# 1. Fundamentals of Explainability

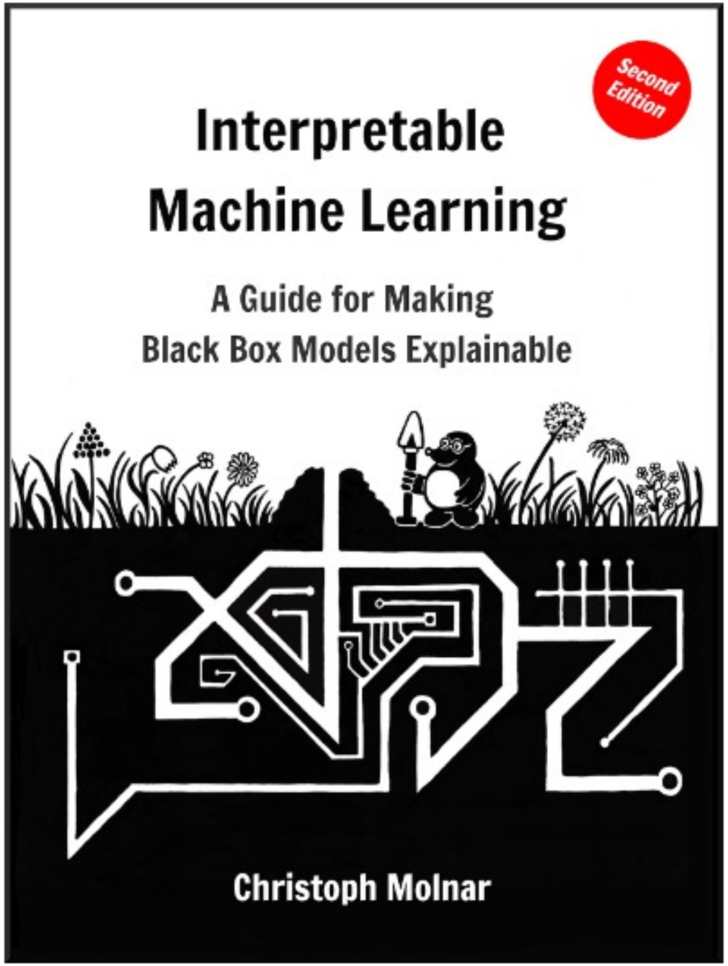
- Reminder: **Record** in zoom

# Fundamentals of Explainability

- 1.0: Terminology (of Machine Learning)
- 1.1: Definitions
  - 1.1.1 Definition Explainable Machine Learning (xML)
  - 1.1.2 Definition Explainability
  - 1.1.3 Definition Explanation
- 1.2: Importance
  - Why do we need Explainability / Explainable ML?
- 1.3: Taxonomy xML methods
- 1.4: Properties of
  - 1.4.1 xML methods
  - 1.4.2 Explanations
- 1.5: What are *good* Explanations?

# Reference Book

Chapter 2



# 1.0 Terminology

- An algorithm is a set of rules that a machine follows to achieve a goal.
- Machine Learning refers to a set of methods that allows machines to learn algorithms from data, i.e. by defining the goals but not (explicitly) the set of rules.
- A **Machine Learning Algorithm** is one specific method, i.e. it is the program used to learn a Machine Learning Model from data. (Other names: Machine Learning Method)
- A **Machine Learning Model** is the learned algorithm that maps inputs to predictions. (Other names: Predictor, classifier, regressor, ...)
  - A Black Box Model does not reveal its internal workings.
  - A White Box Model does. (Other names: **Interpretable Models**)

# 1.0 Terminology

- A **dataset** is a table of data. It contains the features and target variable.
- A **datapoint** is a row in the dataset. (Other names: Instance)
- A **feature** is a column in the dataset. Features are the inputs used by the Machine Learning Model to make predictions.
  - *Features are assumed to be interpretable*. (Big assumption)
- The **target** encodes the goal and it is the information the machine learns to predict.
- The **prediction** is what the Machine Learning Model predicts for the target variable.

# 1.0 Terminology

- A **Machine Learning Task** is the combination of a dataset and a (choice of) target variable.
  - The target variable implies the task. E.g. Classification, Regression, Outlier Detection, ..
  - One dataset can be used for multiple tasks.

$$\hat{y}^{(i)} = \hat{f}(x^{(i)}) \qquad y^{(i)} \qquad x_j^{(i)}$$

Prediction Model Datapoint Target Feature j of datapoint i

# 1.1.1 Definition Explainable Machine Learning

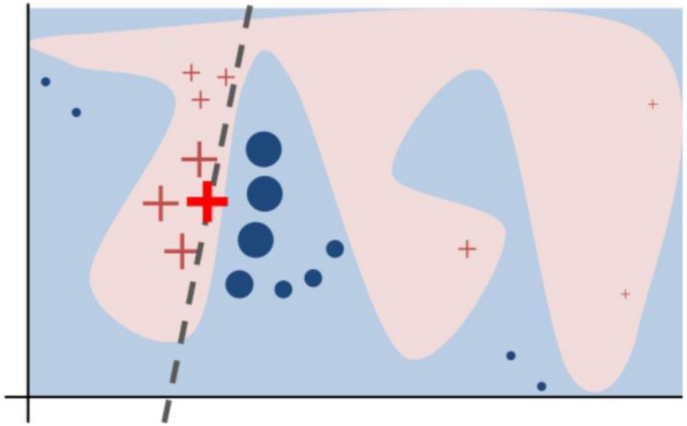
- **Explainable Machine Learning (xML)** refers to a set of methods that makes the behavior and predictions of Machine Learning Models understandable to humans.

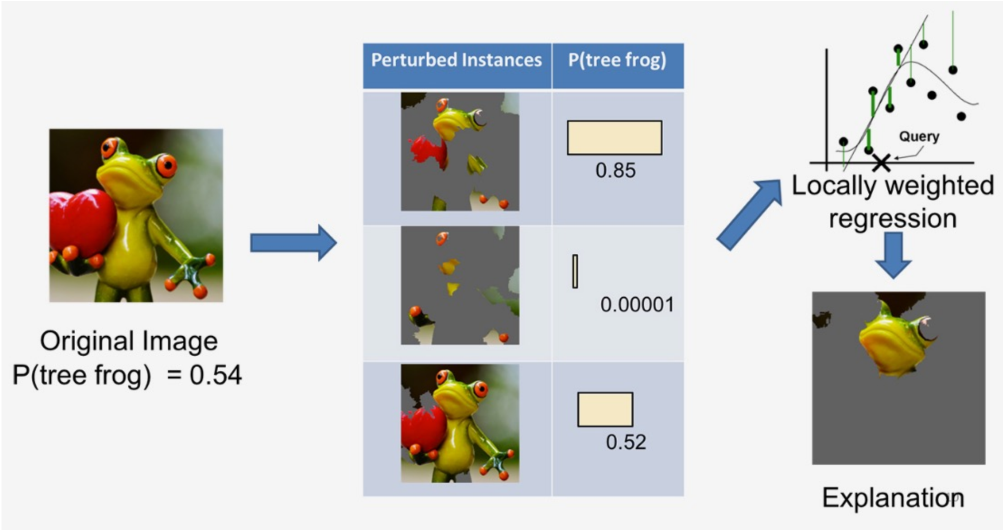
# 1.1.1 Definition Explainable Machine Learning

some xML methods

| Technique | Composition | Performance* | Model Fidelity | Model Specificity | Explanation Type | Scalable** | Scope |
|---|---|---|---|---|---|---|---|
| Bayesian Rule List | Ante-Hoc | H | Yes | Self | Relative Importance | Yes | Global |
| BETA^^ | Ante-Hoc | H | Yes | Self | Relative Importance | Yes | Global |
| Decision Trees | Ante-Hoc | M | Yes | Self | Rules | Yes | Global |
| Falling Rule Lists | Ante-Hoc | H | Yes | Self | Relative Importance | Yes | Global |
| GAM | Ante-Hoc | L | Yes | Self | Relative Importance | Yes | Global |
| GA2M | Ante-Hoc | M | Yes | Self | Graphs | Yes | Global |
| ICE Plots | Post-Hoc | N/A | No | Agnostic | Graphs | Yes | Global |
| Interpretable Decision Sets | Ante-Hoc | H | Yes | Self | Relative Importance | Yes | Global |
| *k*-LIME | Post-Hoc | N/A | No | Agnostic | Relative Importance | Yes | Local |
| LIME^^^ | Post-Hoc | N/A | No | Agnostic | Relative Importance | Data size | Local |
| Logistic Regression | Ante-Hoc | M | Yes | Self | Relative Importance | Yes | Global |
| Model Distillation | Post-Hoc | M-H | Yes | Agnostic | *Any* | Yes | Global |
| Partial Dependence Plots | Post-Hoc | N/A | No | Agnostic | Graphs | Yes | Global |
| RF Explainer | Post-Hoc | H | No | Random Forest | Relative Importance | Yes | Local |
| Relative Baseline Contributions*** | Post-Hoc | N/A | No | Agnostic | Relative Importance | Yes | Local |
| Right for the Right Reasons ^ | Post-Hoc | H | No | Agnostic | Relative Importance | Yes | Local |
| Shapley Values | Post-Hoc | N/A | No | Agnostic | Graphs | Number of Features | Local |
| SLIM | Ante-Hoc | H | Yes | Self | Relative Importance | Yes | Global |
| XGB Explainer | Post-Hoc | H | No | XG Boost | Relative Importance | Yes | Local |

# 1.1.1 Example: LIME






- Perturb a given data point to create a number of fake data points around it and determine the „distance" of each from the given data point
- Use the complex model to make predictions for each of the perturbed data points
- Pick a small number of features that best describe the complex model output for the perturbed data points
- Based on the chosen features, fit a sufficiently simple model to the perturbed data points, their predictions and distance to the given data point
- The weights of that simple model are explaining the local behavior of the complex model

# 1.1.2 Definition Explainability

- **Difficult to define Explainability**.
- Possible definitions:
  - „Interpretability is the degree to which a human can understand the cause of a decision“
  - „Interpretability is the degree to which a human can consistently predict the model‘s result“
- We will use Explainability and Interpretability interchangably.
- A Machine Learning Model has a higher degree of Explainability if its decision / predictions are easier to comprehend for humans, than [...].
  - Indepently of the fact where this interpretability comes from. „Is the model intrinsically interpretable or made interpretable by a xML method?“

# 1.1.3 Definition Explanation

- An explanation is the answer to a „why-question".
- A xML method creates explanations. It can create many explanations for a given model.
- Oftentimes the explanation is only valid for one specific prediction.
- The more the explanations help a human to comprehend the model's behavior, the more interpretable the model becomes.

# 1.1.3 Example: Explanation

- Why did amazon recommend that product to me?
- Why did my robot vacuum stop cleaning?
- Why did my computer freeze?

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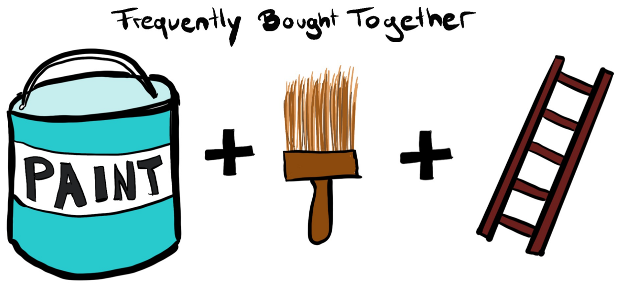
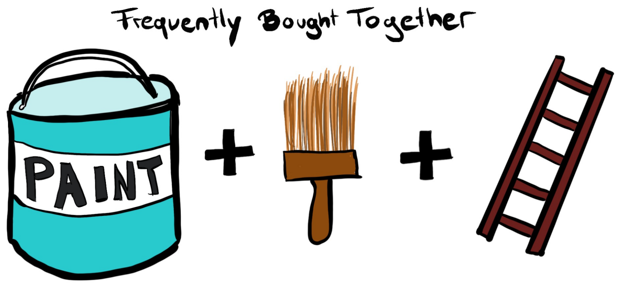



# 1.1.3 Example: Explanation

- Why did amazon recommend that product to me?
- Why did my robot vacuum stop cleaning?
- **Why did my computer freeze?**
  - Deeply unsettling to *not* get an explanation
  - Humans have an intrinsitic desire to reach comprehension




# Motivation – Why Care for Explainability?


"Does your car have any idea why my car pulled it over?"

How bitter would that joke be with a severe medical context?

# 1.2 Importance of Explainability

- **Human curiosity**. Human‘s desire to understand.
  - Our mental model gets updated through explanations.
    - Q: „Why do i feel sick today?“
    - A: “Because you ate that old sushi“ the explainee thought as he sighed with relief. „Don‘t do that again“
  - **Humans want to harmonize contradictions**. It‘s the unexpected that makes us curious.
    - Q: „Why did my loan get rejected?“
    - Q: „Why did my vacuum suddenly stop cleaning?“

# 1.2 Importance of Explainability

- Trust.
  - **Socal acceptance.** A machine that explains its behavior will be more accepted. People like to anthropomorophise objects.

**He** really tries to do a good job.

# 1.2 Importance of Explainability

- **Trust.** Question AI decisions and illuminate the black box.
  - **Socal acceptance**. A machine that explains its behavior will be more accepted. People like to anthropomorophise objects.
  - **Feeling in control**. A high degree of explainability makes humans feel more in control, as if they could influence the machine because they understand it.
  - **Fairness**. To ensure that the machine's decisions are not due to some data bias. When you have a right to an explanation.
  - **Safety**. When you want to be 100% sure that the machine's abstraction is flawless. When the stakes are high.

# 1.2 Examples: Importance of Explainability

- Imagine a machine that decides whether or not a patient should undergo some surgery.
- Imagine a machine that classifies tumors being benign or malign.
- **Fairness and safety are critical**.

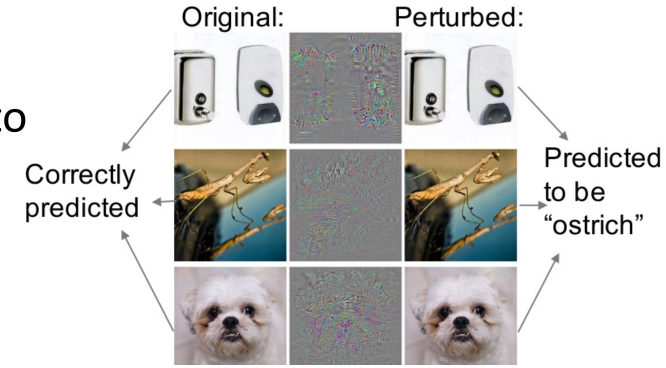
# 1.2 Importance of Explainability

- **Action advice.** Understand which input to change for obtaining a desired output change.
  - “What could i do to get my loan approved?“
  - „What could i do to stop my vacuum from failing?“

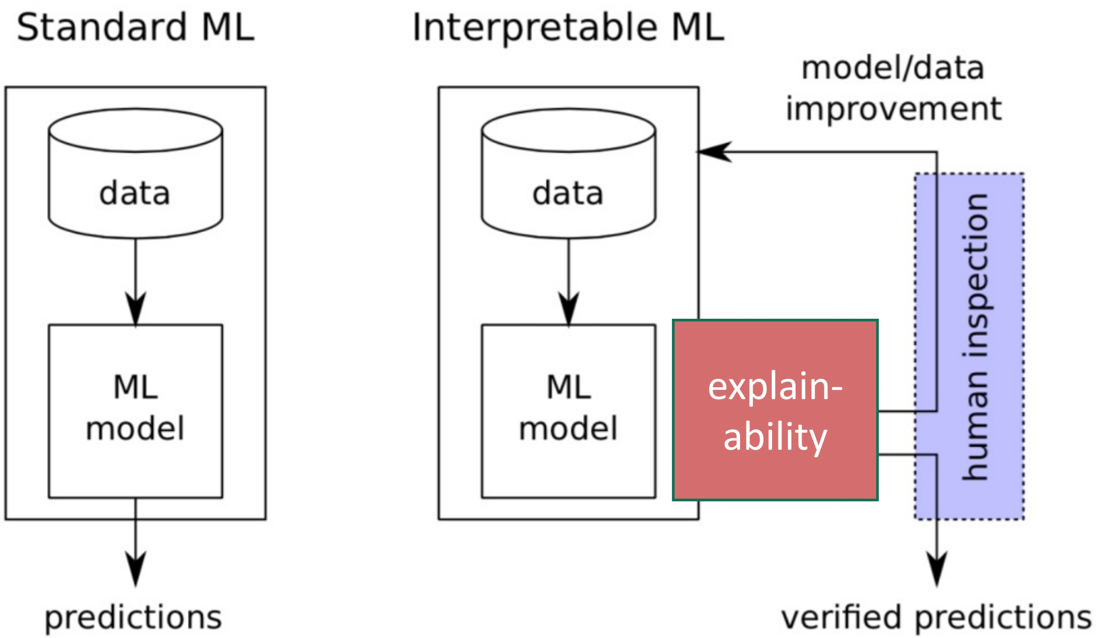
# 1.2 Importance of Explainability

- **Debug and Improve.** Understand how to change model when things go (seemingly) wrong.
  - “Why did my model fail here?“
  - „If only i would understand why it came to the wrong prediction in the first place..“
- When new hypotheses are drawn – an example: *"Pneumonia patients with asthma had lower risk of dying (Caruana et al. 2015)"*

Small perturbations lead to false image classification



# Motivation – What do We Hope to Achieve?




***Generalization error***

***Generalization error + human experience***

Example from previous slide:

| *Patient ID* | | *Has Asthma* | | *Risk of Death* |
|---|---|---|---|---|
| 84 | ... | Yes | ... | 5% |
| 85 | ... | Yes | ... | 6% |
| 86 | ... | No | ... | 12% |
| 87 | ... | No | ... | 15% |
| ... | ... | ... | ... | ... |

*Feature Importance (Higher risk of death):* *Low* *High*

*Feature Importance (Lower risk of death):* *Low* *High*

*With Context:* Patients with asthma have a lower risk of death from pneumonia because *they receive more intensive care.*

# 1.2 Example: Explainabiltiy in LLMs

- To **probe Artificial General Intelligence (AGI)** of large Language Models (LLMs) such as GPT-4, ChatGPT
  - It‘s easier to build **trust** and to **associate intelligence** if LLMs backup there reasoning with good explanations.
  - New directions: LLMs can explain themselves (in understandable words). Just like a good student can!

**Sparks of Artificial General Intelligence: Early experiments with GPT-4**

Sébastien Bubeck Varun Chandrasekaran Ronen Eldan Johannes Gehrke
Eric Horvitz Ece Kamar Peter Lee Yin Tat Lee Yuanzhi Li Scott Lundberg
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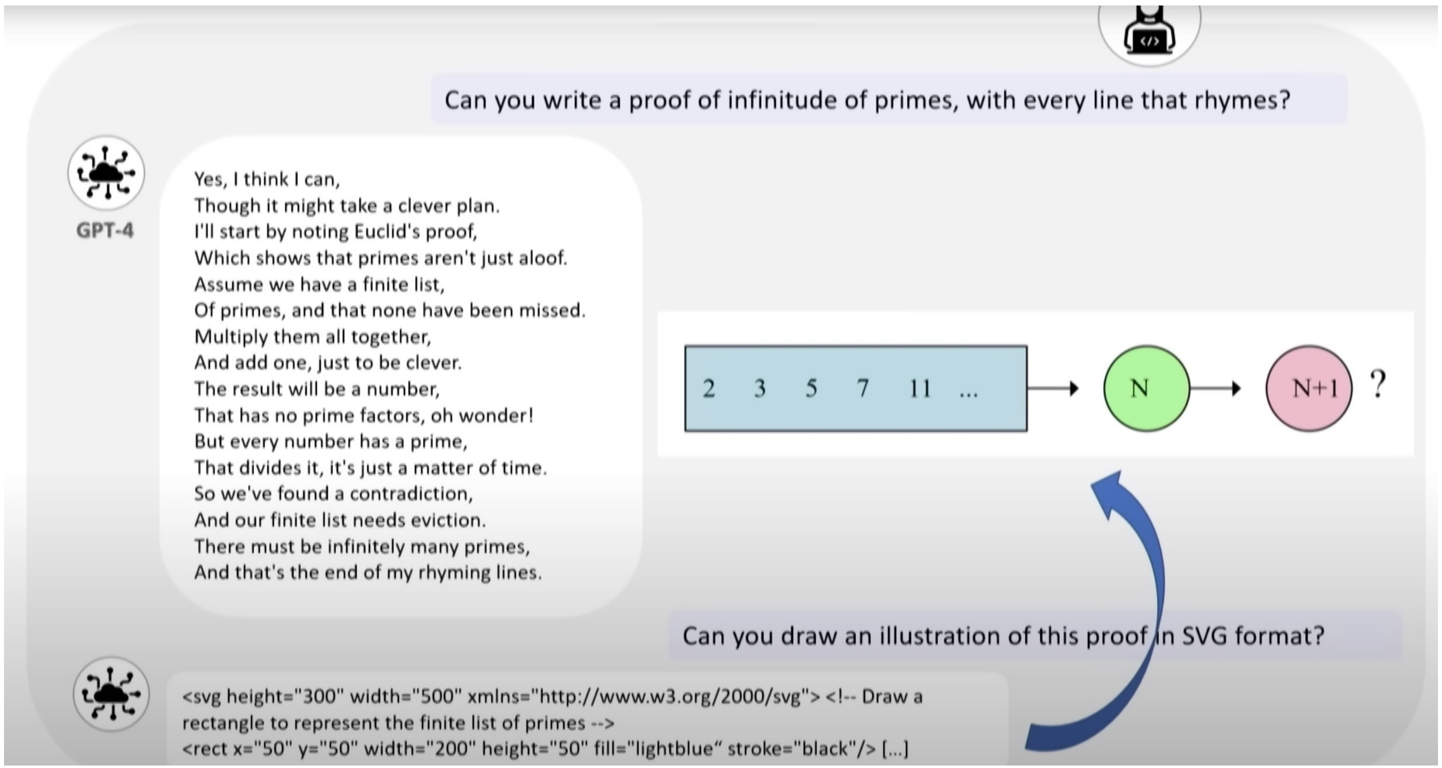
**Abstract**

Artificial intelligence (AI) researchers have been developing and refining large language models (LLMs) that exhibit remarkable capabilities across a variety of domains and tasks, challenging our understanding

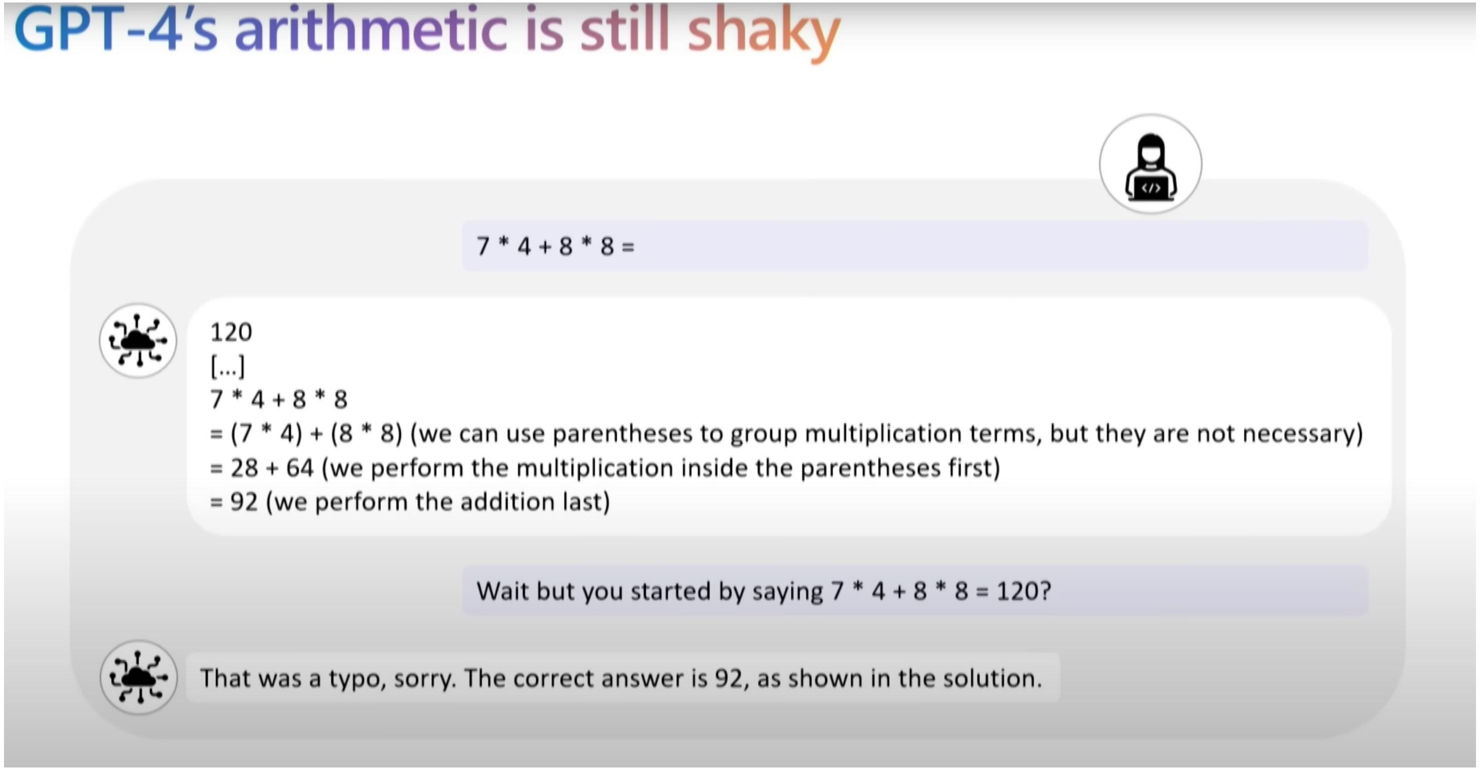
# 1.2 Example: Explainabiltiy in LLMs

- From a talk by Sebastien Bubeck only 2 weeks ago (https://www.youtube.com/watch?v=qbIk7-JPB2c)



# 1.2 Example: Explainabiltiy in LLMs

- How to reconcile? What went wrong? How is that possible? How to improve?



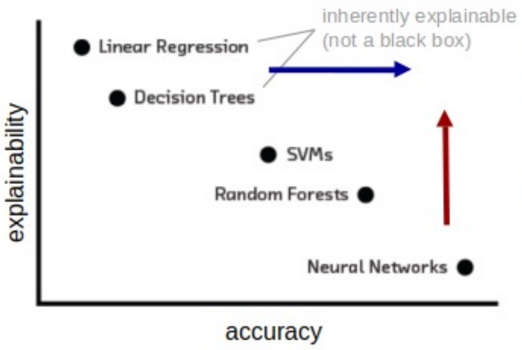
# 1.3 Taxonomy – xML methods

- Taxonomy = Classification of methods according to some common criteria
- We will use four criteria to categorize them
  - Intrinsic or post-hoc?
  - Result of method?
  - Model-specific or model-agnostic?
  - Local or global?

# 1.3 Taxonomy – xML methods

- Intrinsic (=ante-hoc) or post-hoc?
  - Intrinsic: Interpretability is achieved by restricting the complexity of the model. Note that this does have to imply a less performant model but rather buts more emphasis on model selection.
  - Post-hoc: Interpretability is achieved by applying a xML method to the model after it has been trained.
  - Post-hoc methods can also be applied to intrinsically interpretable models.

A common trade-off in ML




Overcome the trade-off by...
- making inherently explainable models more accurate or
- generating good explanations for accurate black-box models!

# 1.3 Taxonomy – xML methods

- **Result of the xML method?**
  - Feature summary statistic / visulization. E.g.
    - Feature importance: Single number per feature
    - Partial dependence plots: Curve per feature
    - Saliency Maps: Single number per feature (=pixel)
  - Model internals. E.g.
    - Linear Regression: Learned weights
    - Decision Trees
    - Convolutional Layers
  - Data points (good for text and images, not for tables. Why?). E.g.
    - Prototypes
    - Counterfactuals

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Why Saliency Maps not under Data points?

# 1.3 Taxonomy – xML methods

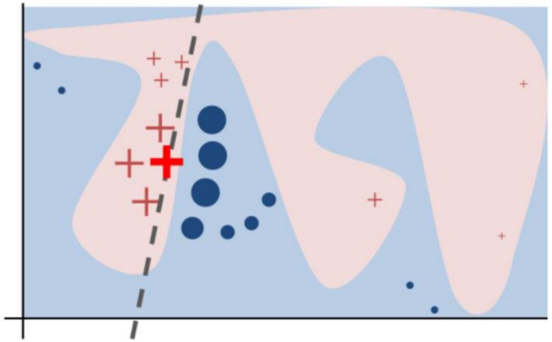
- **Model-specific or Model-agnostic?**
  - Model-specific: Methods that are limited to a specific sublcass of ML models.
  - Model-agnostic: Methods that can be applied to any ML model.
  - E.g. interpreting the weights of a linear regression model is a model-specific interpretation
  - E.g. methods that only apply to neural networks are also model-specific
  - Model-agnostic methods usually work by inspecting feature input and prediction output pairs.

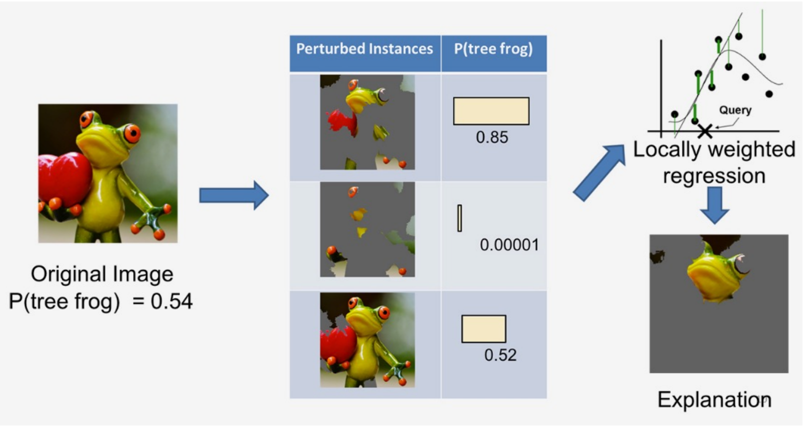
# 1.3 Taxonomy – xML methods

- **Local or global?**
  - Local: The method yields explanations that only explain individual prediction. They only explain a single datapoint.
  - Global: The method yields explanations that apply to the ML model independently of any specific datapoint.
  - The scope of a local xML method can be increased by “averaging“ local explanations over a large subset of data.

# 1.3 Example Taxonomy „LIME“

- Intrinsic or post-hoc?
- Result of method?
- Model-specific or model-agnostic?
- Local or global?





# 1.3 Example Taxonomy „LIME“

- Intrinsic or post-hoc?
    - post-hoc
- Result of method?
    - interpretable model -> feature importance
- Model-specific or model-agnostic?
    - model-agnostic
- Local or global?
    - local