# Link Uncertainty and ML

Emily Sullivan Philosophy and Ethics Eindhoven University of Technology Eindhoven Artificial Intelligence Systems Institute









#### Understanding

















#### Model independence?



#### Model independence?











# MIT Technology Review



Intelligent Machines

#### The Dark Secret at the **Heart of Al**

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

by Will Knight April 11, 2017

KEITH RANKIN





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

> Deep Patient Project Mount Sinai Hospital, New York

KEITH RANKIN

#### MIT Technology Review



"[I]f we're going to use these things and rely on them, then let's get as firm a grip on how and why they're giving us the answers as possible...

If it can't do better than us at explaining what it's doing, then don't trust it."

Daniel Dennett

KEITH RANKIN

### **Opacity Hypothesis**

Complex and opaque models cannot enable understanding of phenomena because the inner workings of the model are opaque, black-boxed, or unintelligible.



#### Understanding





Model



**Explanation** 

### Link Uncertainty Hypothesis

Complex or opaque models fail to explain or enable understanding when the link between the phenomenon and the model is uncertain.



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Complex or opaque models fail to explain or enable understanding when the link between the phenomenon and the model is uncertain.

Understanding world 

**External problem** 

Model

**Explanation** 

# Outline

Explanation for understanding phenomena

Simple models

ML models

LU and model independence in physics?

# Explanation for understanding phenomena

# Explanation

Explanation starts with a question:

Why-questions, how-possibly questions, what-if questions ...

Explanations are a **type of answer** to a question.

Understanding is knowing a correct explanation

# Explanation

Why did the window break?

Glass has x and y physical properties that under great force causes it to break.

Sally threw a rock at a glass window that exhibited great force.

Thus, the window broke





XAI methods allows researchers to **discover an explanation** for the phenomenon of interest.

XAI methods only need to **reveal** aspects of a model that **help to induce an explanation of phenomena**.

# Explanation

#### "how-actually" explanations:

explain actual (causes or dependencies) of a particular event or phenomena how-possibly explanations: explain possible (causes or dependencies)

### Simple models

# Why are so many real-world populations segregated?

### Schelling's Checkerboard Model (1971)



#### Schelling's Checkerboard Model (1971)

Importantly Schelling's model provides insight by help of a simple algorithm.





Coins of (two) different types are placed randomly on a board.



If a coin is adjacent to too many coins of the other type, then that coin is moved to closest empty space.



This is repeated until no more changes are made (reaches equilibrium).

#### def update(self, n): for i in range(n): x = random.randint(0, self.width - 1) y = random.randint(0, self.height - 1) if *self*.is\_unhappy(x,y): self.move\_to\_empty(x, y) def move\_to\_empty(self, x1, y1): new\_cell = random.randint(0, len(self.empty\_spaces) - 1) x2, y2 = self.empty\_spaces[new\_cell] self.race\_array[x1][y1], self.race\_array[x2][y2] = self.race\_array[x2][y2], self.race\_array[x1][y1] tile w = self.canvas\_w / self.width tile\_h = self.canvas\_h / self.height self.canvas.coords(self.tk\_array[x1][y1], x2 \* tile\_w, y2 \* tile\_h, (x2+1) \* tile\_w, (y2+1) \* tile\_h) self.tk\_array[x1][y1], self.tk\_array[x2][y2] = self.tk\_array[x2][y2], self.tk\_array[x1][y1] self.empty\_spaces[new\_cell] = (x1,y1) def is\_unhappy(self, x, y): """A square is unhappy if it does not have at least two similar neighbours. me = self.race\_array[x][y] if me == 0: return False count = 0 if x > 0 and self.race\_array[x-1][y] == me: count += 1if x < self.width - 1 and self.race\_array[x+1][y] == me:</pre> count += 1 if y > 0 and self.race\_array[x][y-1] == me: count += 1 if y < self.height - 1 and self.race\_array[x][y+1] == me:</pre>

count += 1
return count < 2</pre>







Original State

30% preference







Original State

50% preference






Original State

80% preference

How does the algorithm work?

How does Schelling's Model explain segregation?

How is it possible that segregation could occur without institutional racism?

Why are so many real-world populations segregated?

How does the algorithm work?

How is it possible that segregation could occur without institutional racism?

Why are so many real-world populations segregated?

Depending on the question, the algorithm will play a different role in the explanation and understanding.



Look at the details of the program, including input and expected output.

How is it possible that segregation could occur without institutional racism?



- The dots represent people of different races; the empty spaces represent possible houses.
- Identify the key feature behind the algorithm and how it maps onto a possible population.
- Need some external support to motivate

- how the algorithm simulates a <u>real population</u>.

- What is the key feature of the algorithm and how does it map onto real-world populations.

- Must go beyond the model
- Need external evidence that people's preferences primarily determined housing choices
- The appropriate link between the phenomenon and the model must be established.
- In Schelling's case, it is that individual preferences alone can cause segregation in real-world populations.

Why are so many real-world populations segregated?

### ML models

### SO Model



Identify if an individual is gay or straight through facial recognition.

### SO Model

### **Possible Questions**



Identify if an individual is gay or straight through facial recognition.

Is it possible to identify one's sexual orientation based on facial features?

### SO Model

### **Possible Questions**



Identify if an individual is gay or straight through facial recognition.

What would cause facial features to depend on sexual orientation?

### SO Model

### **Possible Questions**



Identify if an individual is gay or straight through facial recognition. Why is the model able to with a high accuracy classify sexual orientation through facial images?

### Melanoma Model



Identify if a mole is likely to be a melanoma.

### Melanoma Model

### **Possible Questions**



Identify if a mole is likely to be a melanoma.

What are the visual signs of melanoma?

### Melanoma Model

### **Possible Questions**



Identify if a mole is likely to be a melanoma.

How does a melanoma differ from a mole?

### Melanoma Model

### **Possible Questions**



Identify if a mole is likely to be a melanoma.

Why should a particular patient's mole be biopsied for melanoma?

### **Opacity Hypothesis**

Complex and opaque models cannot enable understanding of phenomena because the inner workings of the model are opaque, black-boxed, or unintelligible.



#### Understanding





Model



**Explanation** 

Implementation Black-Box

Low-level details of algorithm implementation is obscured, unknown, or illegible. Example: Computing factorials

(factorial 6)

There is a black-box around how (factorial 6) is implemented.

#### Recursive process



Figure 1.3: A linear recursive process for computing 6!.

Example from *SICP* Sussman and Abelson

#### Iterative process

```
(fact-iter 1 1 6)
(fact-iter 1 1 6)
(fact-iter 1 2 6)
(fact-iter 2 3 6)
(fact-iter 6 4 6)
(fact-iter 24 5 6)
(fact-iter 120 6 6)
(fact-iter 720 7 6)
720
```

Figure 1.4: A linear iterative process for computing 6!.

Example from *SICP* Sussman and Abelson

Implementation Black-Box

Low-level details of algorithm implementation is obscured, unknown, or illegible. Explanation / Understanding?

Black boxes do not prohibit understanding in virtue of abstracted *implementation*.

Don't need to know how (factorial 6) is implemented to understand, say a climate model, that utilizes factorials.

For higher level questions the exact implementation does not need to be known in order to enable understanding.

When implementation matters

### Implementation Black-Box

Low-level details of algorithm implementation is obscured, unknown, or illegible. How is this feature of the algorithm implemented?

Why is this implementation better (or faster) than this other implementation?

### Levels of black-boxes



### Levels of black-boxes



### Levels of black-boxes

```
(define (factorial n)
  (fact-iter 1 1 n))
(define (fact-iter product counter max-count)
  (if (> counter max-count)
      product
      (fact-iter (* counter product)
      (+ counter 1)
      max-count)))
```

Levels of black-boxes

What levels of implementation black boxes undermine explanation and understanding?

If the algorithm is indeterminate?

If it changes or updates while running it?

Levels of black-boxes

What levels of implementation black boxes undermine explanation and understanding?

If the algorithm is indeterminate?

If it changes or updates while running it?



Levels of black-boxes

# Highest-level of black-box output

### The entire algorithm is obscured.

Levels of black-boxes

# Highest-level of black-box input output

Goal of algorithm (model) Way (model / algorithm) achieves goal

Levels of black-boxes

# Highest-level of black-box input output

### Goal of algorithm (model) Way (model / algorithm) achieves goal

Levels of black-boxes

# Highest-level of black-box input output

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Levels of black-boxes

What about DNN models?

Highest-level of black-box input output

Goal of algorithm (model) Vay (model / algorithm) achieves goal

Levels of black-boxes

### What about DNN models?

Highest-level of black-box

input

output

Goal of algorithm (model) Vay (model / algorithm) achieves goal

# We know the high-level algorithmic structures of DNNs.





functions: Sigmoid, hyperbolic tangent function (tanh), rectified linear units (ReLu)





(a) Husky classified as wolf





Ribeiro et al. 2016

LIME

### Link Uncertainty Hypothesis

Complex or opaque models fail to explain or enable understanding when the link between the phenomenon and the model is uncertain.





Model

**Explanation**






How-possibly?

Male

alc

How-actually?







The idealized assumptions underlying the model—

e.g. that sexual orientation is binary and static, that those who are openly gay on social media are representative of the whole gay population, and ignoring gender and racial variance—

distort important difference makers in real-world populations.

Model **Explanation** 

world

#### Understanding











(Esteva, A., et. al, 2017)

#### Any difference in the level of understanding we gain from these models must be due to something other than opacity.

Black-box / Opacity



(Wang, Y. and Kosinski, M., 2018)



(Esteva, A., et. al, 2017)

The level of link uncertainty between the phenomenon and the model differs.



(Wang, Y. and Kosinski, M., 2018)

## Reducing Link Uncertainty

- requires connecting data, model architectures, and counterfactual the model makes inferences to the target phenomena
  - Robustness analysis (e.g. over different data distributions)
  - traditional empirical research
  - Improve ground truth methods for data labeling

There is a special worry with DNN models.

The power of these models mean that we need to take special care to make sure the models do not have high levels of link uncertainty before we rely on their results.

We need to be clear when a model is **merely exploratory** and not a **new discovery**.



- Difference between explaining the model and explaining phenomena with models.
- Model opacity is not in-principle a problem for explaining phenomena.
- For explaining phenomena, the problem of model opacity is an external problem of link uncertainty

# Model independence?

How could the notion of LU be helpful?



## Model independence

### Disanalogies

- "single class categorization"
- Don't know what you are looking for
- Searching 'without an alternative'
- Opacity a worry?

### Analogies

- similar threat of treating data in non-realistic ways
- Searching in large space of parameters for a significant pattern
- Needing to know when findings are worth investigating further

### Model independence

When could there high link uncertainty that would prevent explanation and understanding?

Some ideas I heard yesterday....

Misalignment (or uncertainty of alignment) between ML architectures and data --- (Kyle Cranmer)

Uncertainty concerning inter-dependency between choice of operator bases --- (Christophe Grojean)

Bottom-up approaches to SMEFT *before* 'fit into global explanation theory'--- (Martin King)

# Model independence?

What do you think?

Does this add more than EFT validity?



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