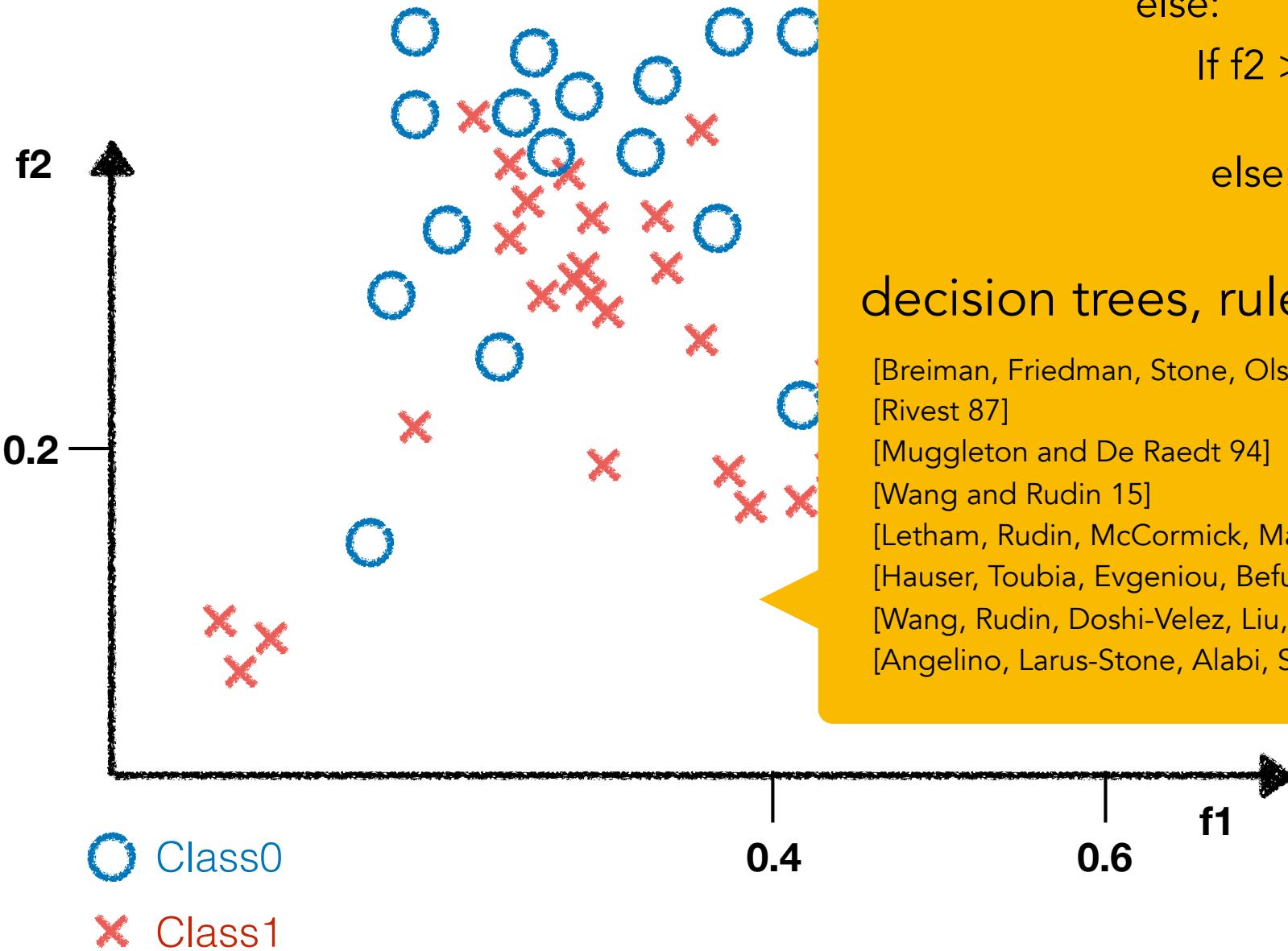
○ Class0

✗ Class1

Building a new model



Building a new model



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

Building a new model



Which ones are the limitations of rule-based methods?

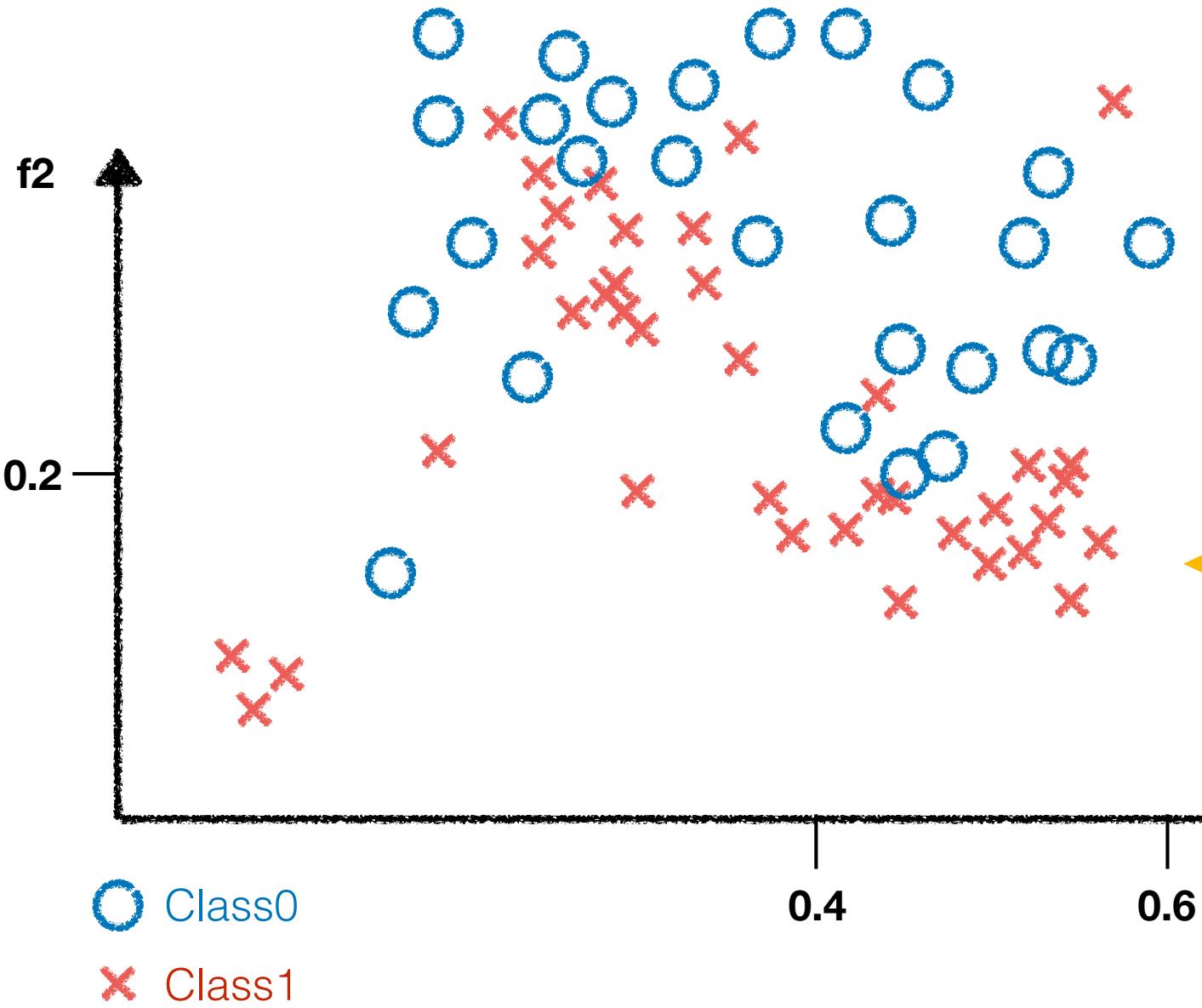
- A. It may not be as interpretable as you may think
- B. It only works if the original features are interpretable
- C. The data might not cluster
- D. None of the above

Which ones are the limitations of rule-based methods?

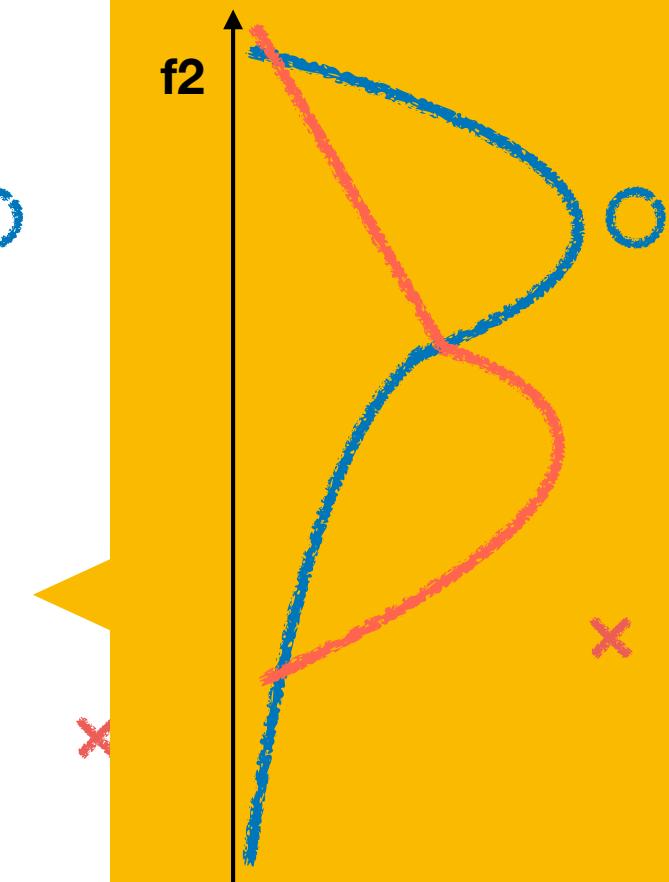
- Depth/Length of the tree might be too big
- Complexity of rules might be high
- Might not work for audio/images/embeddings

- A. It may not be as interpretable as you may think
- B. It only works if the original features are interpretable
- C. The data might not cluster
- D. None of the above

Building a new model

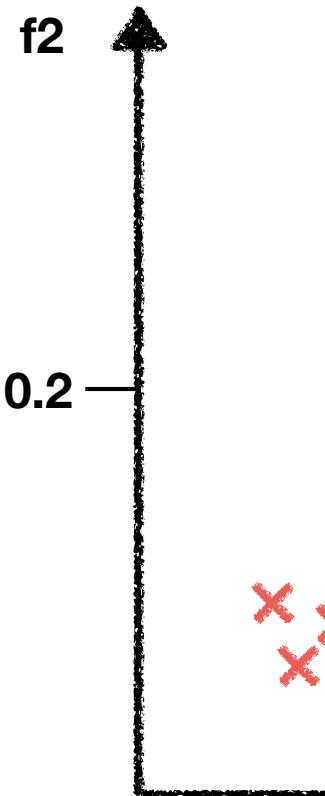


Fit a simpler function
for each feature



Building a new model

Fit a simpler function



Linear model

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

generalized linear model

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

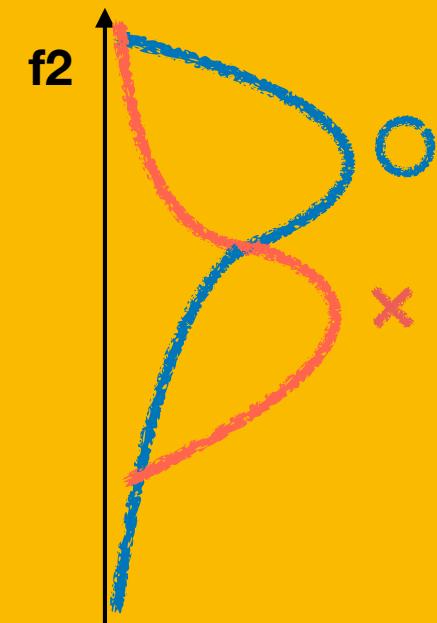
○ Class 0

generalized additive model

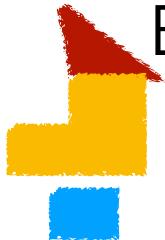
$$g(y) = f_1(x_1) + \dots + f_n(x_n)$$

✗ Class 1

Table from [Gehrke et al. '12]



Building a new model



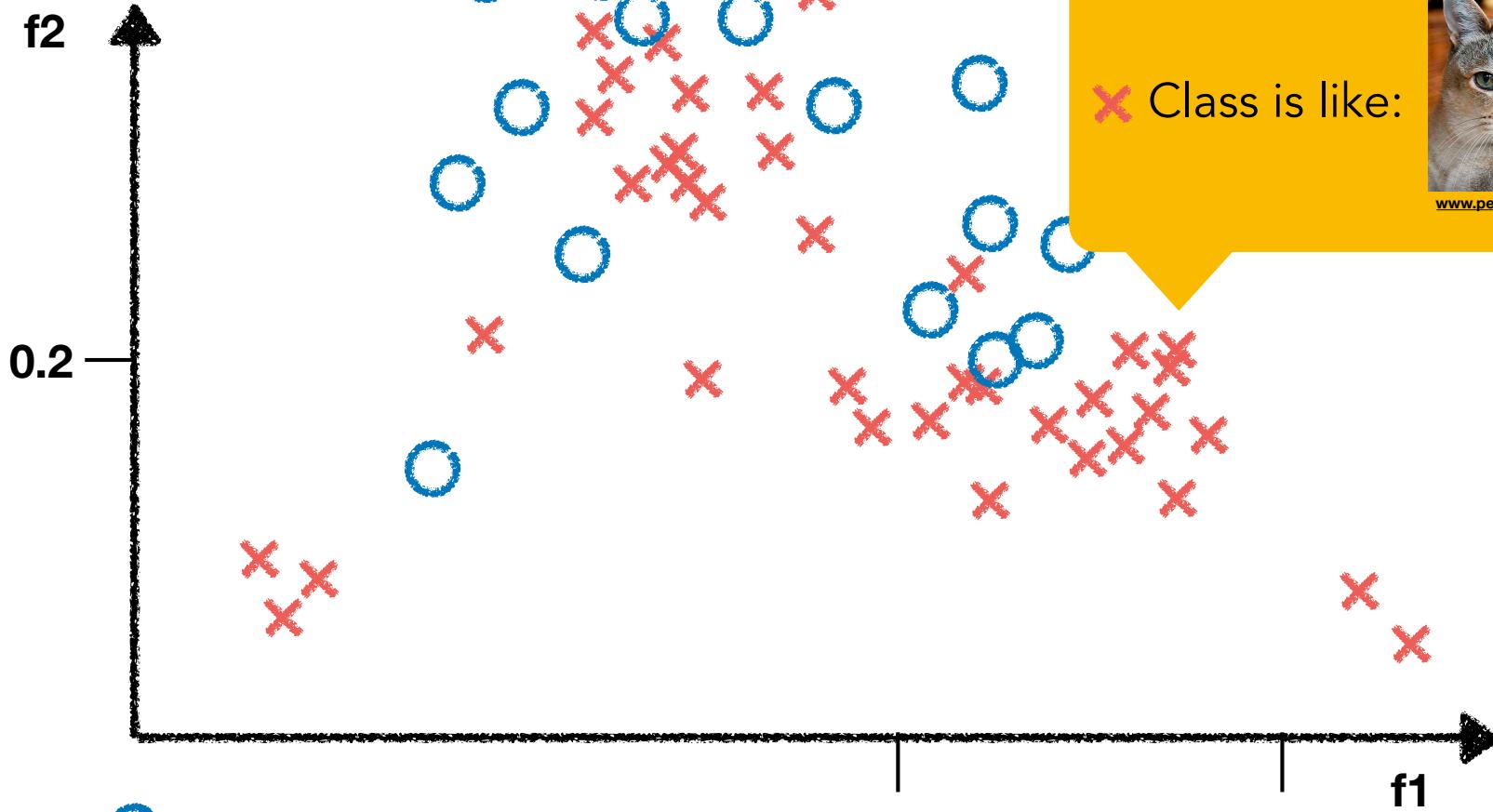
Example based



Class is like:



Class is like:



○ Class0
✗ Class1

- [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]

Building a new model



Example based



Class is like:



Class is like:



Building a new model

Interactive Bayesian Case Model (BCM) [K. Rudin, Shah'14]

Cluster Prototypes and Subspaces

Demote from Prototype

```
def dotProduct(listA,listB):
    total=0
    for(a,b)in zip(listA,listB):
        product=a*b
        total+=product
    return total
```

id: 1

Promote to Prototype

```
def dotProduct(listA,listB):
    iB=0
    length=len(listA)
    total=0
    while iB<length:
        total+=listA[iB]*listB[iB]
        iB+=1
    return total
```

id: 45

Demote from Prototype

```
def dotProduct(listA,listB):
    assert len(listA)==len(listB)
    return sum(a*b for(a,b)in zip(listA,listB))
```

id: 15

Promote to Prototype

```
def dotProduct(listA,listB):
    listC=[]
    iB=0
    while iB<len(listA)and iB<len(listB):
        listC.append(listA[iB]*listB[iB])
        iB+=1
    return sum(listC)
```

id:

Demote from Prototype

```
def dotProduct(listA,listB):
    length=len(listA)
    iB=0
    total=0
    while iB<length:
        total+=int(listA[iB])*int(listB[iB])
        iB+=1
    return total
```

id: 62

Promote to Prototype

```
def dotProduct(listA,listB):
    total=0
```

id: 54

Most prototypical homework submission in cluster 3.

Homework submissions in cluster 3

Building a new model

Interactive Bayesian Case Model (BCM) [K. Rudin, Shah'14]

Cluster Prototypes and Subspace

Demote from Prototype

```
def dotProduct(listA, listB):
    total=0
    for(a,b) in zip(listA, listB):
        product=a*b
        total+=product
    return total
```

Change
important
keywords in the
cluster

Demote from Prototype

```
def dotProduct(listA, listB):
    assert len(listA)==len(listB)
    return sum(a*b for(a,b) in zip(listA, listB))
```

Demote from Prototype

```
def dotProduct(listA, listB):
    length=len(listA)
    iB=0
    total=0
    while iB<length:
        total+=int(listA[iB])*int(listB[iB])
        iB+=1
```

Promote to Prototype

id: 45

```
def dotProduct(listA, listB):
    iB=0
    length=len(listA)
    total=0
    while iB<length:
        total+=listA[iB]*listB[iB]
        iB+=1
    return total
```

Make this example
prototype, and
recluster!

Promote to Prototype

id: 52

```
def dotProduct(listA, listB):
    listC=[]
    iB=0
    while iB<len(listA) and iB<len(listB):
        listC.append(listA[iB]*listB[iB])
        iB+=1
    return sum(listC)
```

Promote to Prototype

id: 54

```
def dotProduct(listA, listB):
    total=0
```

Tool A

dot product

Ready for Input

Cluster Prototypes and Subspaces

```
def dotProduct(listA, listB):
    total=0
    iB=0
    while iB<len(listA):
        product=listA[iB]*listB[iB]
        total+=product
        iB+=1
    return total
```

```
def dotProduct(listA, listB):
    total=0
    for(a,b) in zip(listA, listB):
        product=a*b
        total+=product
    return total
```

```
def dotProduct(listA, listB):
    if len(listA)!=len(listB):
        print 'length of A and B need to be the same'
    return None
```

Cluster members

Show all stacks

Promote to Prototype

```
def dotProduct(listA, listB):
    length=len(listA)
    total=0
    for i in range(0,length):
        product=listA[i]*listB[i]
        total=total+product
    return total
    print total
```

Promote to Prototype

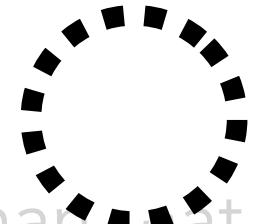
```
def dotProduct(listA, listB):
    length=len(listA)
    iB=0
    total=0
    while iB<length:
        total=total+listA[iB]*listB[iB]
        iB+=1
    return total
```

Which ones are the limitations of case-based models?

- A. The complexity of explanation is higher than that of data points
- B. There may not be a good representative examples
- C. Human may overgeneralize
- D. None of the above

Which ones are the limitations of case-based models?

None of data points are representative!



- A. The complexity of explanation is higher than that of data points
- B. There may not be a good representative examples
- C. Human may overgeneralize
- D. None of the above

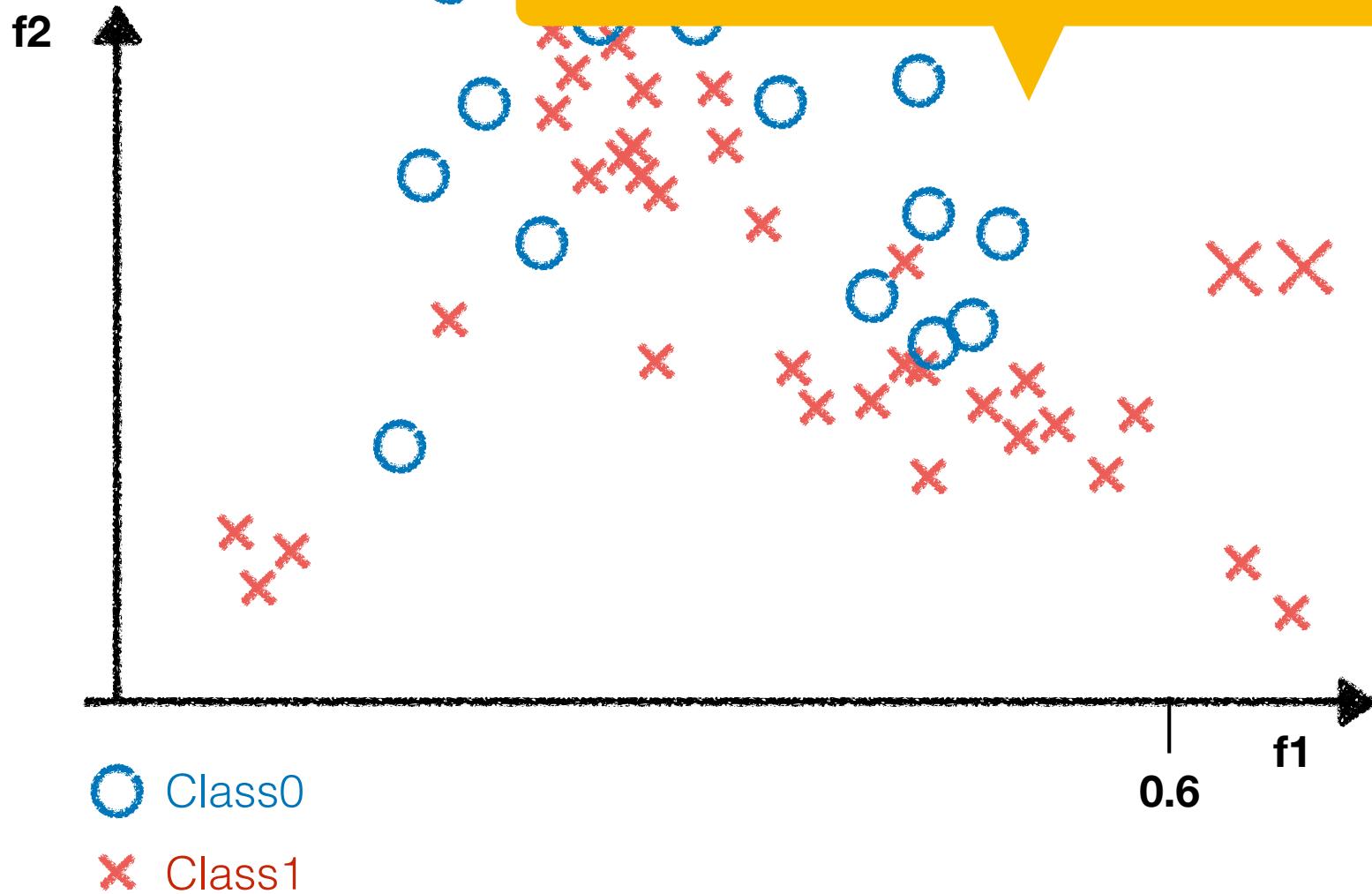


Building a new model

Build a sparse model

$$y = a_0 + a_1x_1 + a_{21}x_{21} + a_{1002}x_{1002}$$

(all other a_i 's set to zero)



Which ones are the limitations of sparsity methods?

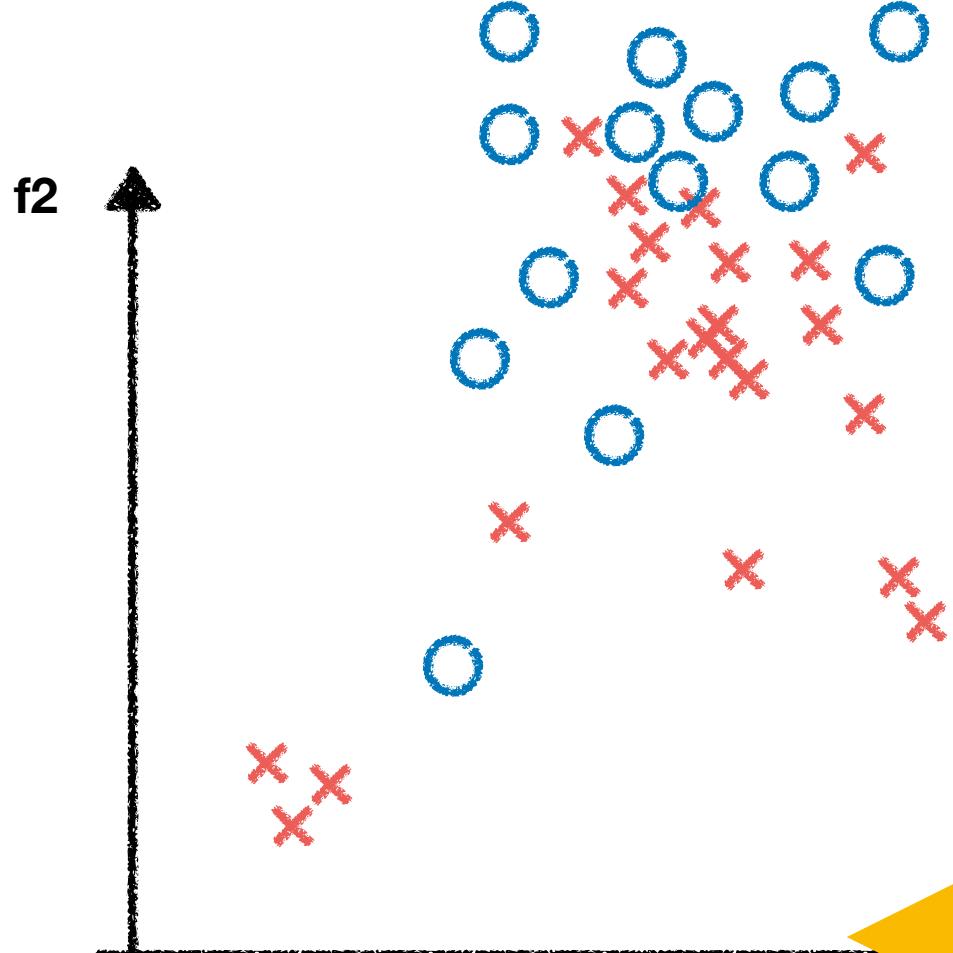
- A. The model may not be able to represent what it learned in a sparse fashion.
- B. There might be the case that only the collections of factors make more sense
- C. None of the above

Which ones are the limitations of sparsity methods?

- A. The model may not be able to represent what it learned in a sparse fashion.
- B. There might be the case that only the collections of factors make more sense
- C. None of the above

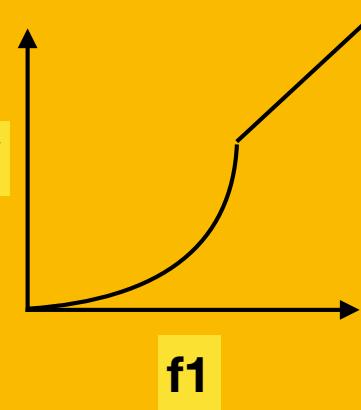
“Sparsity is good, but not enough. Just because it is sparse, doesn’t mean it’s interpretable.” [Freitas ‘10]

Building a new model



Piecewise
monotonic

Monotonicity



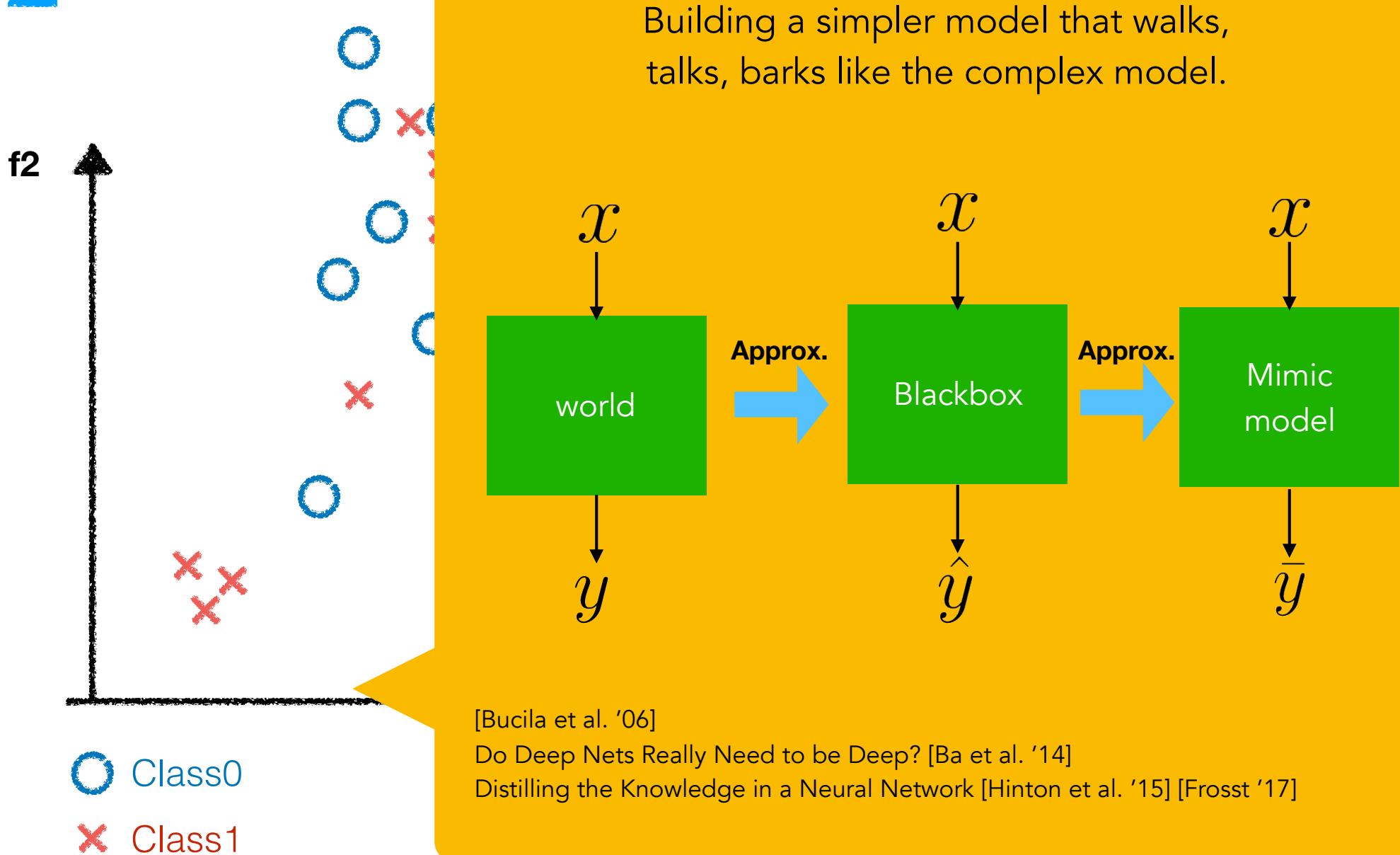
Learn piecewise monotonic function within a user specified lattice (intervals) [Gupta et al. '16]

Monotonic neural networks by constraining weights [Neumann et al.'13, Riihimaki and Vehtari '10]

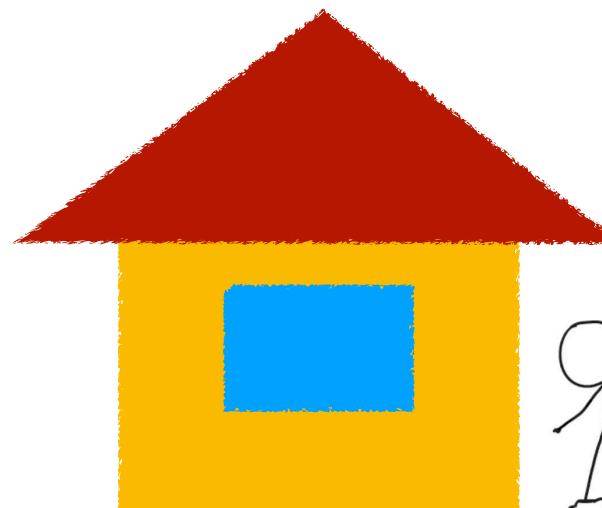


Building a new model

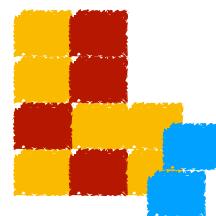
Mimic models, model distillation



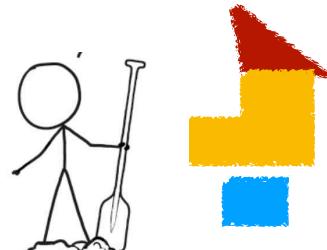
Types of interpretability methods



My ML



Before building
any model



Building
a new model

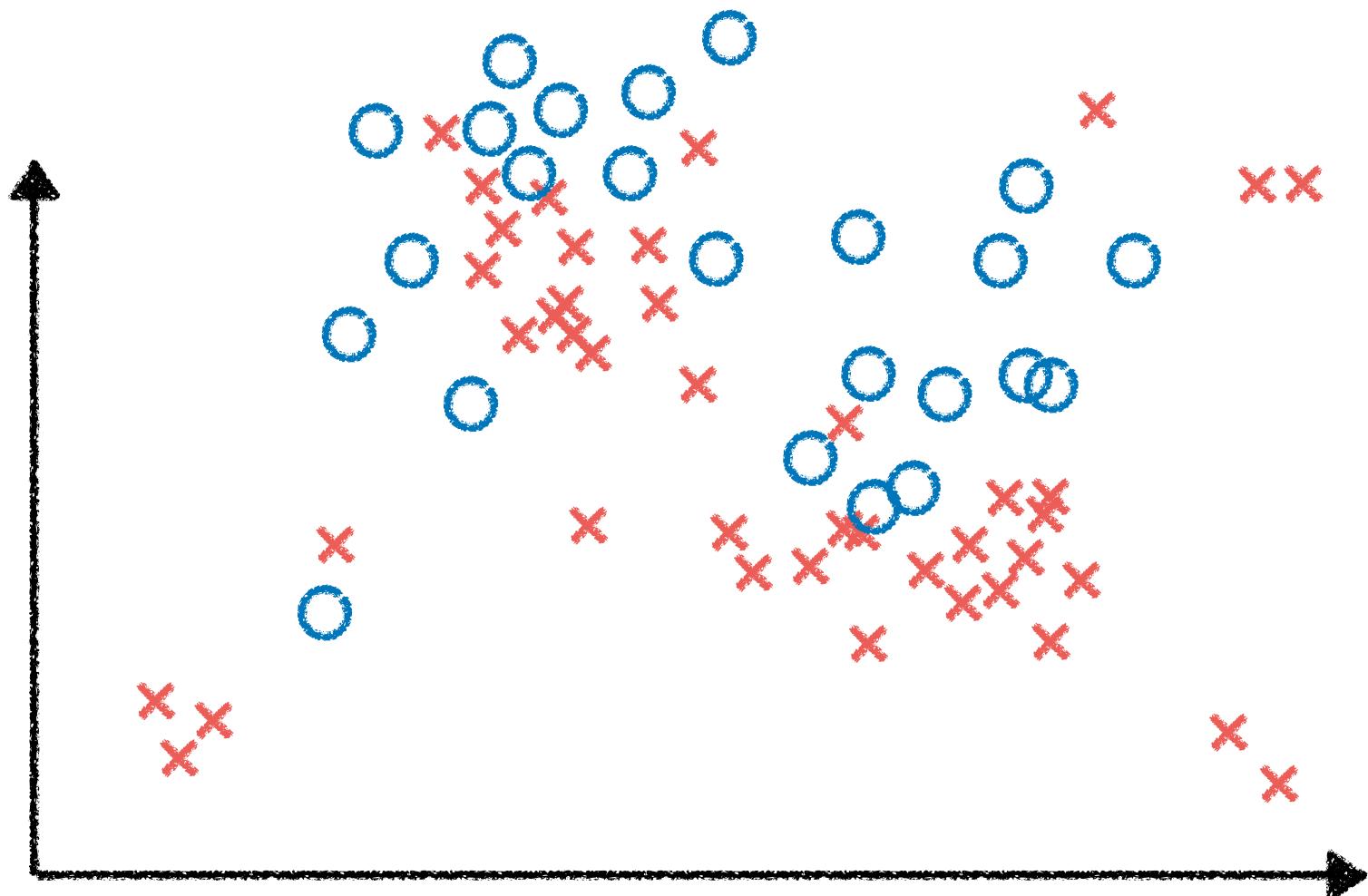


After
building a model

Ablation test

Input-feature importance

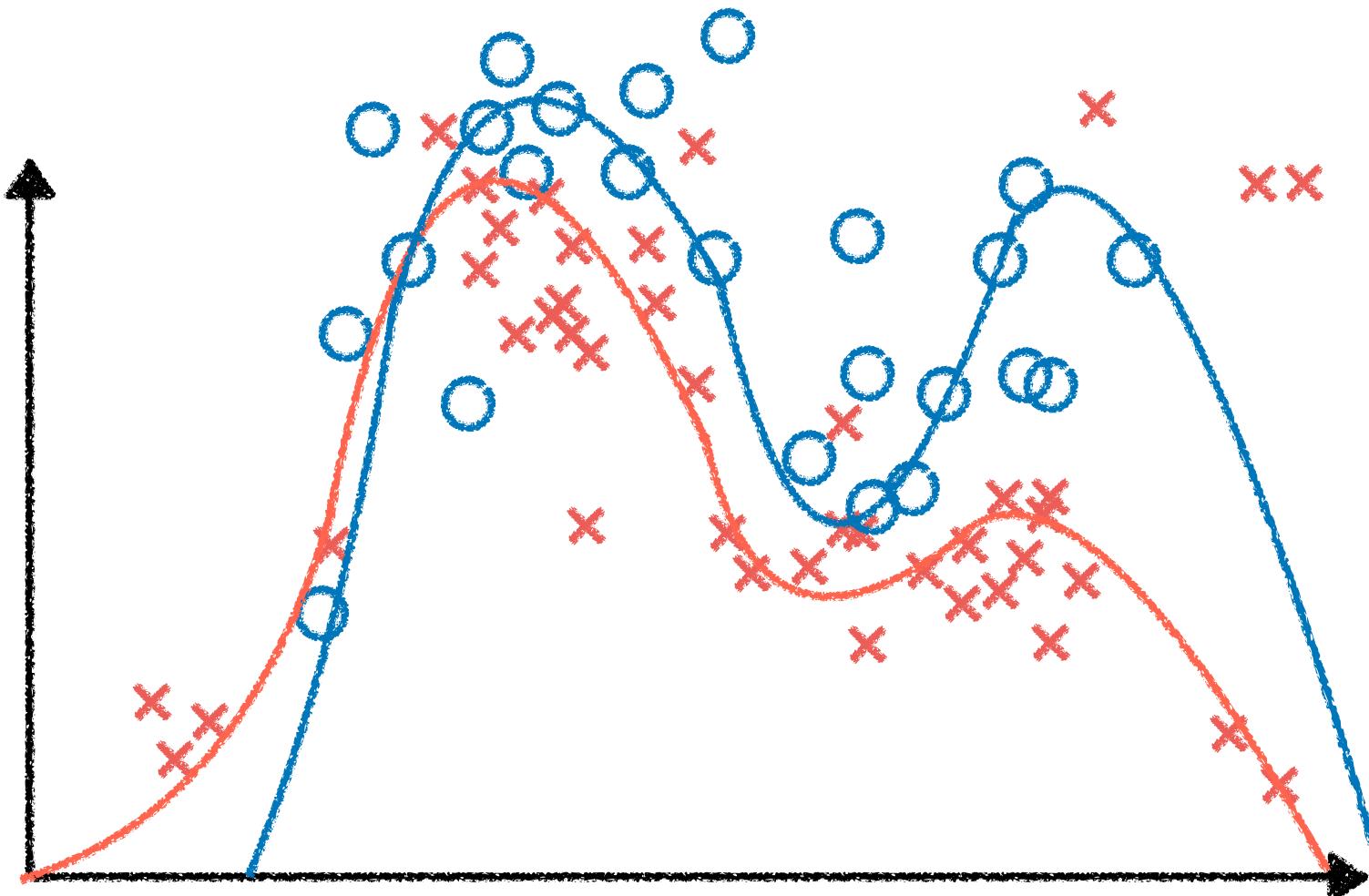
Concept importance



○ Class0

✗ Class1

After building a model



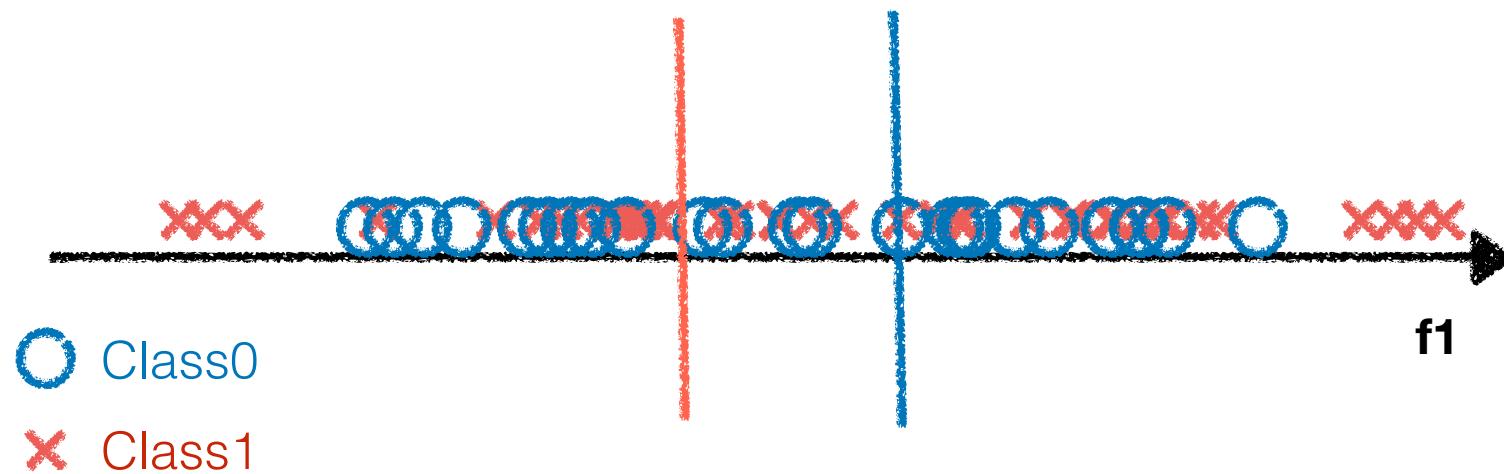
○ Class0

✗ Class1



After building a model

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



After building a model



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

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

To classify this image:

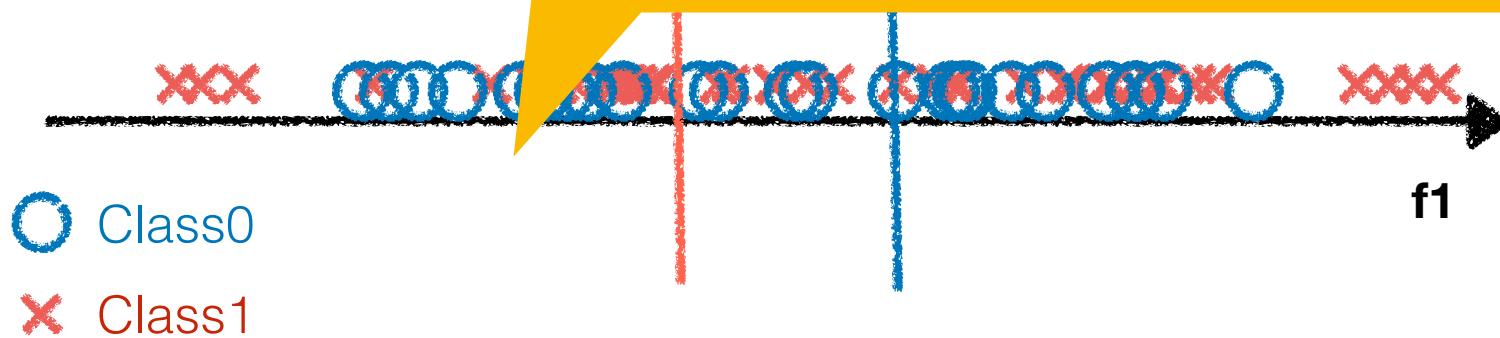


Model found these images most helpful

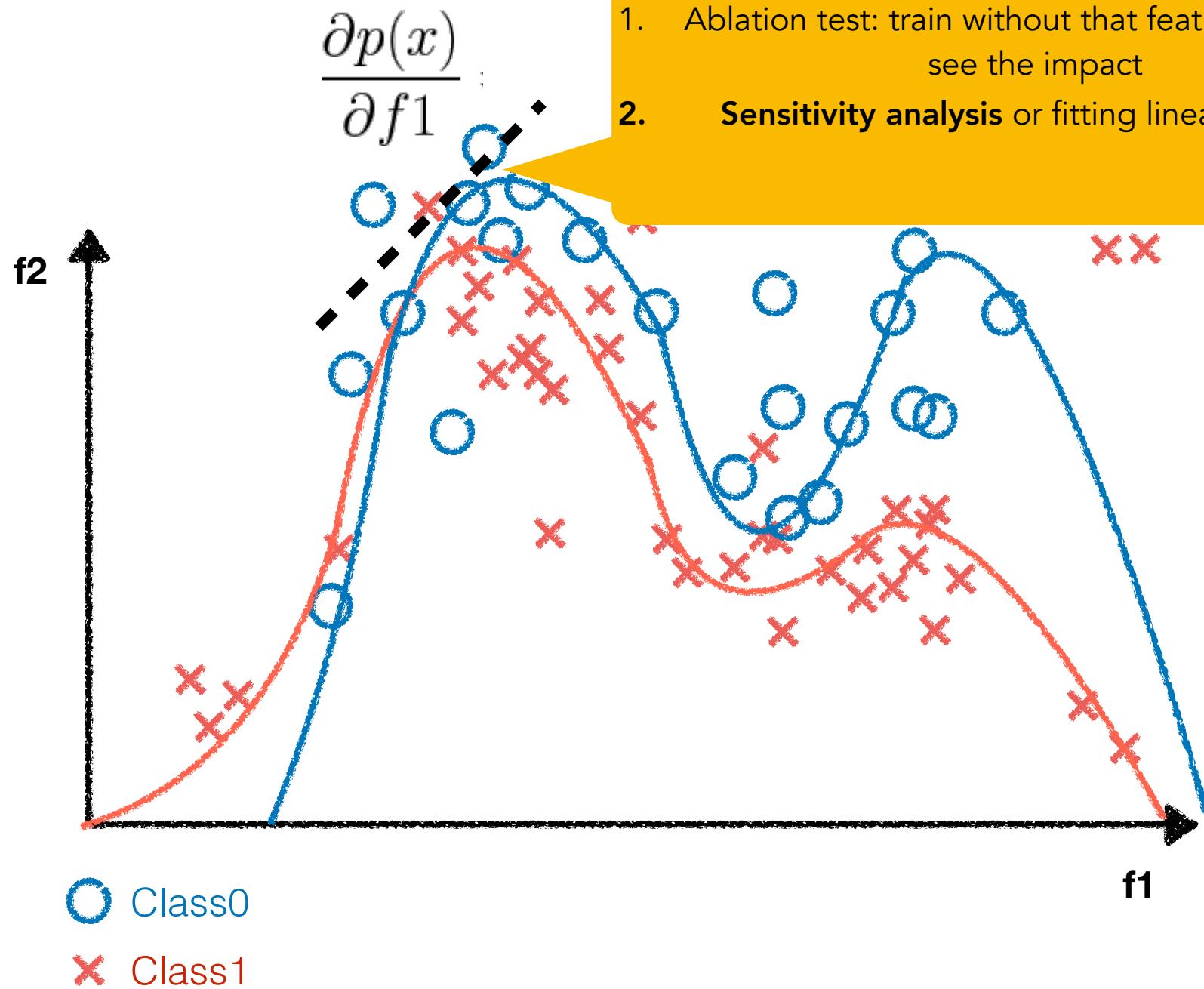
SVM



Inception

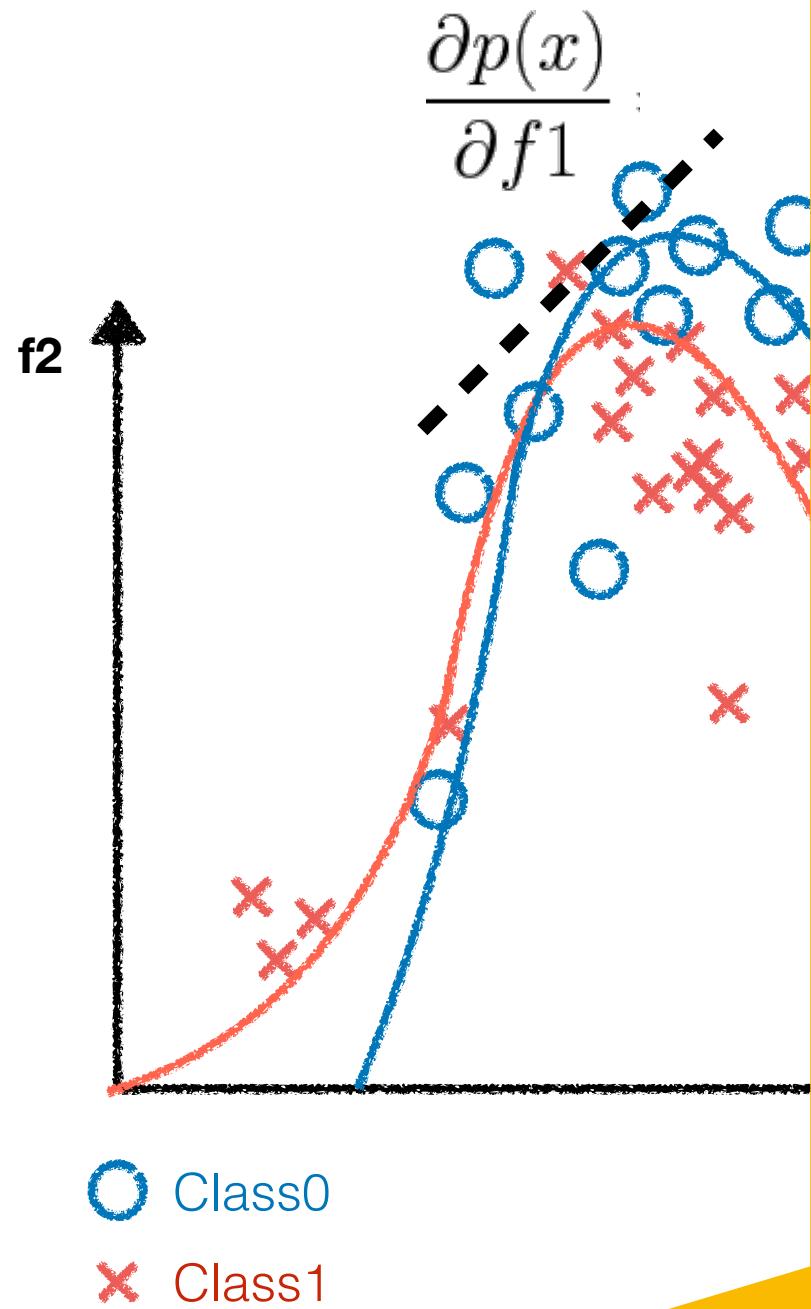


After building a model



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

After building a model

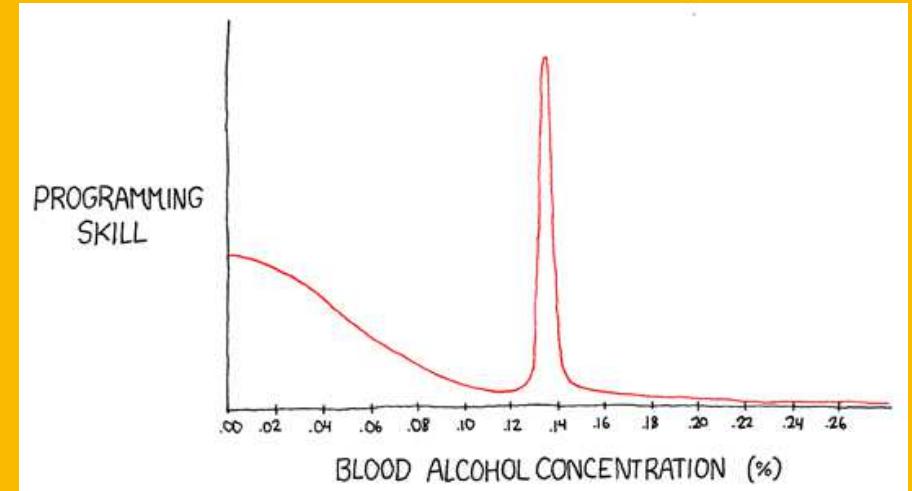


1. Ablation test: train without that feature/data and see the impact

2. **Sensitivity analysis** or fitting linear function

What happened to the output, \hat{y} if we perturb input $x \rightarrow x + \epsilon$

For nonlinear functions $\hat{y} = f(x)$ higher order derivatives will get involved.

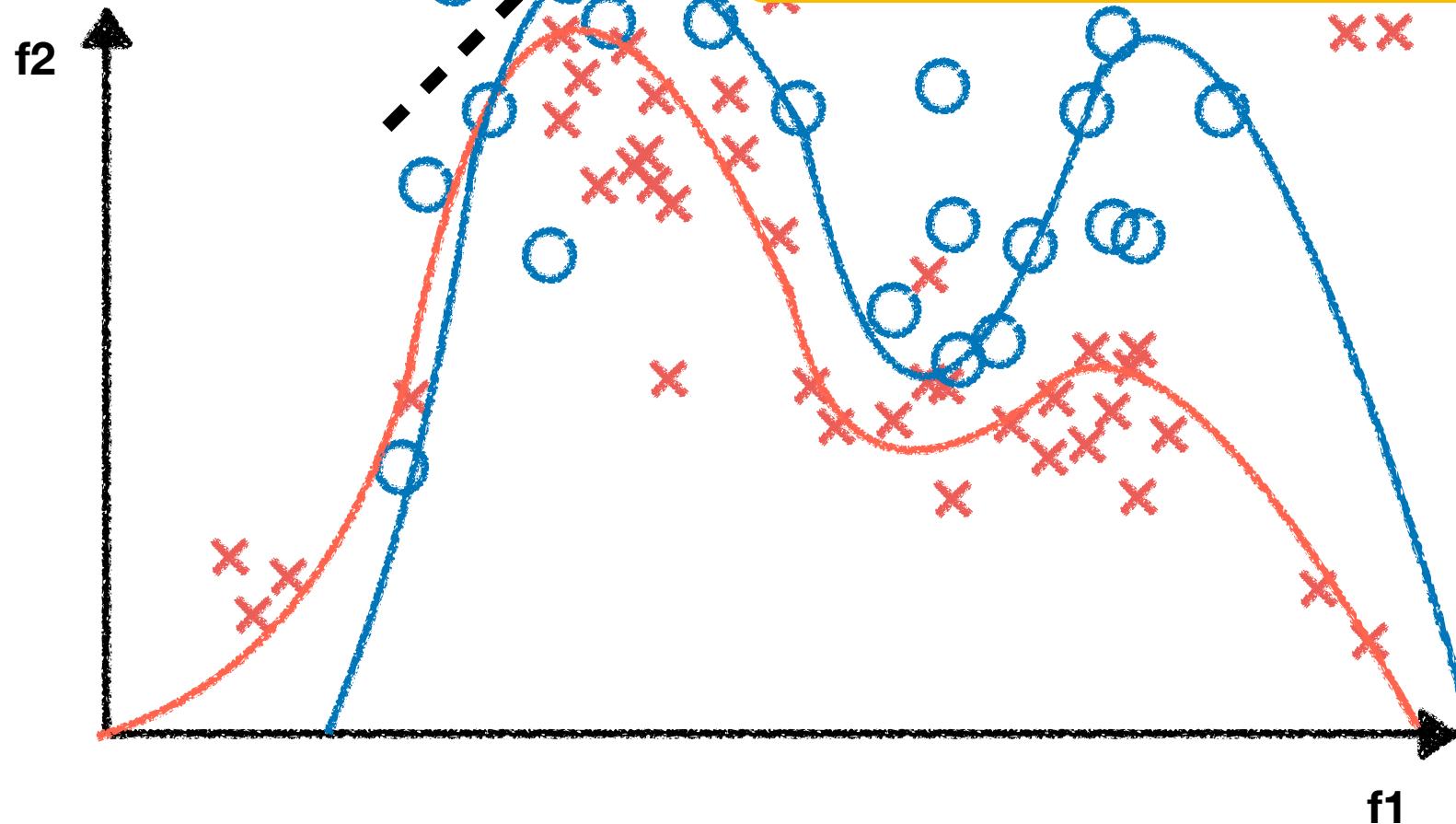


After building a model

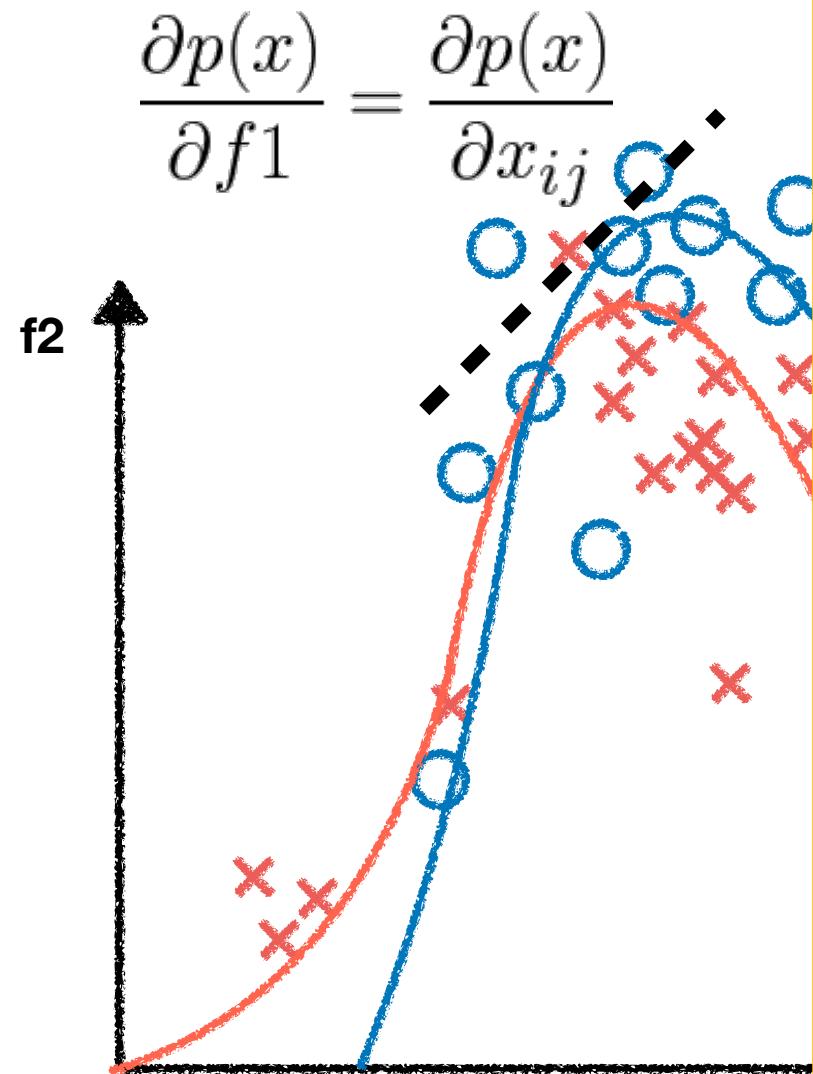


$$\frac{\partial p(x)}{\partial f_1} = \frac{\partial p(x)}{\partial x_{ij}}$$

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



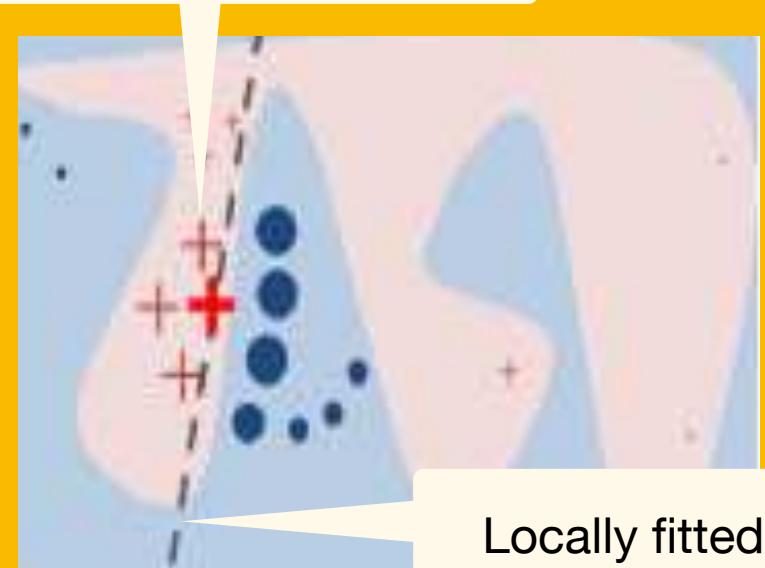
After building a model



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

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

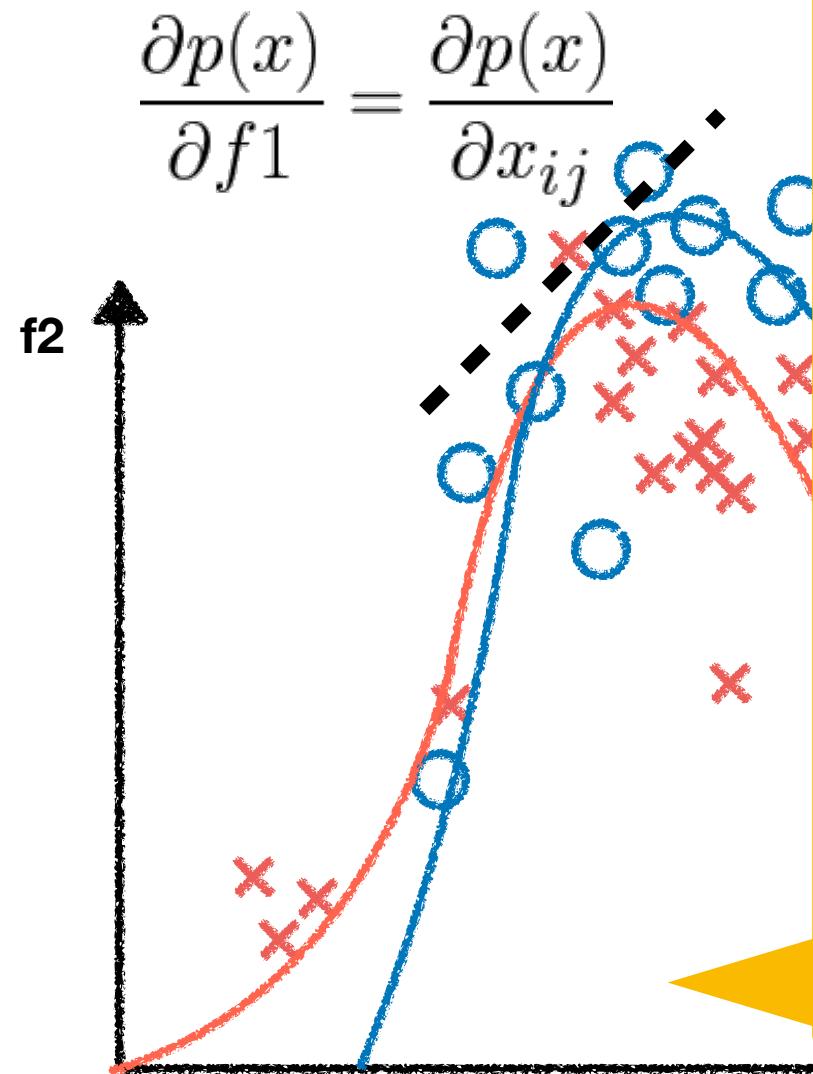
Want local explanation
of the **+** data point



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

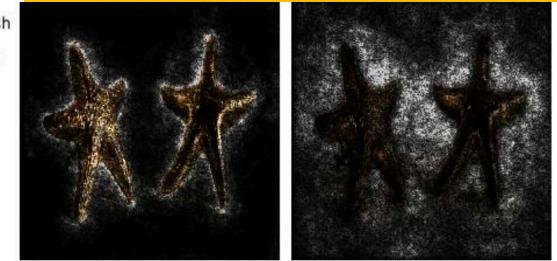


1. Ablation test: train without that feature/data and see the impact
2. **Sensitivity analysis or fitting linear function**

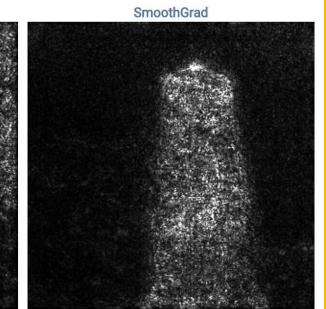
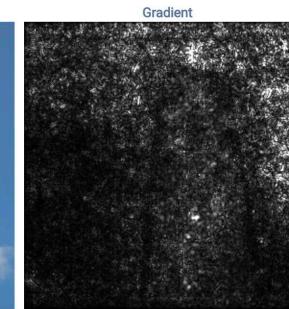
Integrated gradients [Sundararajan et al. 17]



Top label: starfish
Score: 0.999992



SmoothGrad [Smilkov et al. 17]



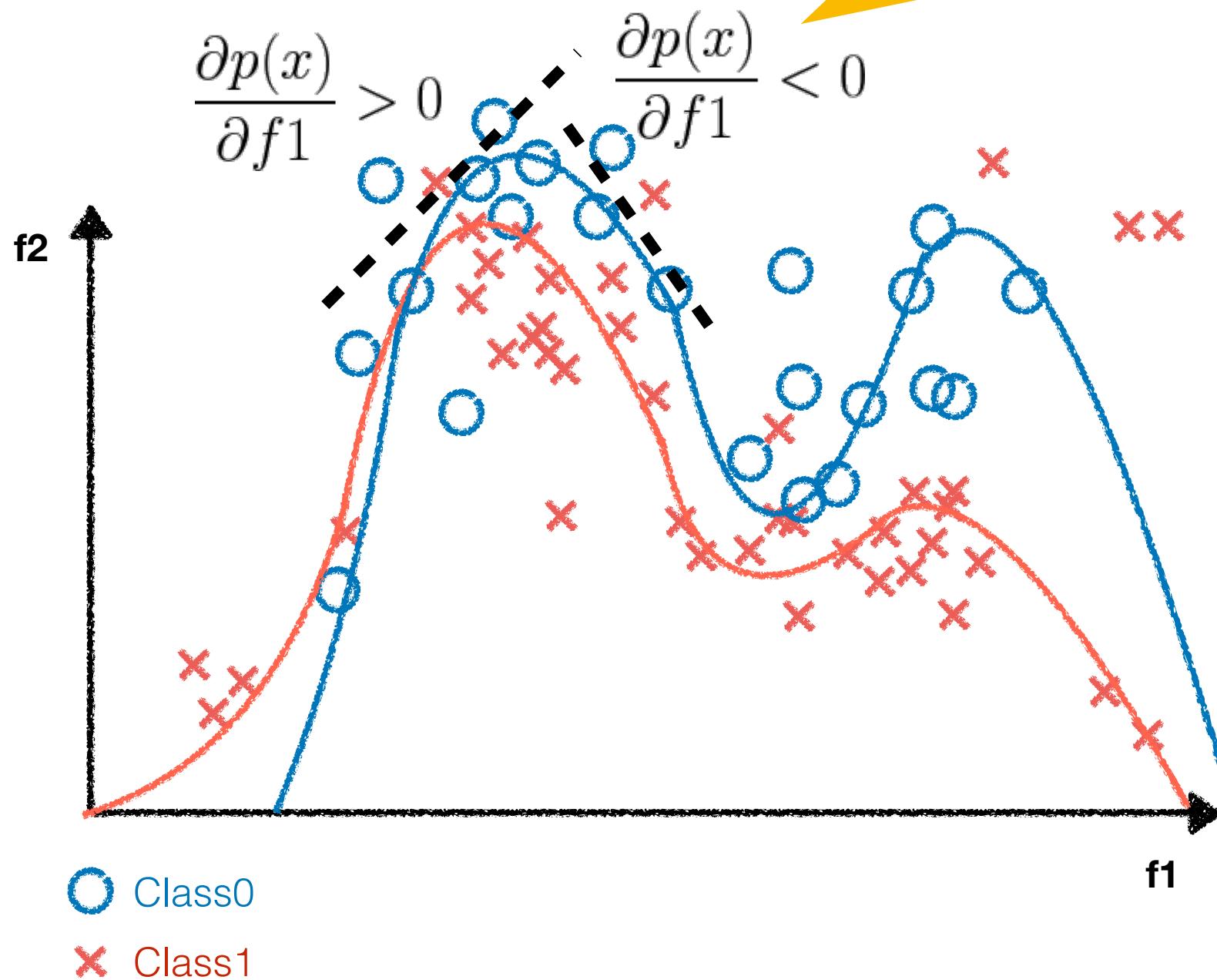
[Zeiler et al. '13] [Selvaraju et al. 16]

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

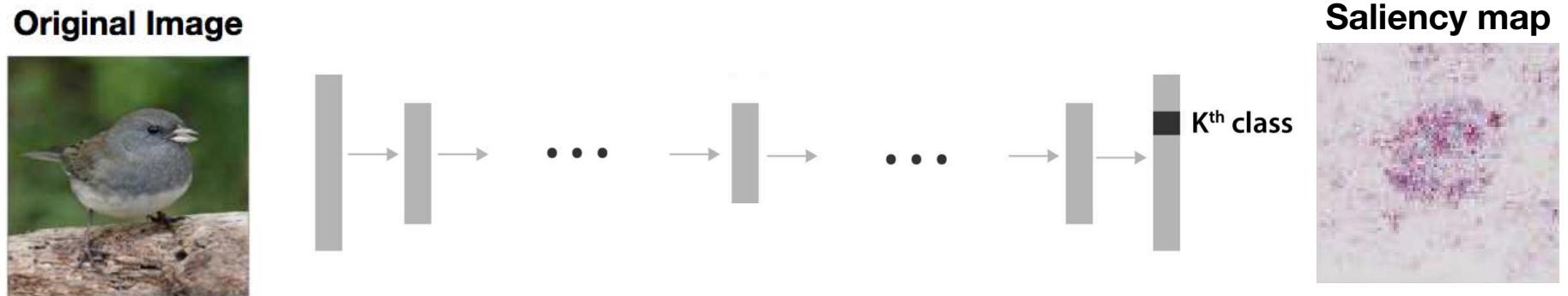
f1

After building a model

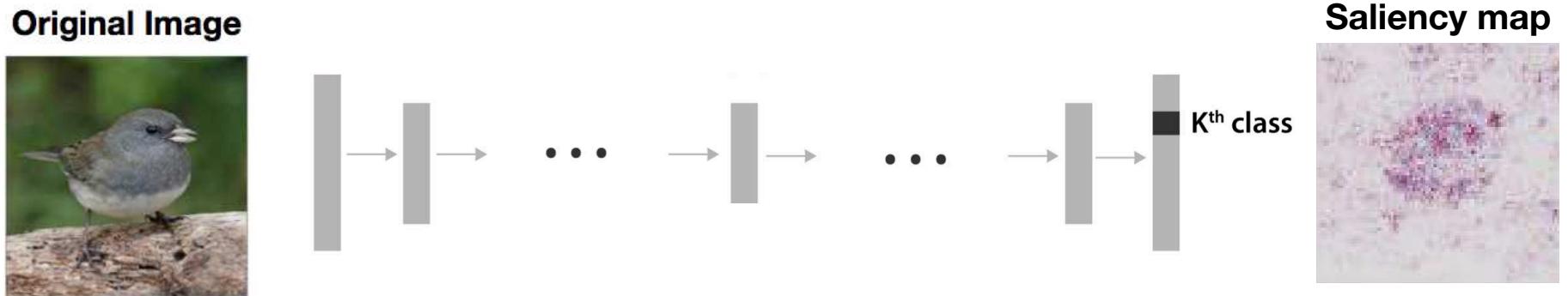
Local explanations



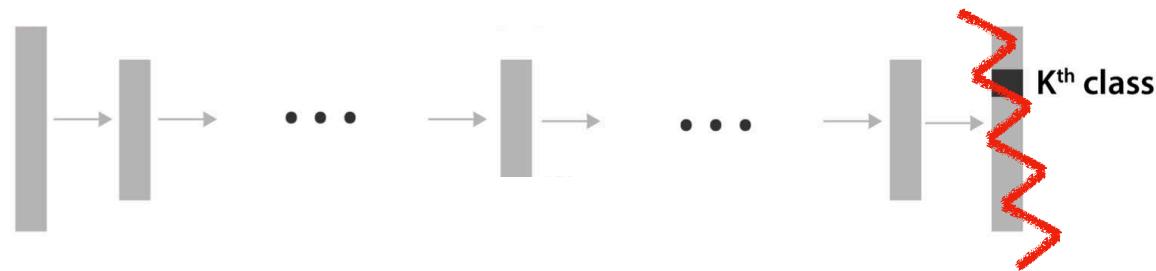
Some confusing behaviors of saliency maps.



Some confusing behaviors of saliency maps.

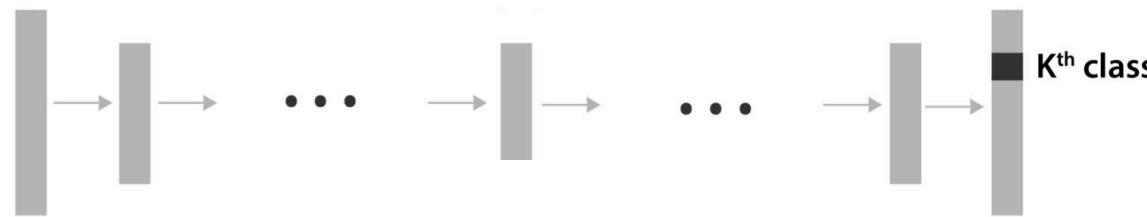


Randomized weights!
Network now makes garbage prediction.

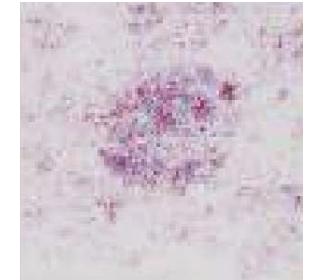


Some confusing behaviors of saliency maps.

Original Image

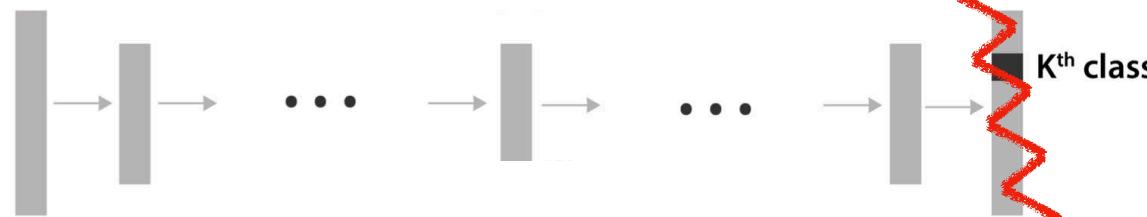


Saliency map



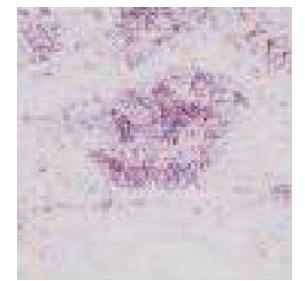
!!!!!!??!?

Original Image

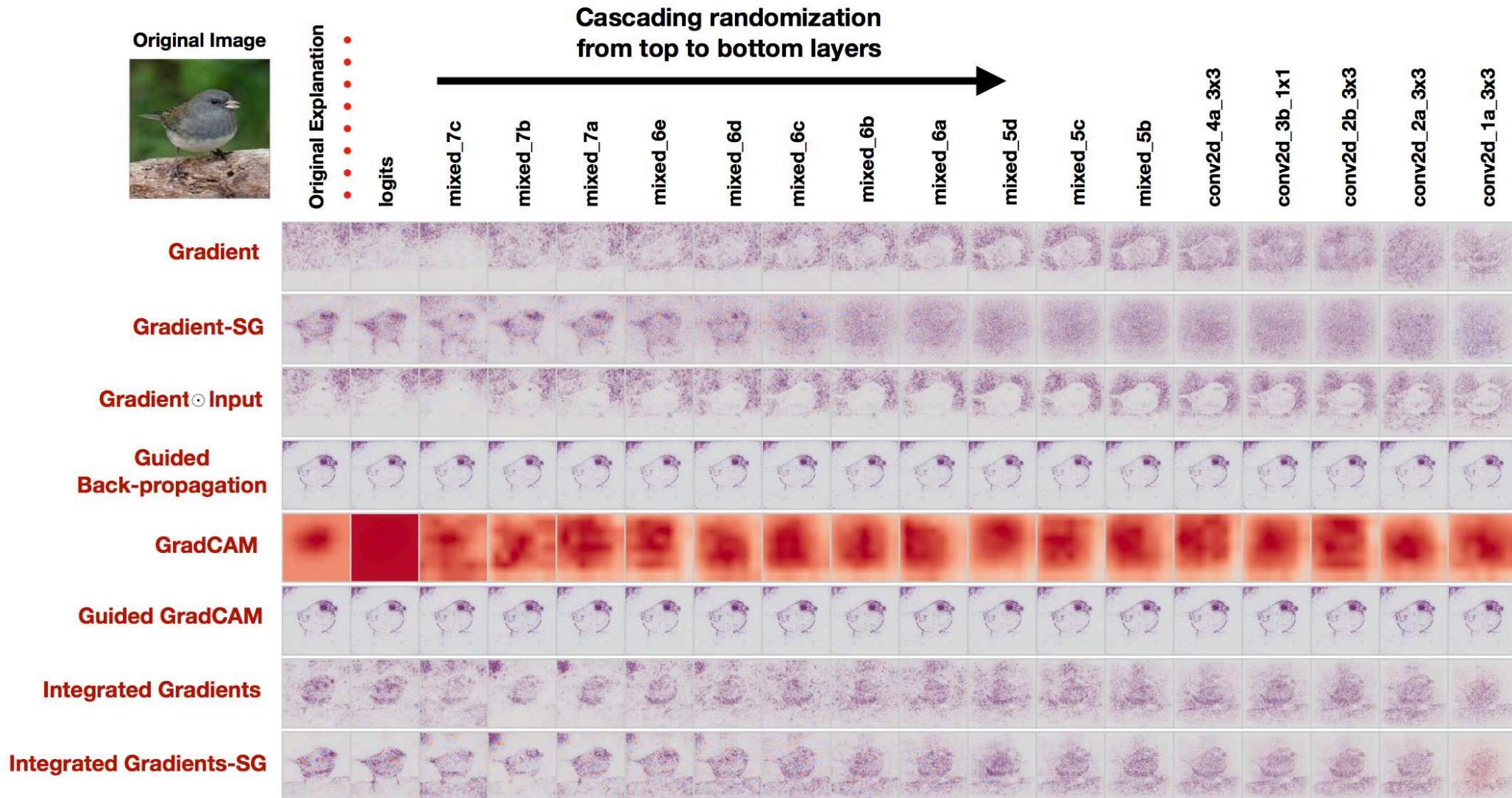


Randomized weights!

Network now makes garbage prediction.



Some saliency maps look similar when we randomize the network.



Which ones are the limitations of sensitivity analysis/gradient-based methods?

- A. It may not be truthful to the model
- B. The model may not allow sensitivity analysis
- C. Two local explanations may conflict
- D. The perturbed x may not be from the data distribution
- E. Interactions of sensitivity (changing two variables) is expensive

Which ones are the limitations of sensitivity analysis/gradient-based methods?

- A. It may not be truthful to the model
- B. The model may not allow sensitivity analysis
- C. Two local explanations may conflict
- D. The perturbed x may not be from the data distribution
- E. Interactions of sensitivity (changing two variables) is expensive



After building a model



Common misunderstanding:
An explanation IS how the model works.



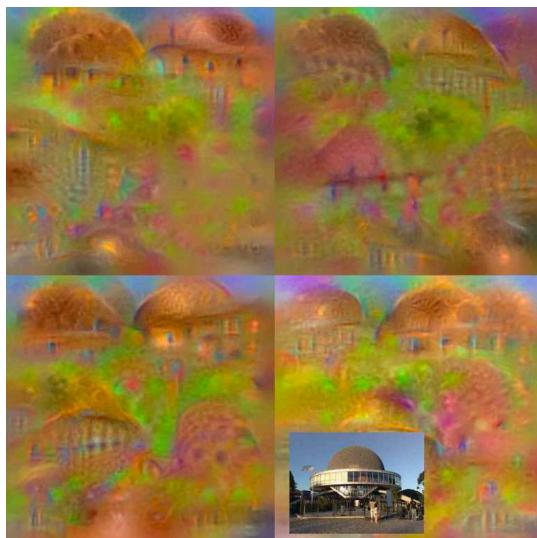
Local explanations may return
contradictory explanations.

After building a model

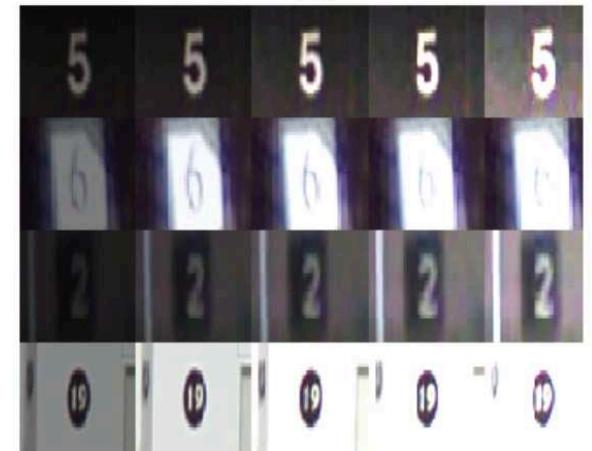


Investigation on hidden layers

[Mahendran and Vedaldi '18]



[Adel et al. '18]

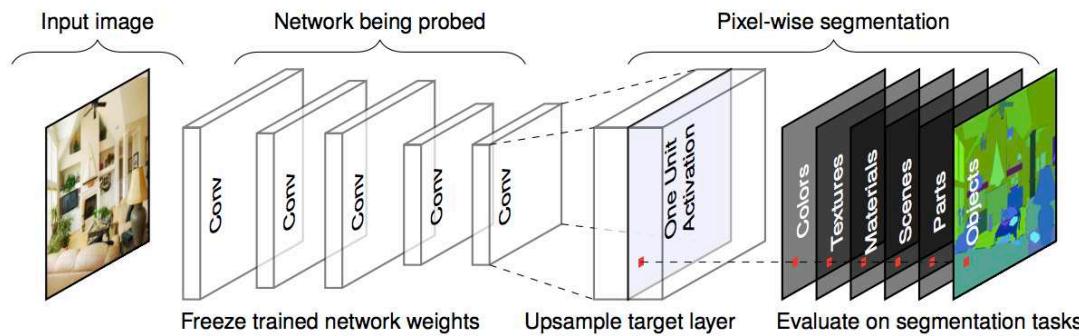


[Mordvintsev et al. '15]



[Bau and Zhou et al. '17]

[Zhou et al. '18]



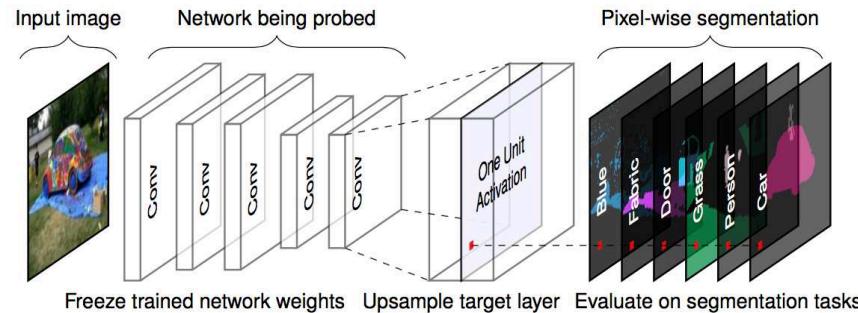
concept-based:
NN learns concepts!

After building a model

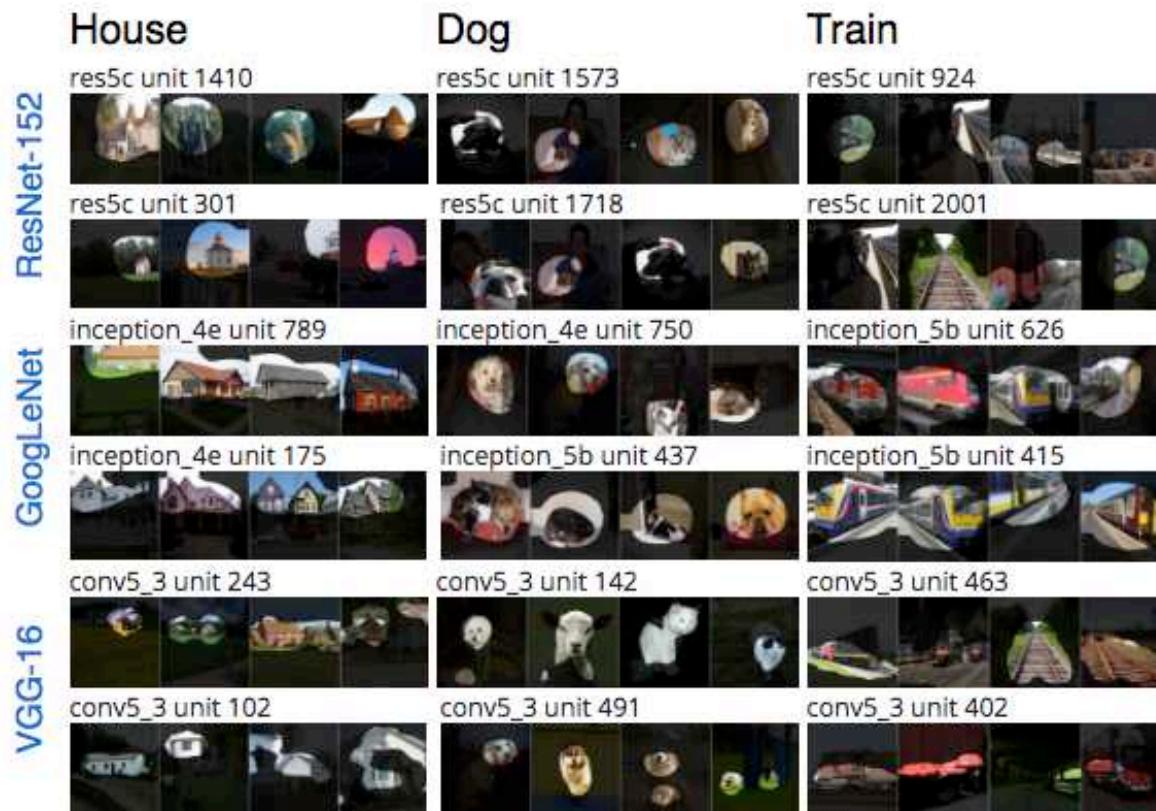


Investigation on hidden layers

[Bau and Zhou et al. '17] [Zhou et al. '18]



concept-based:
NN learns concepts!



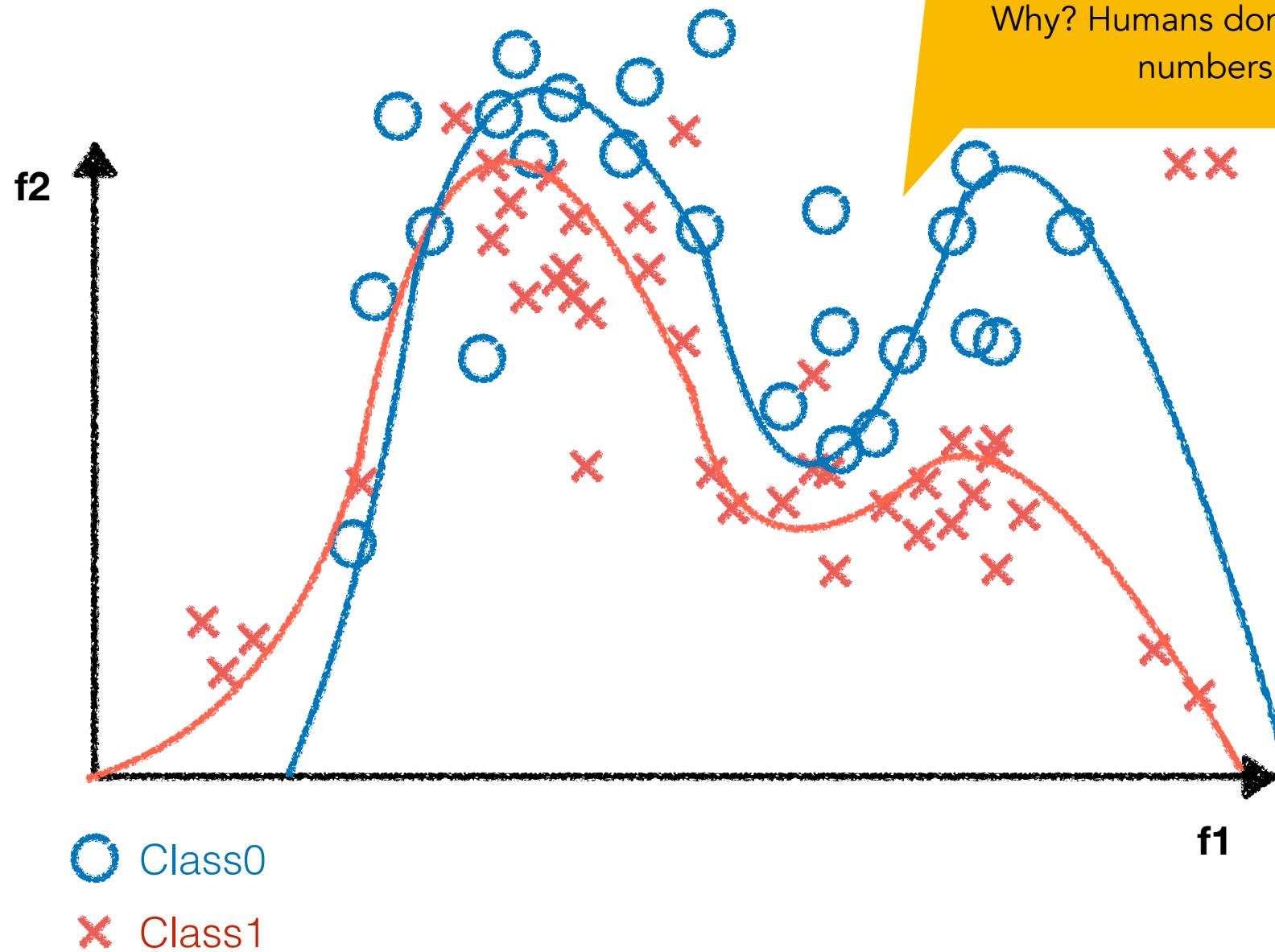
After building a model



$$\frac{\partial p(x)}{\partial \text{concept}}$$

Concept-based:

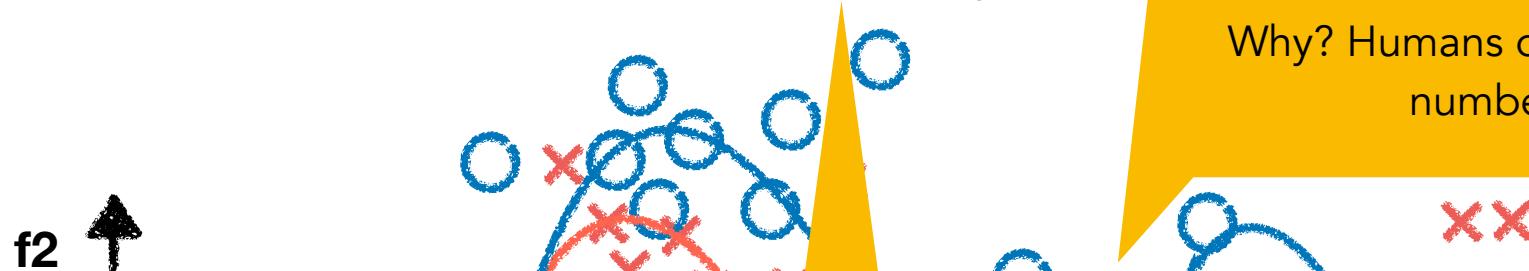
Why? Humans don't think in numbers!



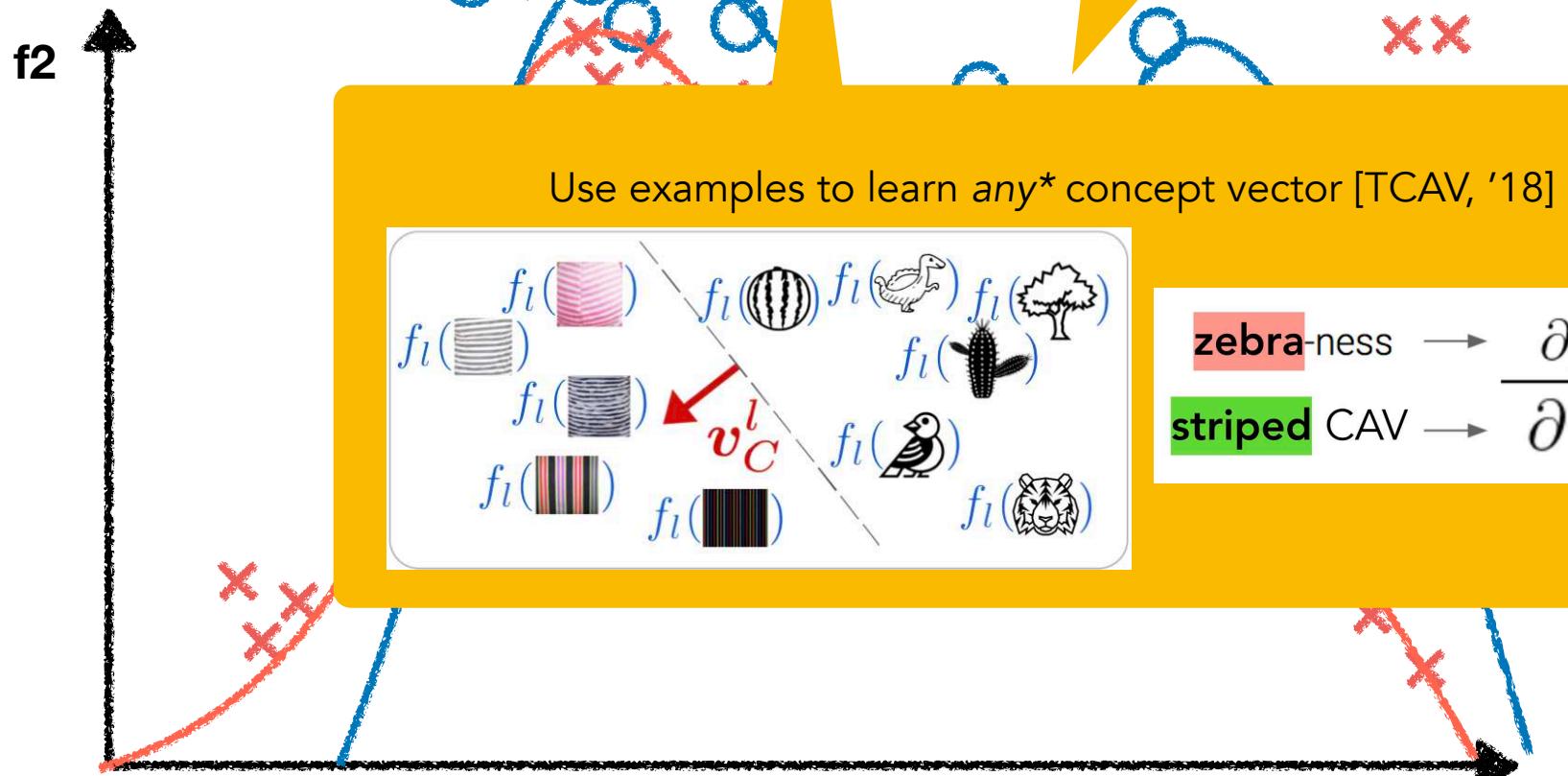
After building a model



$$\frac{\partial p(x)}{\partial \text{concept}}$$



Concept-based:
Why? Humans don't think in numbers!



○ Class0

✗ Class1

*only if it exists; statistical testing can tell you.

TCAV [K, Wattenberg, Gilmer, Cai, Wexler, Viegas, Sayres] ICML18



Defining concept activation vector (CAV)

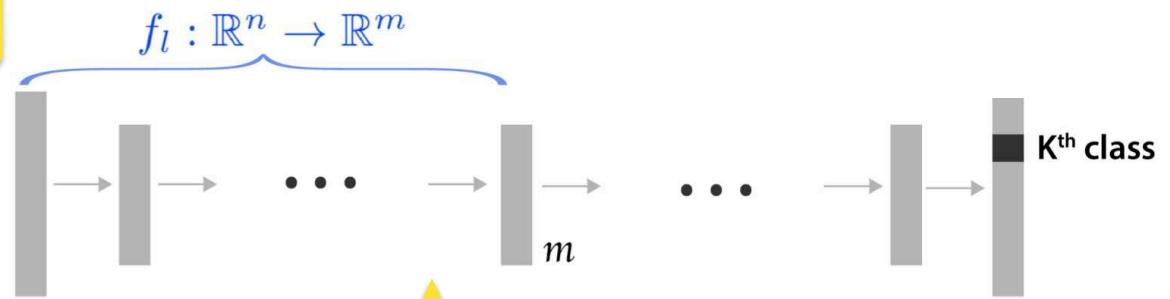
Inputs:

a



Examples of
concepts

Random
images



A trained network under investigation
and
Internal tensors



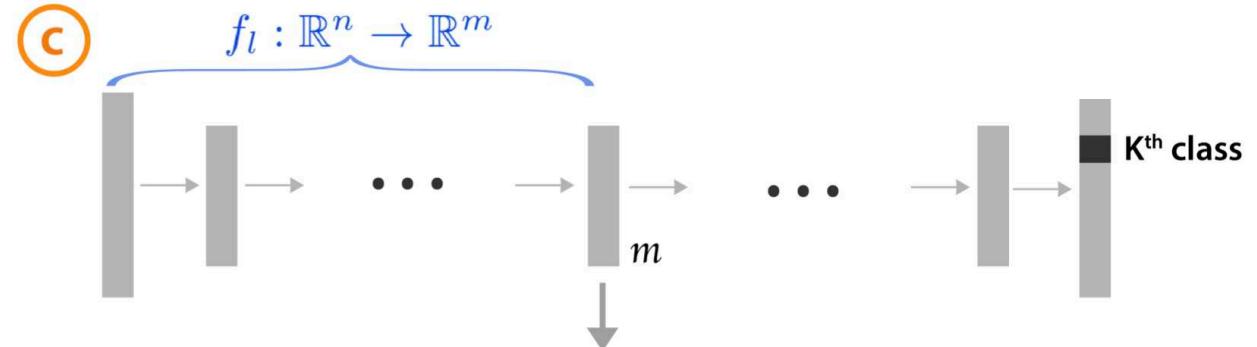
Defining concept activation vector (CAV)

Inputs:

a



c

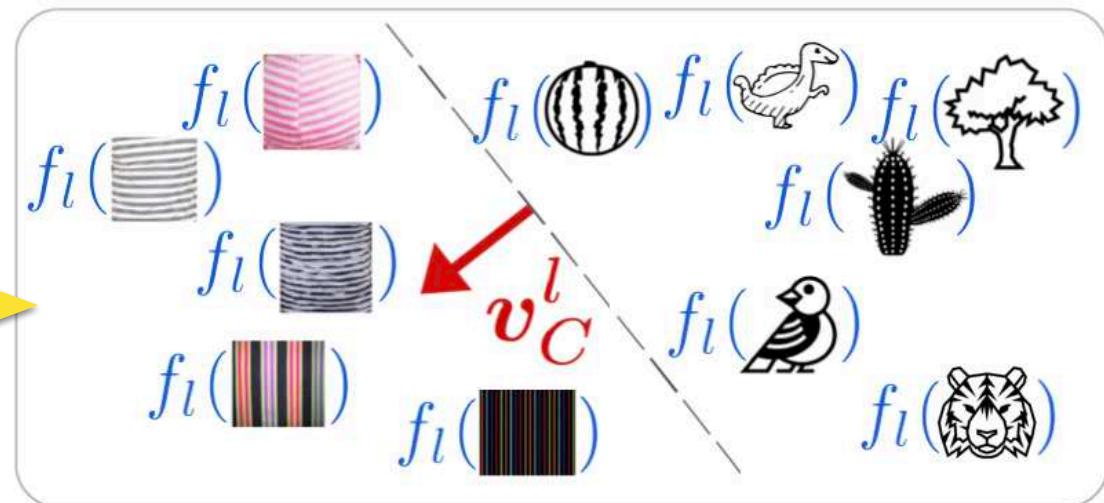


d

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]



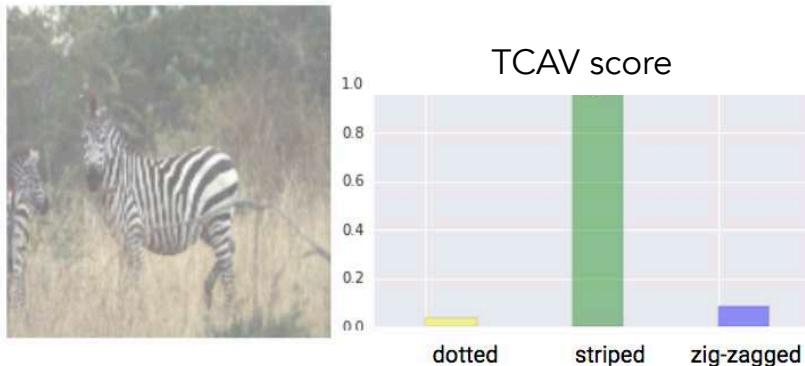
After building a model



TCAV core idea:

Derivative with CAV to get prediction sensitivity

TCAV



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

Directional derivative with CAV

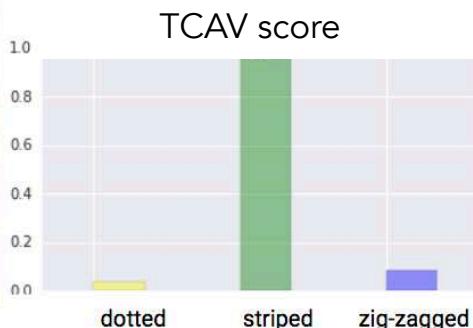
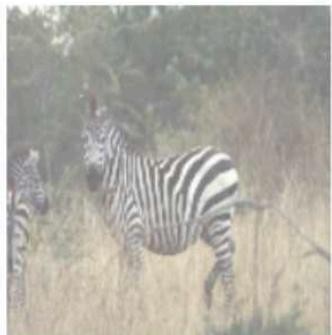
After building a model



TCAV core idea:

Derivative with CAV to get prediction sensitivity

TCAV



$$\begin{aligned} & S_{C,k,l}(\text{zebra}) \\ & S_{C,k,l}(\text{dotted}) \\ & S_{C,k,l}(\text{striped}) \\ & S_{C,k,l}(\text{zig-zagged}) \end{aligned} \quad \left. \right\}$$

zebra-ness $\rightarrow \frac{\partial p(z)}{\partial \mathbf{v}_C^l} = S_{C,k,l}(\mathbf{x})$

striped CAV $\rightarrow \frac{\partial \mathbf{v}_C^l}{\partial \mathbf{v}_C^l} = S_{C,k,l}(\mathbf{x})$

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

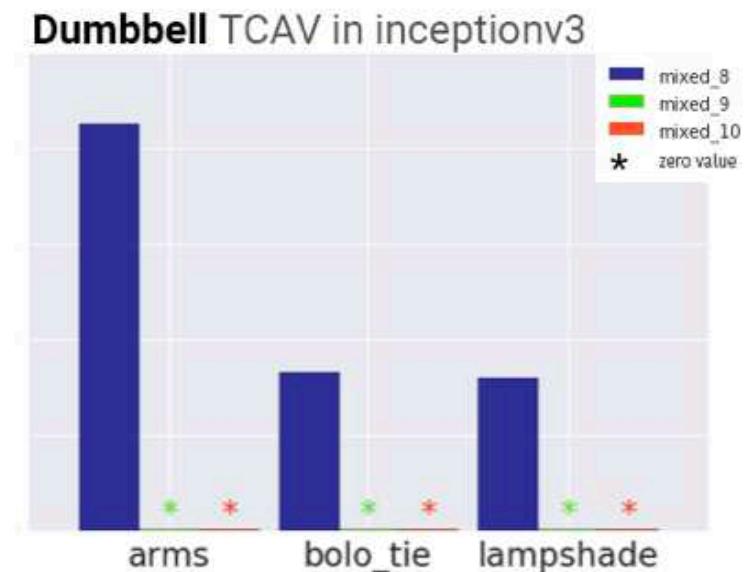
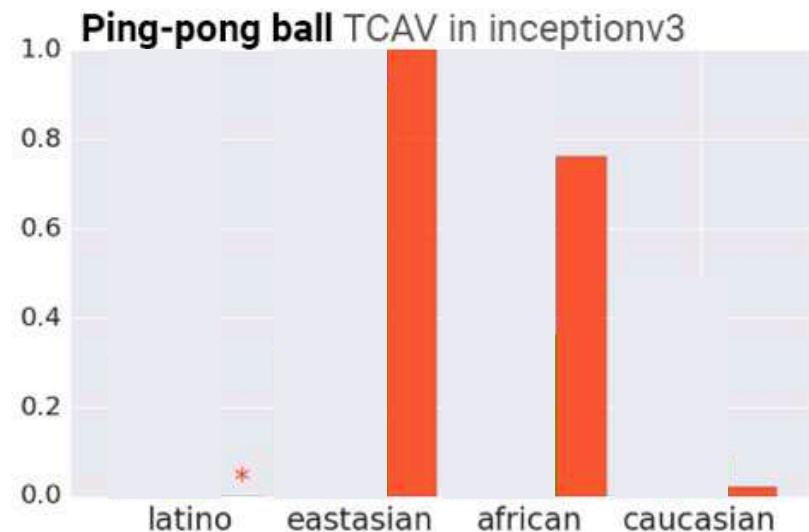
Directional derivative with CAV

After building a model



TCAV for widely used image prediction models

Quantitative confirmation to previously qualitative findings
[Stock & Cisse, 2017]
[Mordvintsev et al. '15]



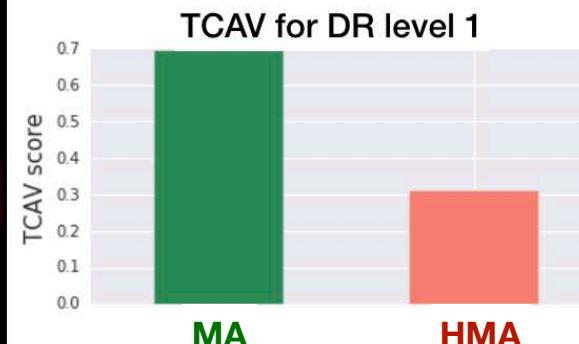
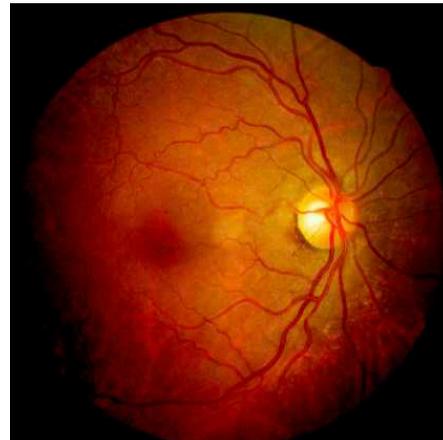
After building a model



TCAV for Medical application: Diabetic Retinopathy

DR level 1

Med

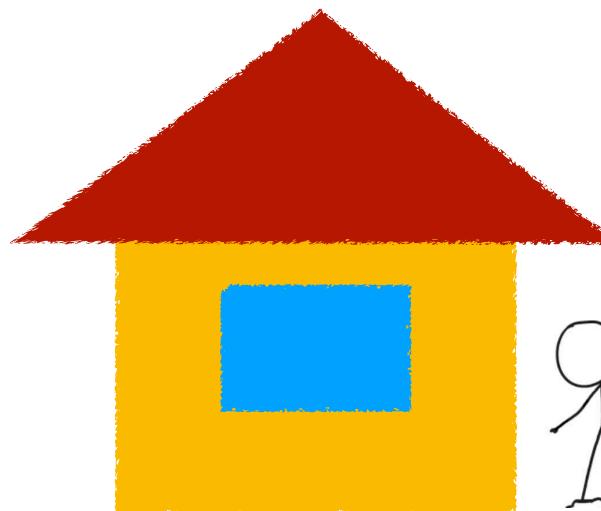


TCAV shows the model is **inconsistent** with doctor's knowledge for classes when model is less accurate

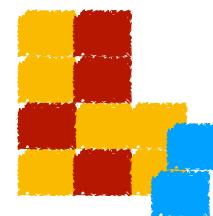
Green: domain expert's label on concepts belong to the level

Red: domain expert's label on concepts does not belong to the level

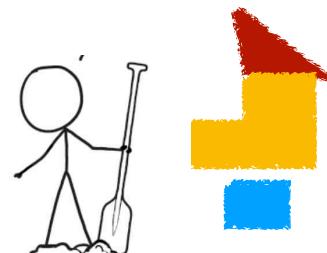
Types of interpretability methods



My ML



Before building
any model



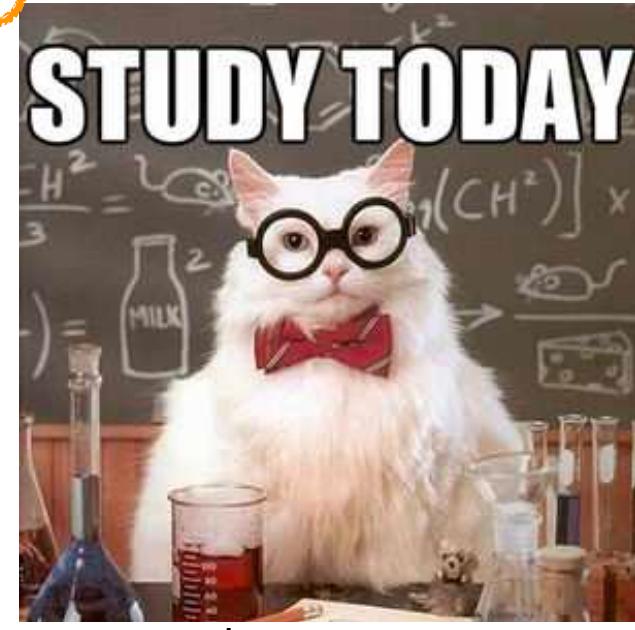
Building
a new model



After
building a model

Agenda

- **When** and **why** interpretability
- **Overview** of interpretability methods.
- How to **Evaluate** interpretability methods.





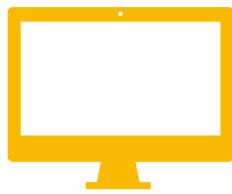
One way to evaluation interpretability...

“You know it when you see it”





Spectrum of evaluation in machines learning



Machine Learning

Function-based

a variety of synthetic
and standard
benchmarks
e.g., UCI datasets,
imagenet



Application-based

Backing up claims
e.g., performance on a
cool medical dataset,
winning Go games



Spectrum of evaluation in interpretable machine learning

Interpretable Machine Learning



Function-based

How sparse are
the features?

Does it look
reasonable?



Application-based

How much did
we improve patient
outcomes?

Do scientists find
the explanations
useful?

Quantitative Qualitative



Spectrum of evaluation in interpretable machine learning

Interpretable Machine Learning

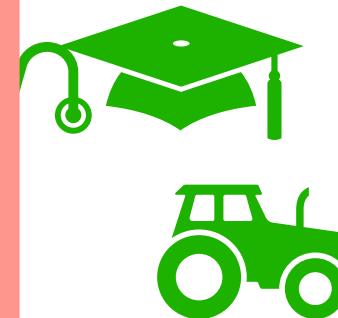


Function-based

How sparse are
the features?

Does it look
reasonable?

It's easy to formalize,
optimize, and evaluate... but
may not solve a real need.



Application-based

How much did
we improve patient
outcomes?

Do scientists find
the explanations
useful?

Quantitative Qualitative



Spectrum of evaluation in interpretable machine learning

Interpretable Machine Learning



Function-based

How sparse are
the features?

Does it look
reasonable?



Application-based

How much did
we improve patient
outcomes?

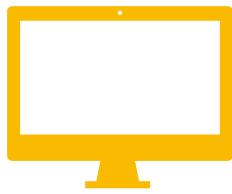
Do scientists find
the explanations
useful?

Quantitative Qualitative



Spectrum of evaluation in interpretable machine learning

Interpretable Machine Learning



Function-based

How sparse are
the features?

Does it look
reasonable?

It's real evaluation, but it's
costly and hard to compare
work A to B.



Application-based

How much did
we improve patient
outcomes?

Do scientists find
the explanations
useful?

Quantitative Qualitative



Spectrum of evaluation in interpretable machine learning



Function-based

How sparse are
the features?

Does it look
reasonable?

cognition-based

What factor should
change to change
the outcome?

What are the
discriminative
features?

Application-based

How much did
we improve patient
outcomes?

Do scientists find
the explanations
useful?

Quantitative Qualitative

Low cost

High cost

Low validity

High validity



Spectrum of evaluation in interpretable machine learning



Factor-based

Prediction task: 1. Show explanations to humans.
2. Ask humans what would the machine do.

Q. Which group does this new data belong to?



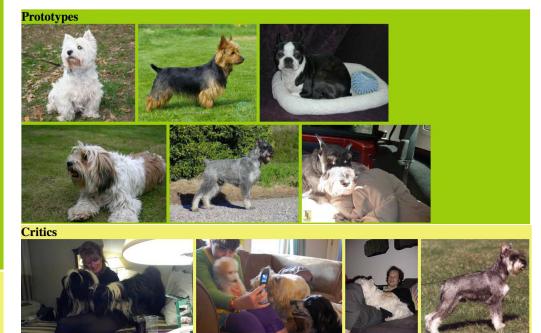
- Group A
- Group B

Group A



110

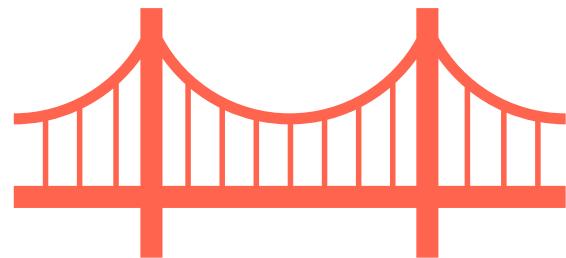
Group B



[K. 16]



Spectrum of evaluation in interpretable machine learning



Factor-based

Validation task: 1. Show explanations to humans.
2. Ask humans whether the machine's answer was correct.

Q. Machine thinks this image belongs to Group B. Is this correct?



- Yes
- No



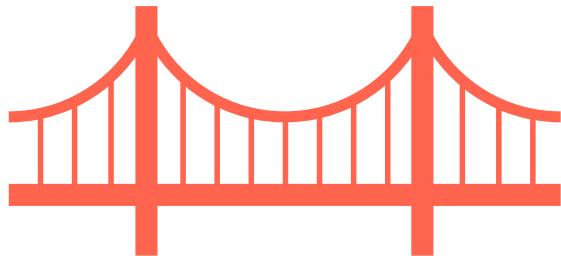
11/17



[K. 16]



Spectrum of evaluation in interpretable machine learning



Factor-based

Formulate an experiment where you have the **ground-truth** when you can.



An example of ground-truth experiment setup in TCAV



Goal: find out what was
important for a prediction



An example of ground-truth experiment setup in TCAV

caption
concept



image
concept

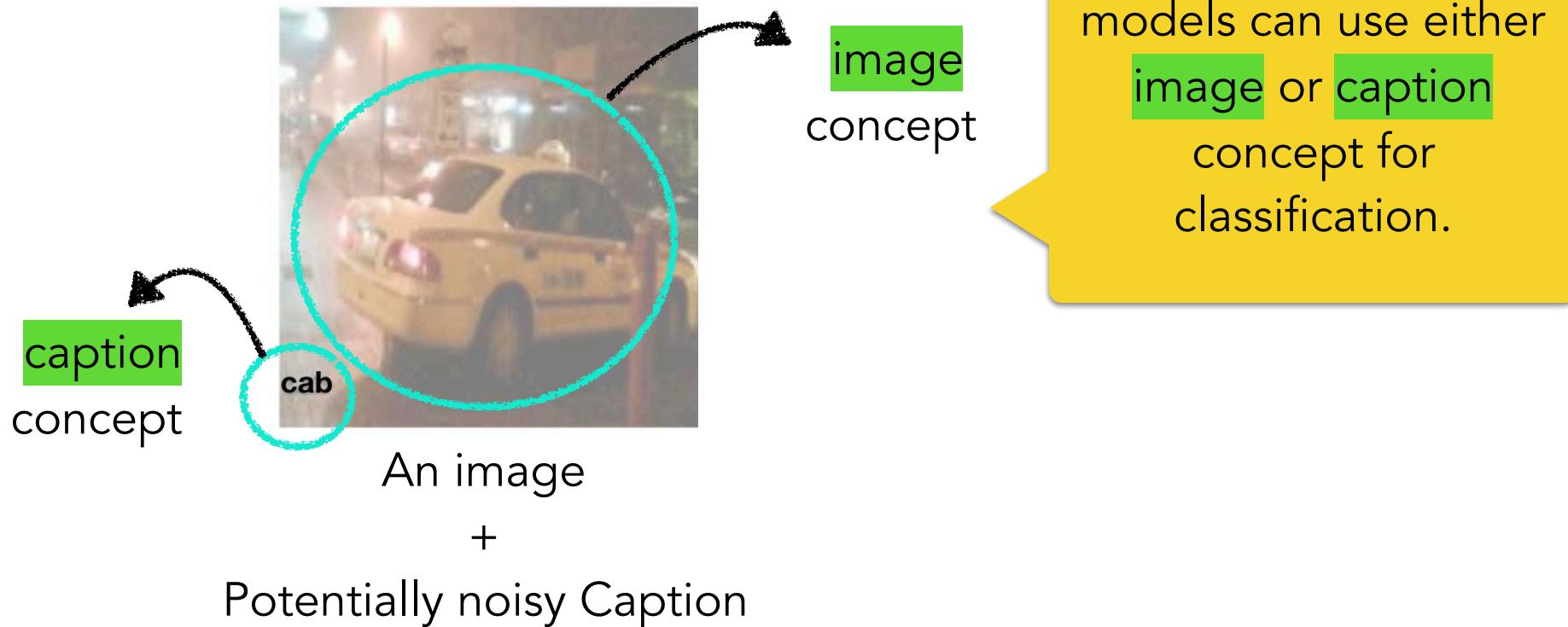
An image

+

Potentially noisy Caption

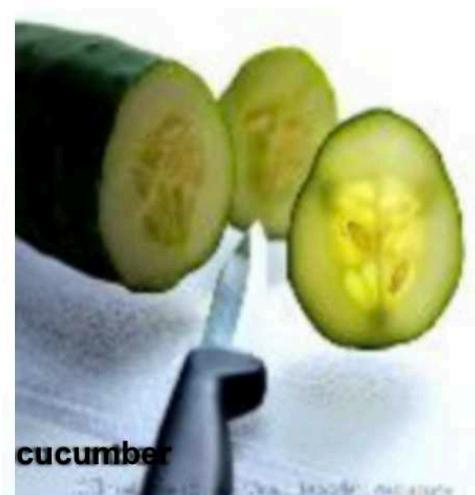


An example of ground-truth experiment setup in TCAV





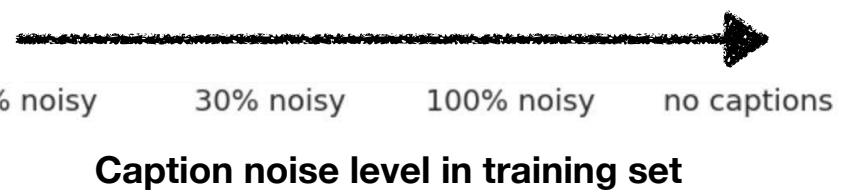
An example of ground-truth experiment setup in TCAV



Image

+

Potentially noisy Caption





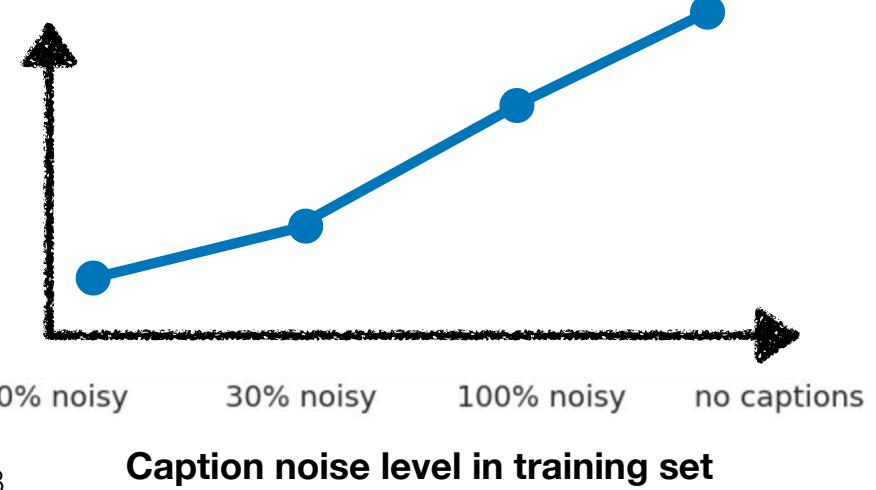
An example of ground-truth experiment setup in TCAV



models can use either image or caption concept for classification.



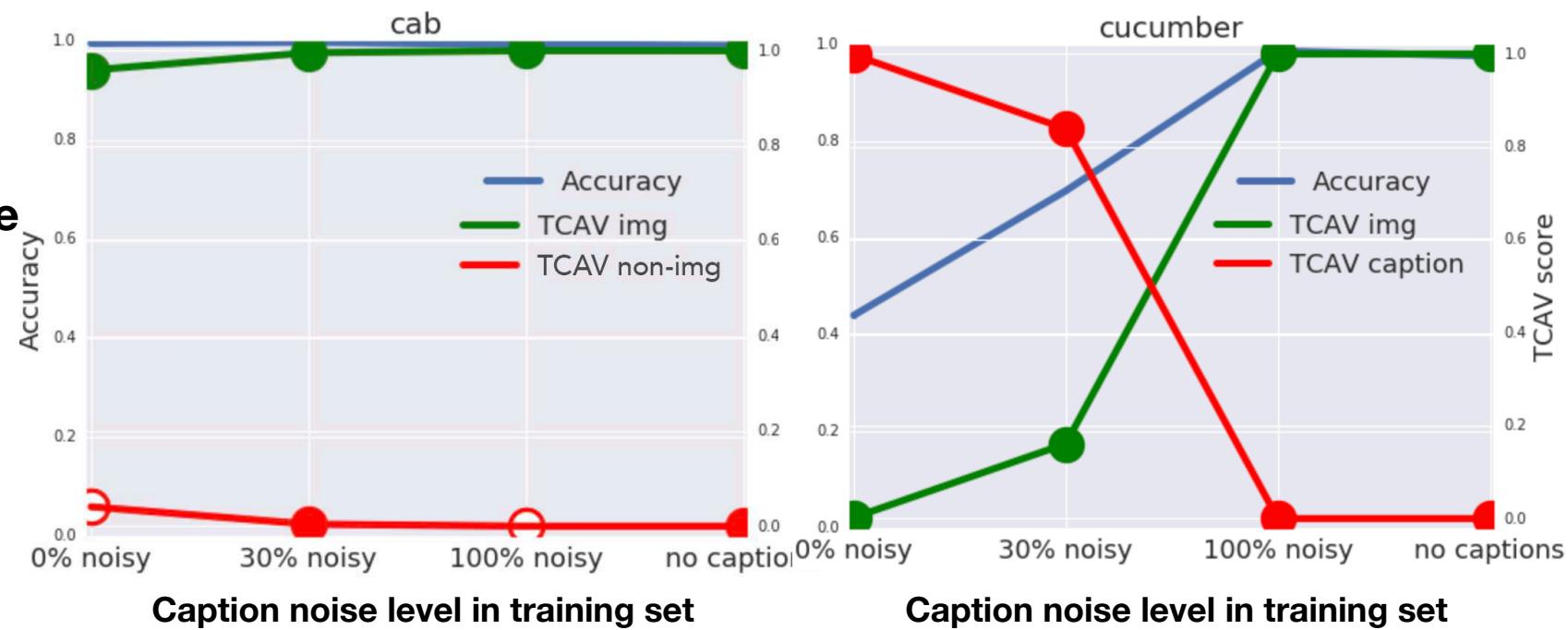
Test accuracy with no caption image = Importance of image concept





An example of ground-truth experiment setup in TCAV

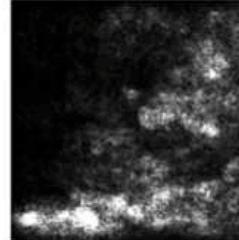
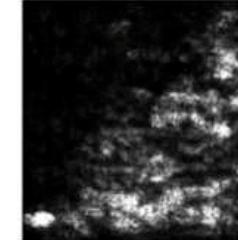
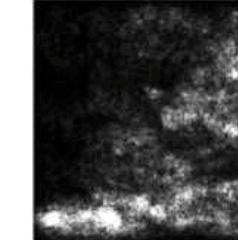
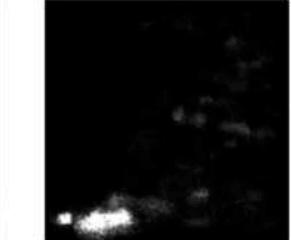
**Test accuracy
with
no caption image**





An example of ground-truth experiment setup in TCAV

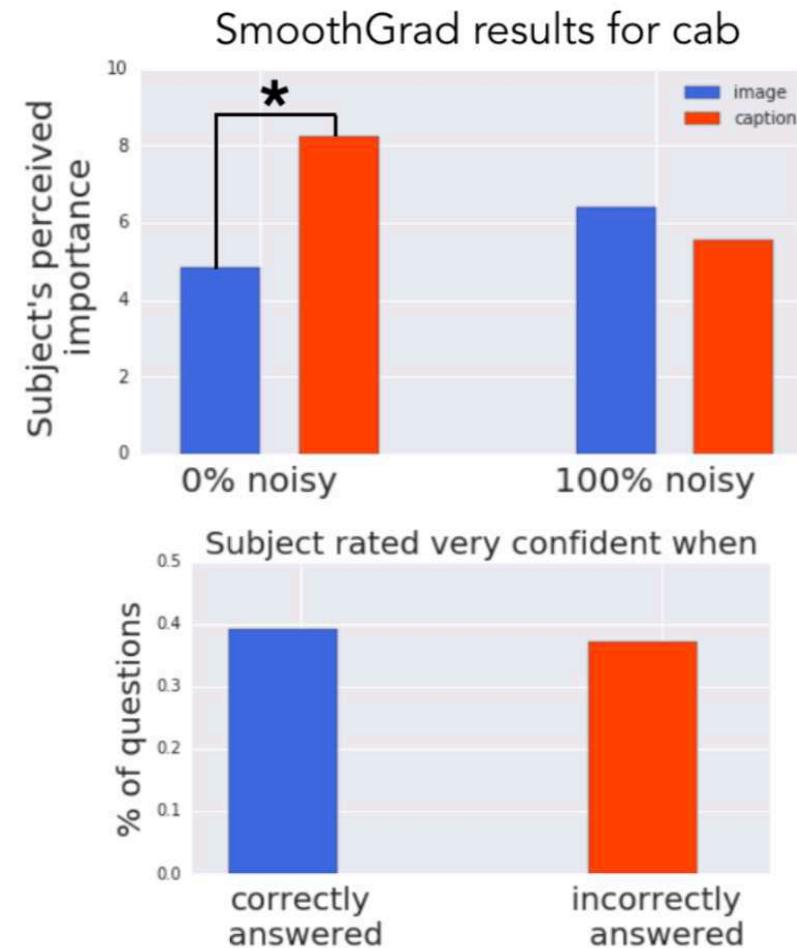
Cool, cool.
Can saliency maps do it too?

Ground truth	Input image (with caption)	Vanilla gradient	Guided backprop	Integrated gradient	Smoothgrad
Image concept Cab					



Human subject experiment: Can saliency maps communicate the same information?

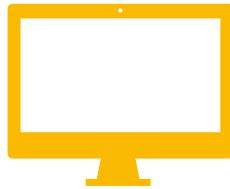
- Correctly communicated 52% (50% random)
- More than 50% no significant consensus among turkers
- Humans are **very** confident even when they are wrong.



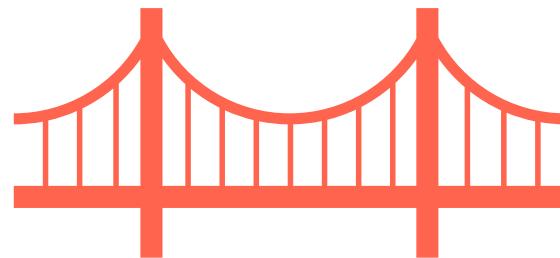
50 turkers, shown 3 classes and 2 saliency maps



Evaluating interpretability methods



Function-based



Factor-based



Application-based

- Decide which level of evaluation is needed.
- Do **human experiments** when you can.
- **Formulate an experiment** where you have the **ground-truth** when you can.

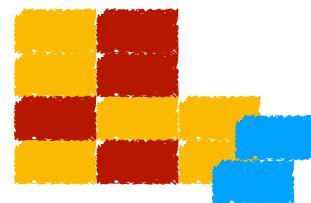
Conclusion

Why and when?

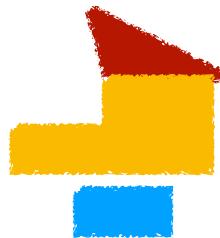
Fundamental underspecification

How?

Before building
any model



Building
a new model



After
building a model



How to evaluate?

Human experiment and ground-truth experiment

Google's Interpretability best practices:

<https://ai.google/education/responsible-ai-practices>



<https://imgflip.com>

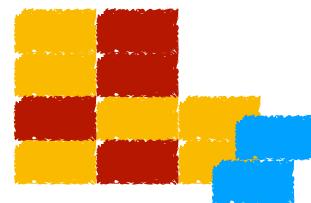
Conclusion

Why and when?

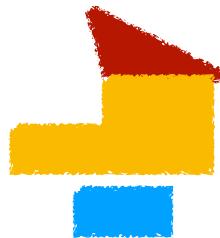
Fundamental underspecification

How?

Before building
any model



Building
a new model



After
building a model



How to evaluate?

Human experiment and ground-truth experiment

Google's Interpretability best practices:

<https://ai.google/education/responsible-ai-practices>