Interpretable Machine Learning: The fuss, the concrete and the questions







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

Been Kim Google Brain



with Finale Doshi-Velez, Harvard university Tutorial, ICML 2017



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Contents of this tutorial is largely based on our paper Towards A Rigorous Science of Interpretable Machine Learning https://arxiv.org/abs/1702.08608



https://xkcd.com/



https://xkcd.com/

Potentially serious consequences? Yes.

- Cost-effective Health Care (CEHC) built models to predict probability of death for patients [Cooper et al. 97]
 - HasAsthma(x) \Rightarrow LowerRisk for pneumonia (x)



Example borrowed from [Caruana et al. '15]

Potentially serious consequences? Yes.

Cost-effective Health Care (CEHC) by the second description of death for patients [Coc What else did it learn?!



Example borrowed from [Caruana et al. '15]

ML community is responding



Year

Why now?

Widespread data collect + vast computation resources

→ ML everywhere!



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 an input, and you do:



Input = [Owl, ICML]

Animal



 I will show you a decision tree. Follow the Input = [Kangaroo, ICML] right path given an input, and you do:



Sample decision tree #1 Input: [ICML, 2017, Australia, Kangaroo, Sunny]



Sample decision tree #2

Input: [ICML, 2017, Australia, Kangaroo, Sunny]



Sample decision tree #3 Input: [ICML, 2017, Australia, Kangaroo, Sunny]



Sample decision tree #3 Input: [ICML, 2017, Australia, Kangaroo, Sunny]

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

1990

Clap! Stomp

nal =

Can you guess which feature (e.g., animal, year ,conference) was more 'important' (i.e., used in more number of examples) given a decision tree given lots of data?

Left

Year



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
Else if (sunny and cold)	then
Else if (wet and weekday)	then
Else if (at ICML)	then
Else if (cloudy and hot)	then
Else if (snowing)	then
Else if (New Dr. Who)	then
Else if (paper deadline)	then
Else if (sick and bored)	then
Else if (tired)	then
Else if (advisor might come)	then
Else if (code running)	then
Else	then

n	go swim
n	go ski
n	go work
n	attend tutorial
n	go swim
n	go ski
n	watch TV
n	go work
n	watch TV
n	watch TV
n	go work
n	watch TV
n	go work

Maybe rule sets are better?

IF (sunny and hot) OR (cloudy and hot) 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

Wait... Why am I here then?



https://ameblo.jp/kamar-saya-meg/entry-12247929580.html

Is interpretability possible at all?

WIRED

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

The new availability of huge amounts of data, along with the statistical tools to crunch these numbers, offers a whole new way



SHARE

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

Key Point:

It's about knowing enough for your downstream tasks.

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



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

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

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

What is interpretability?

- Not as simple as decision rules
- Not as simple as rule lists or rule sets.
- Not about understanding every bits and bytes of the model.

Our goal:

Bring us toward more precise notion of what interpretability entails, when it is needed, and how to evaluate it.

Just the **start of a discussion**!

Interpretability

Dictionary definition:

Interpretation is the process of giving **explanations**

Interpretability

Dictionary definition:

Interpretation is the process of giving **explanations**

To Humans

Interpretability

Why and when?

How can we do this?

Interpretation is the process of giving explanations

How can we measure 'good' explanations?

To Humans



Agenda

1. Why and when?

2. How can we do this?

Interpretation is the process of giving explanations

3. How can we measure 'good' explanations?

To Humans

Why interpretability?

Fundamental **underspecification** in the problem

Why interpretability?

Fundamental **underspecification** in the problem

More data or more clever algorithm won't help.

Underspecification example 1: safety



https://www.ll.mit.edu/publications/labnotes/automation.html

Underspecification example 1: safety

- Cost-effective Health Care (CEHC) built models to predict probability of death for patients [Cooper et al. 97]
 - HasAsthma(x) \Rightarrow LowerRisk for pneumonia (x)



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Example borrowed from [Caruana et al. '15]

Underspecification example 2: debugging

We want to understand why the system doesn't work, and

fix it.



https://yorktown.cbe.wwu.edu/sandvig/mis314/lectures/images/rubber-duck-debugging.jpg

Underspecification example 3: mismatched objectives and multi-objective trade-offs

• What you optimize is not what you meant to optimize.

All of these may address depression. Which side-effects are you willing to risk?



http://img.medscapestatic.com/pi/features/drugdirectory/octupdate/MYN62330.jpg,, http://img.medscapestatic.com/pi/features/drugdirectory/octupdate/PLV04411.jpg, https://www.google.com/url? sa=i&rct=j&q=&esrc=s&source=images&cd=&cad=rja&uact=8&ved=0ahUKEwjKgaaZkZbVAhXDPT4KHSZ3D-MQjRwIBw&url=http%3A%2F%2Fwww.webmd.com%2Fdrugs%2F2%2Fdrug-4870-5047%2Fvenlafaxineoral%2Fvenlafaxine-oral%2Fdetails&psig=AFQjCNHMQN9D8bhQZUFyxfHd9AoY5yxq5g&ust=1500580783703785

Underspecification example 4: science

Get me something new. Something... new.



http://cdn.playbuzz.com/cdn/a6006912-25e4-4cb5-867d-36c333b437c2/f2519ae0-e3d9-48e9-8f0d-4e68e2c99e26.jpeg

Underspecification example 5: legal/ethics

• We're legally required to provide an explanation and/or we don't want to discriminate against particular groups.



http://leap.utah.edu/_images/program-options/Pre-Law.jpg
Examples of underspecification

- **Safety**: We want to make sure the system is making sound decisions.
- **Debugging**: We want to understand why a system doesn't work, so we can fix it.
- Science: We want to understand something new.
- Mismatched Objectives and multi-objectives trade-offs: The system may not be optimizing the true objective.
- Legal/Ethics: We're legally required to provide an explanation and/or we don't want to discriminate against particular groups.

+ Your case?

Fundamental **underspecification** in the problem

What is NOT underspecification?



Underspecification is not uncertainty



https://www.pinterest.com/pin/461126449319612657/



[K., Kaess, Fletcher, Leonard, Bachrach, Roy and Teller '10]

Our cousins are not us



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

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

 $\underline{http://www.cinemablend.com/pop/Netflix-Using-Amazon-Cloud-Explore-Artificial-Intelligence-Movie-Recommended to the second se$



Agenda

1. Why and when?

2. How can we do this?

Interpretation is the process of giving **explanations**

3. How can we measure 'good' explanations?

To Humans





Not mutually exclusive categories Nor Exhaustive list of literatures

Before building any model



Visualization

• Exploratory data analysis



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

Before building any model



- Visualization
- Exploratory data analysis [Tukey 77]













Before building any model



- Visualization
- Exploratory data analysis

Building a new model



- rule-based, per-featurebased
- case-based
- sparsity
- monotonicity

Building a new model



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

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]



Building a new model: Per-feature based



Linear model

generalized linear model

generalized additive model

generalized additive² model

Table from [Gehrke et al. '12]

$$y = eta_0 + eta_1 x_1 + ... + eta_n x_n$$

 $g(y) = eta_0 + eta_1 x_1 + ... + eta_n x_n$
 $g(y) = f_1(x_1) + ... + f_n(x_n)$
 $g(y) = f_1(x_1) + ... + f_n(x_n)$
 $+ \sum_{i \neq j} f_{ij}(x_i, x_j).$

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Which one is NOT 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

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- Depth/Length of the tree might be too big
- Complexity of rules might be high
- May need lots of splits to fit complex function

Building a new model



- rule-based, per-featurebased
- case-based
- sparsity
- monotonicity



"I recommend treatment X because it worked for other patients like you..."

[Frey, Dueck '10] [Yen, Malioutov , Kumar '16] [Arnold , El-Saden , Bui , Taira '10] [Floyd , Aha '16] [Homem, Perico , Santos , Bianchi , de Mantaras '16] [Jalali , Leake '15] [Reid , Tibshirani '16]



- Explain clustering results using examples (Bayesian Case Model)
- Joint inference on prototypes, subspaces and cluster labels

Cluster A







[K. Rudin, Shah '14]

Building a new model: Case-based

iBCM + OverCode system



[K. Glassman, Johnson, Shah '15]



```
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</pre>
```

[K. Glassman, Johnson, Shah '15]

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Which one is NOT the limit None of data points are representative! of case-based models? A. The complexity of explanation is higher than an of

- 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

Break-y 5 mins

Need more coffee, need more coffee....



UH-OH, It's kicking in!!!!

http://weknowmemes.com/generator/meme/Coffee-kicking-in/335689/

After the break: Interpretability methods when you already have a model (e.g., deep learning) How to evaluate explanations

Building a new model



- rule-based, per-featurebased
- case-based
- sparsity
- monotonicity



$y = a_0 + a_1 x_1 + a_{21} x_{21} + a_{1002} x_{1002}$ (all other a,'s set to zero)

[Jain , Rao , Dhillon '16] [Yang , Barber , Jain , Lafferty '16] [Greenlaw , Szefer , Graham , Lesperance , Nathoo '17] [Kim , Xing '10] [Meier , Van De Geer , Buhlmann '08] [Bach , Jenatton , Mairal , Obozinski '12]


Which one is NOT 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, but just because it is sparse, doesn't mean it's interpretable." [Freitas '10]

Types of interpretable methods

Building a new model



- rule-based, per-featurebased
- case-based
- sparsity
- 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]

Types of interpretable methods

- Sensitivity analysis, gradient-based methods
- mimic/surrogate models
- Investigation on hidden layers

After building a model



Types of interpretable methods

- Sensitivity analysis, gradient-based methods
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After building a model





If we perturb the input $x \to x + \epsilon$?

• ϵ can be group of features, data points, specific inputs

xkcd.com

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



After building a model: Sensitivity analysis

Locally fitted

linear function

Sensitivity analysis on model [Ribeiro et al. '16] Influential functions [Koh et al.'17]

Want local explanation

of the 🕂 data point





Model found these images most helpful

SVM

Inception



[Simonyan et al., '13] [Li et al., '16] [Datta et al. '16] [Adler et al., '16]

After building a model: Saliency/attribution Maps

• Give me the features in the input space that mattered for the classification

 $\frac{\partial y}{\partial x_{ij}}$



Grad-CAM [Selvaraju et al. 16]





(a) Original Image (c) Grad-CAM 'Cat'









Integrated gradients [Sundararajan et al. 17]



Top label: starfish Score: 0.999992







Grad-CAM [Selvaraju et al. 16]



(a) Original Image



(c) Grad-CAM 'Cat'

SmoothGrad [Smilkov et al. 17]







Oh yeah, gradients makes sense. Integrated It's about how much the label would changes as I change the data...

[Erhan 2009] [Springenberg, '14] [Shrikumar '17]









	2016	2017	Only this feature changed
а	4	5	(5-4)*1* 3 = 3
р	1	2	4*(2-1)*3 = 12
С	3	4	4*1*(4-3) = 4
е	12	40	

Increase in e: 28!





	2016	2017	Only this feature changed		What?	<u>'</u> !	
а	4	5	(5-4)*1* 3 = 3				
р	1	2	4*(2-1)*3 = 12		PO		
С	3	4	4*1*(4-3) = 4		2		
е	12	40	19	-		07	
Increase in e 28! Where is my 9?							

Which one is NOT 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

Types of interpretable methods

- Sensitivity analysis, gradient-based methods
- mimic models
- Investigation on hidden layers

After building a model





After building a model: Mimic models

- \bullet Train a black box on $x\,$ and $\,y\colon\,f(x)=\hat{y}\,$
- \bullet Train an interpretable model on x and $\; \hat{y}: f(x) = \; \bar{y} \;$





After building a model: Mimic models

- Model compression or distillation [Bucila et al. '06, Ba et al. '14, Hinton et al. '15]
- Visual explanations [Hendricks et al. '16]



Which one is NOT the limitations of mimic models?

- A. You may not be able to distill there may not be simpler model at all
- B. There might be a gap between what the actual model is doing and your mimic model is doing
- C. The simpler model may not be interpretable
- D. None of the above

Types of interpretable methods

- Sensitivity analysis, gradient-based methods
- mimic/surrogate models
- Investigation on hidden layers





After building a model: Investigation on hidden layers

[Dosovitskiy et al. '16]





Starfish

Hartebeest





Anemone Fish

Banana Parachute

Screw

[Bau and Zhou et al. '17]





Which one is NOT the limitations of investigation on hidden layers?

- A. They may be lack of actionable insights
- B. It is unclear if visualizing neuron vs. per layer vs. per subspaces is more meaningful than others
- C. A golden dataset with detailed labels with human concepts are often not available
- D. None of the above

What's the best interpretability method for me?





Agenda

1. Why and when?

2. How can we do this?

Interpretation is the process of giving **explanations**

3. How can we measure 'good' explanations?

To Humans

"You know it when you see it"

"You know it when you see it"



"You know it when you see it"

Generalized additive models (GAMs) are the gold standard for intelligibility when low-dimensional terms are considered [4, 5, 6]. Standard GAMs have the form

$$g(E[y]) = \beta_0 + \sum f_j(x_j), \qquad (1)$$

where g is the link function and for each term f_j , $E[f_j] = 0$. Generalized linear models (GLMs), such as logistic regresThese are great papers and I had definitely also made these claims in my work!

accurate, yet are highly interpretable. These predictive models will be in the form of sparse *decision lists*, which consist of a series of *if...then...* statements where the *if* statements define a partition of a set of features and the *then* statements correspond to the predicted outcome of interest. Because of this form, a decision list model naturally provides a reason for

"You know it when you see it"

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We want **evidencebased** so that we can compare work A to work B, and to generalize.

"You know it when you see it" measure how well they do

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Q. Which group does this new data point belong to?

accurate, yet are highly interpretable. These predictive modes the form of sparse *decision lists*, which consist of a series of statements where the *if* statements define a partition of a series and the *then* statements correspond to the predicted outcomes and the *then* statements form, a decision list model naturally provides the series of this form.

A. Group 1





B. Group 2



K. 16]

"You know it when you see it" measure how well they do

provide

A. Group 1



Because

Q. Which group does this new data point belong to?

B. Group 2



Spectrum of evaluation



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

Function-based

How sparse are

the features?

Does it look

reasonable?



How much did we improve patient outcomes?

Do scientists find the explanations useful?



 Does providing interpretability assist with a down-stream task, such as increasing fairness, safety, scientific discovery, or productivity?



Commonly used in HCI, visualization communities



https://www.bu.edu/today/2012/do-scholarly-articles-want-to-be-free/



 Does providing interpretability assist with a down-stream task, such as increasing fairness, safety, scientific discovery, or productivity?



It's real evaluation, but it's costly and hard to compare work A to B
Evaluation: Function-based



Evaluation: Function-based



It's easy to formalize, optimize, and evaluate...

but may not solve a real need

e.g., 5 unit sparsity will save more patients than 10 unit sparsity?



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Evaluations: cognition-based

• Human subject experiments on general forms



Evaluations: cognition-based

• Human subject experiments on general forms



Problem-related Factors

- 1. Global vs. Local
- 2. Time budget
- 3. Severity of

underspecification

Method-related factors

- 4. Cognitive chunks
- 5. Audience training

Cognition-based

What factor should change to change the outcome?

What are the discriminative features?

Problem-related Factors

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 - underspecification

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Cognition-based

What factor should change to change the outcome?

What are the discriminative features?

e.g., Humans capacity as function of factors, Set of factors that carries over well to application

Problem-related factor: global vs. local





Problem-related factor: time budget



https://www.greek-names.info/names-of-ancient-greek-astronomers/



http://www.idonme.com/application-medical.php

Problem-related factor: severity of underspecification

solve f(x) + a bounded term

(stop if obstacle within 2m)

VS.

make a safe autonomous car

solve Al



Method-related factor: Audience Training



http://www.ufo-blogger.com

• The expert's background will affect what cognitive chunks and relations they have available

Recommendations List these factors in your work so that others can compare your work to theirs. Find more factors.

Does it look reasonable?

What are the discriminative features?

Cognitive-based

What factor should

change to change

the outcome?

Problem-related Factors

- 1. Global vs. Local
- 2. Time budget
- 3. Severity of

underspecification

alitative

Method-related factors

- 4. Cognitive chunks
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the explanations useful?

Wrap up

1. Why and when?

Interpretation is the process of giving **explanations**

3. How can we measure 'good' explanations?

2. How can we do

this?

To Humans

How shall we move the field forward?



https://imgflip.com

...and PAIR @ Brain, we are hiring.

ai.google/pair

QnA

Recommendations List these factors in your work so that others can compare your work to theirs. Find more factors.

Cognitive-based

What factor should change to change to the outcome?

Does it look reasonable?

What are the discriminative features?

Problem-related Factors

- 1. Global vs. Local
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Method-related factors

- 4. Cognitive chunks
- 5. Audience training

the explanations useful?