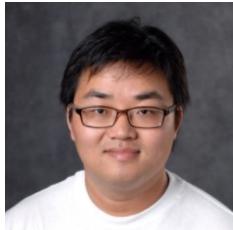
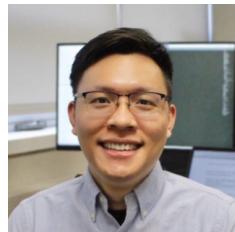


Introduction



Privacy



Safety & Robustness



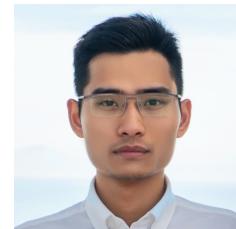
Jiliang Tang

Xiaorui Liu

Yixin Li



Explainability



Non-discrimination & Fairness

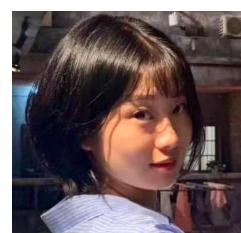


Wenqi Fan

Environmental Well-being

Haochen Liu

Accountability & Auditability

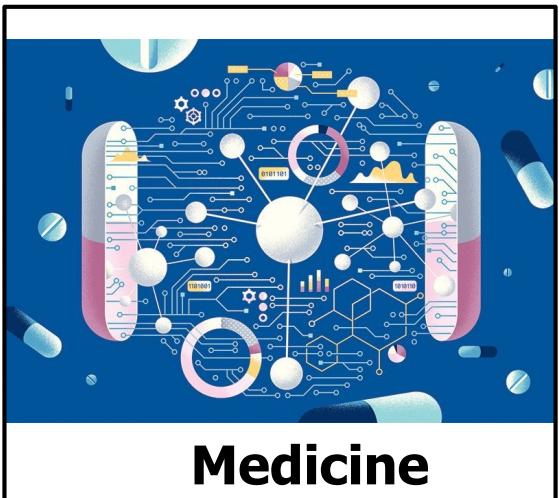
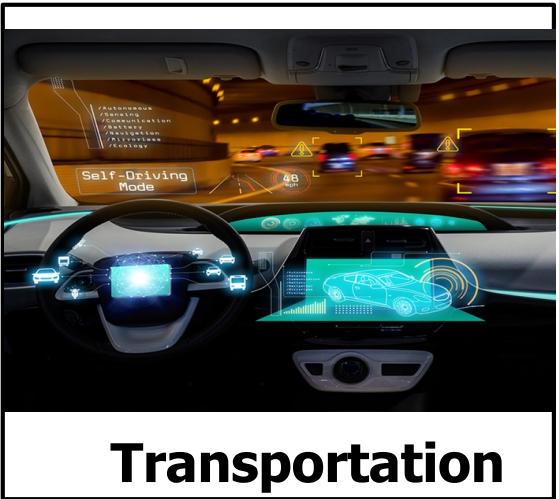


Dimension Interactions

Yiqi Wang

Future Directions

AI in Critical Systems

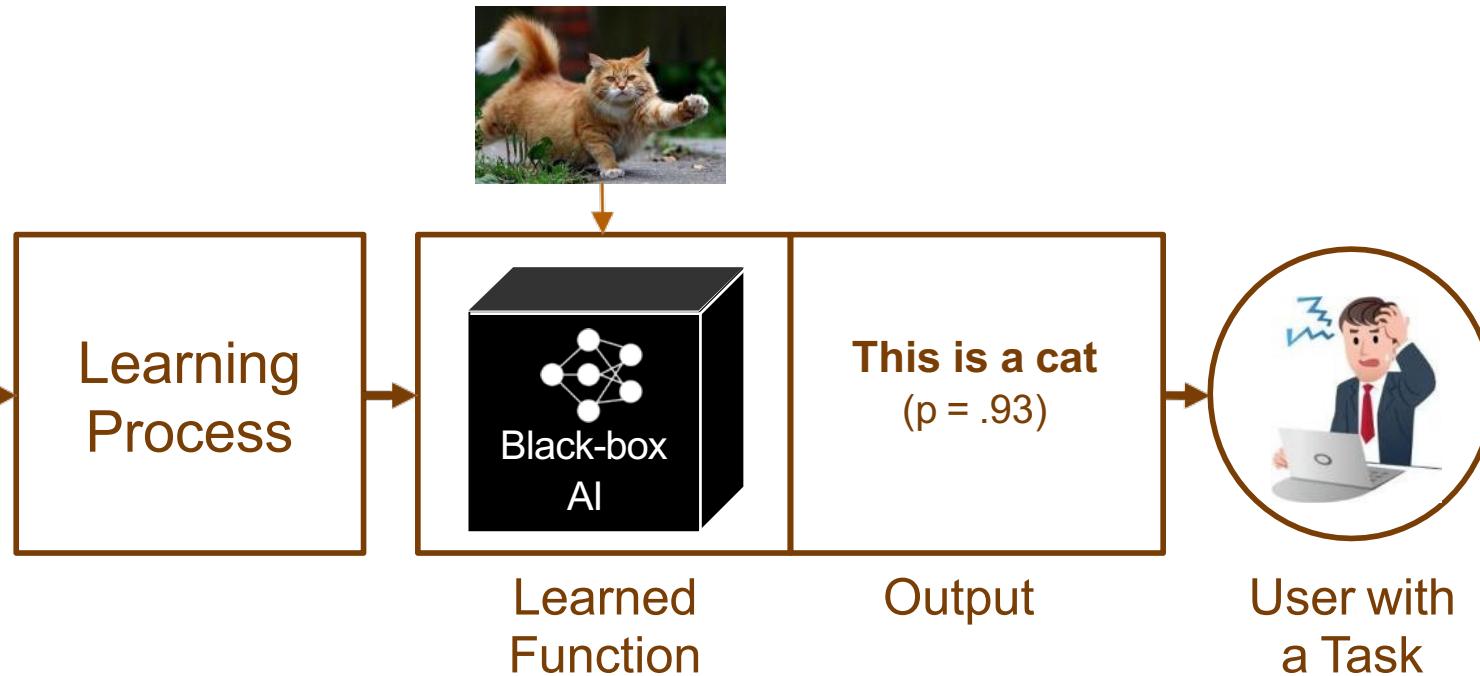


How an AI model works?

Today

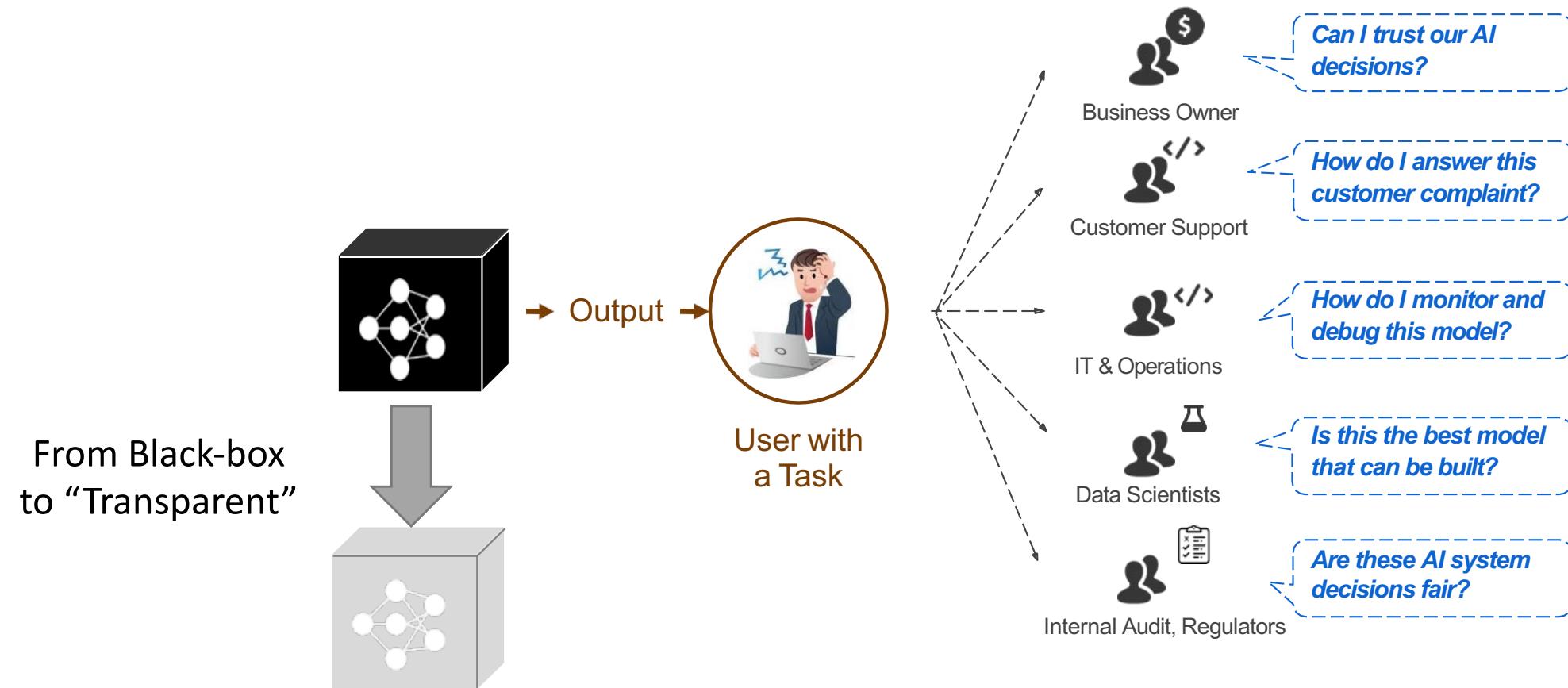


Training
Data



- Why did you do that?
- Why not something else?
- When do you succeed?
- When do you fail?
- When can I trust you?
- How do I correct an error?

Black-box AI creates confusion and doubt



The Need for Explainable AI

Explainable AI

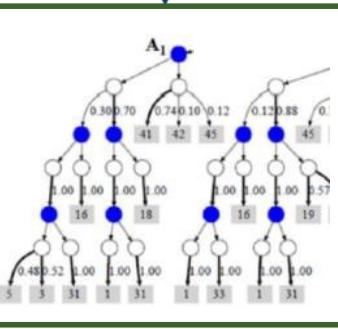
Tomorrow



Training
Data



New
Learning
Process



Explainable
Model



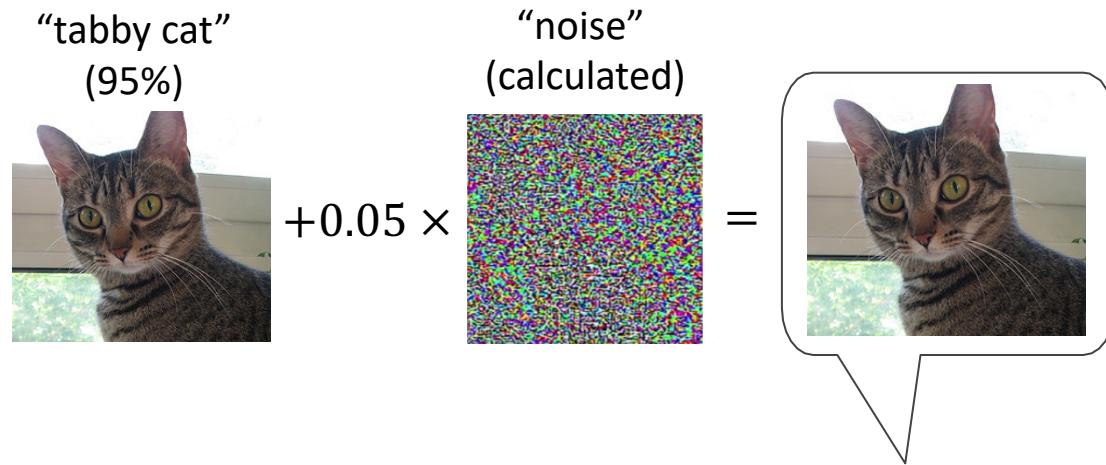
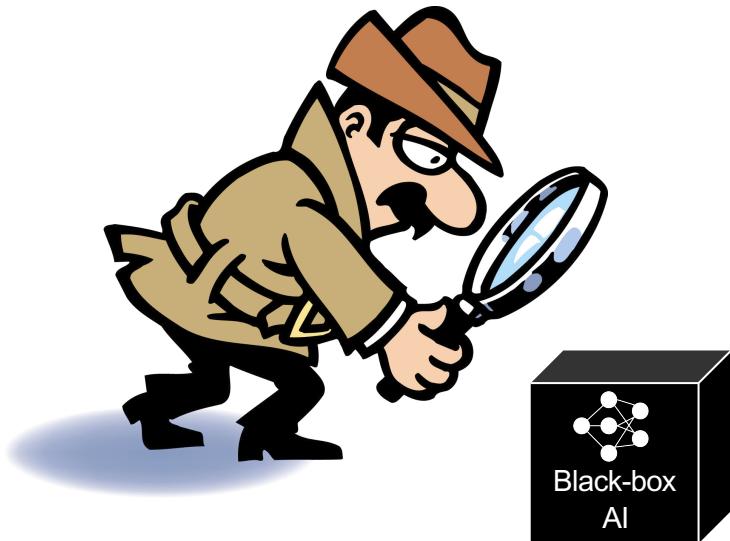
Explanation
Interface



User with
a Task

- I understand why
- I understand why not
- I know when you'll succeed
- I know when you'll fail
- I know when to trust you
- I know why you erred

Why Explainability: Debug (Mis-)Predictions



Top label: **"strawberry"** (99%)

Why did the network label this image as **"strawberry"**?

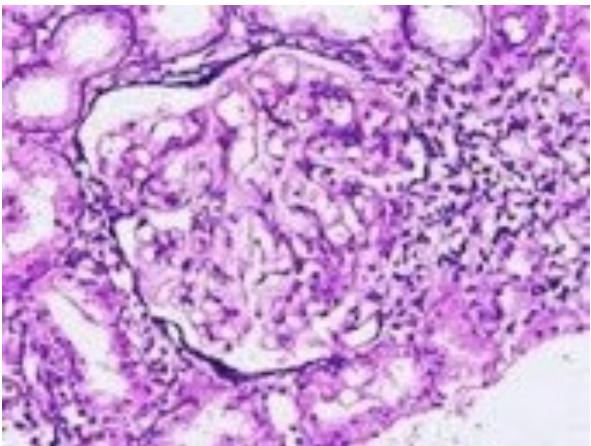
Why Explainability: Verify the AI System

Wrong decisions can be costly and dangerous.

*“Autonomous car crashes,
because it wrongly recognizes ...”*

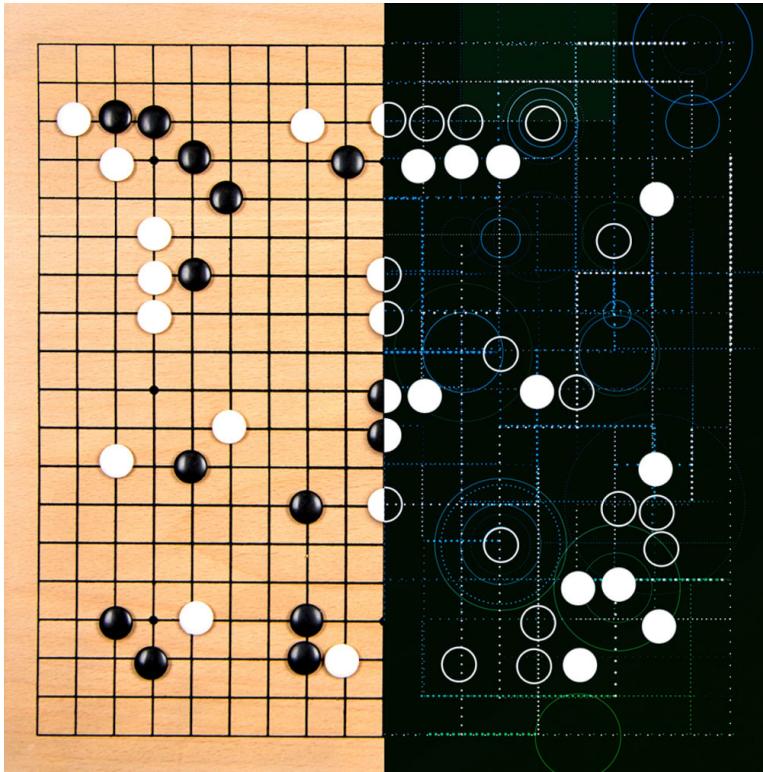


*“AI medical diagnosis system
misclassifies patient’s disease ...”*

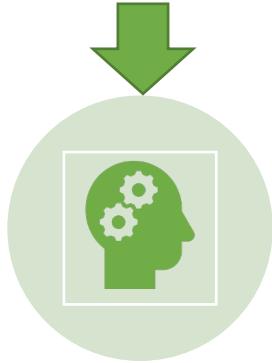


Why Explainability: Learn New Insights

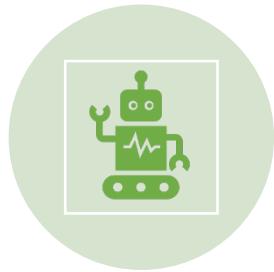
“It's not a human move. I've never seen a human play this move... so beautiful.” -- Fan Hui vs. AlphaGo



Outline



CONCEPTS AND TAXONOMY



TECHNIQUES FOR
EXPLAINABILITY IN AI
(XAI)



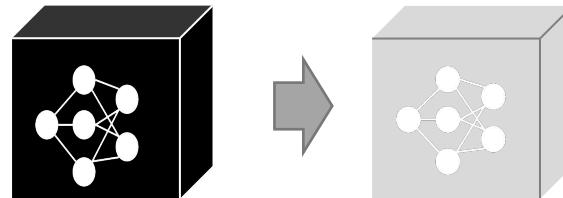
APPLICATIONS IN REAL
SYSTEMS



SURVEYS AND TOOLS

What is Explainable AI (XAI)?

- The degree to which a human can understand the cause of a decision.
 - **Interpretable AI:** intrinsically transparent and interpretable, rather than black-box/opaque models, such as decision trees and linear regression.
 - **Explainable AI:** additional (post hoc) explanation techniques, but still black-box and opaque, such as DNN.



From Black-box to “Transparent”



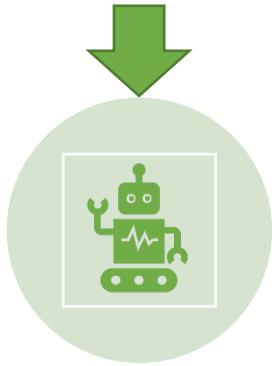
Taxonomy

- **Model usage:** model-intrinsic and model-agnostic
 - Only restrict to a specific architecture of an AI model or not
- **Differences in the methodology:** gradient-based and perturbation-based
 - Employ the partial derivatives on inputs or change input data
- **Scope of explanation:** local and global
 - Provide an explanation only for a specific instance or for the whole model
- **Counterfactual explanations**
 - “If X had not occurred, Y would not have occurred.”

Outline



CONCEPTS AND TAXONOMY



TECHNIQUES FOR
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APPLICATIONS IN REAL
SYSTEMS



SURVEYS AND TOOLS



Model usage

- Only restrict to a specific architecture of an AI model or not

- Model-intrinsic Explanations
 - Transparent or white-box explanation (model-specific)

- Model-agnostic Explanations
 - Interpret already well-trained models
 - Post-hoc or black-box explainability methods

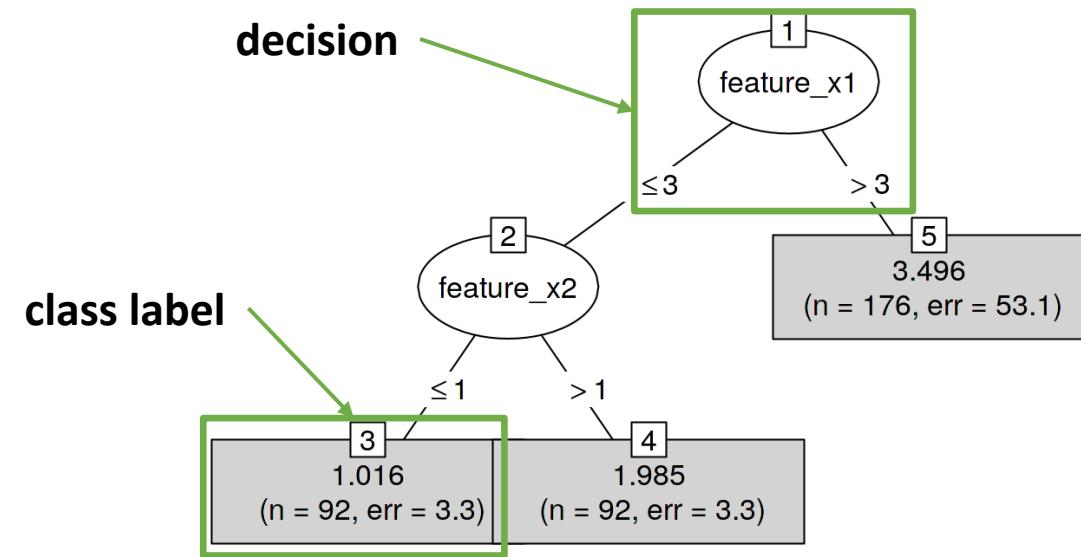
Model usage: Model-intrinsic Explanations

- Transparent, or white-box explanation (model-specific)
 - linear/logistic regression, decision trees, rule-based models, etc.

$$\hat{y} = \mathbf{w}^T \mathbf{x} + b = w_1 x_1 + \dots + w_d x_d + b$$

feature weight

linear regression model



Decision tree

Model usage: Model-agnostic Explanations

❑ Interpret already well-trained models

- Post-hoc or black-box explainability methods

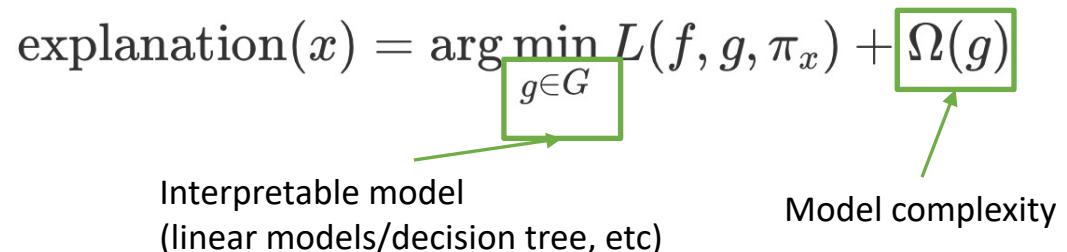
❑ Local Interpretable Model-Agnostic Explanations (LIME)

- Approximating the black-box model by an interpretable one (such as linear model) learned on perturbations of the original instance.

$$\text{explanation}(x) = \arg \min_{g \in G} L(f, g, \pi_x) + \Omega(g)$$

Interpretable model
(linear models/decision tree, etc)

Model complexity



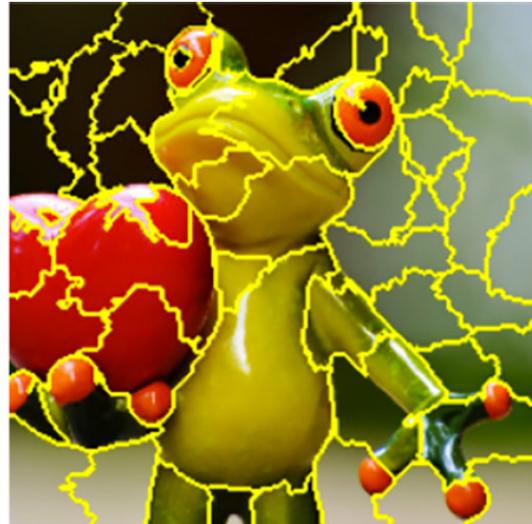
The diagram shows the LIME explanation formula. A green bracket encloses the term $\arg \min_{g \in G} L(f, g, \pi_x)$. An arrow points from this bracket to the text "Interpretable model (linear models/decision tree, etc)". Another green bracket encloses the term $\Omega(g)$. An arrow points from this bracket to the text "Model complexity".

Model usage: Model-agnostic Explanations

LIME:



Original Image

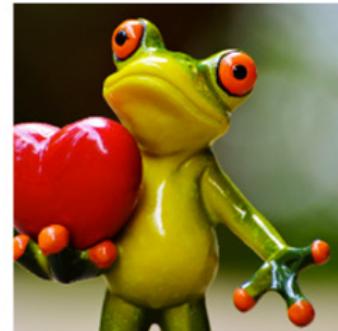


Interpretable
Components

Transforming an image into interpretable components

Model usage: Model-agnostic Explanations

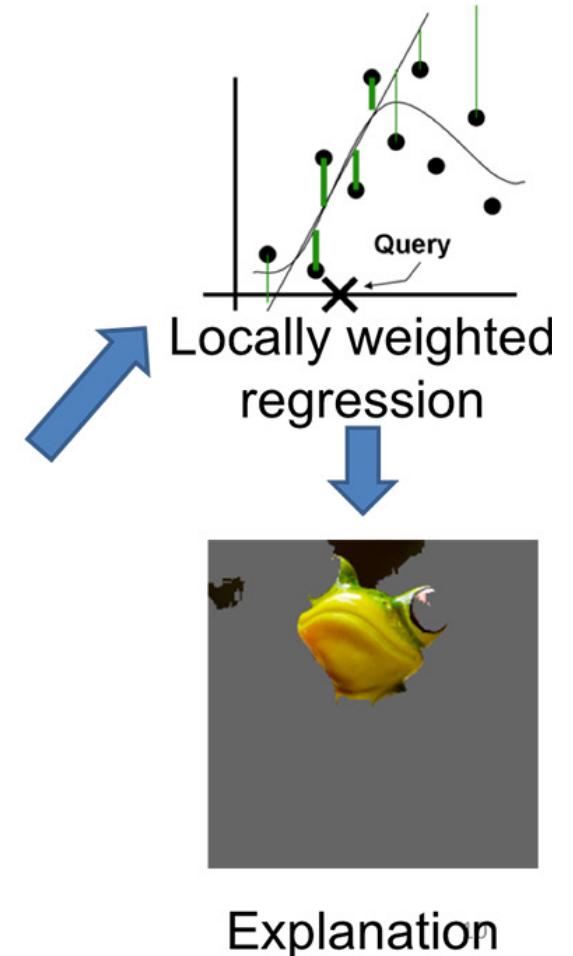
LIME:



Original Image
 $P(\text{tree frog}) = 0.54$



Perturbed Instances	$P(\text{tree frog})$
	0.85
	0.00001
	0.52



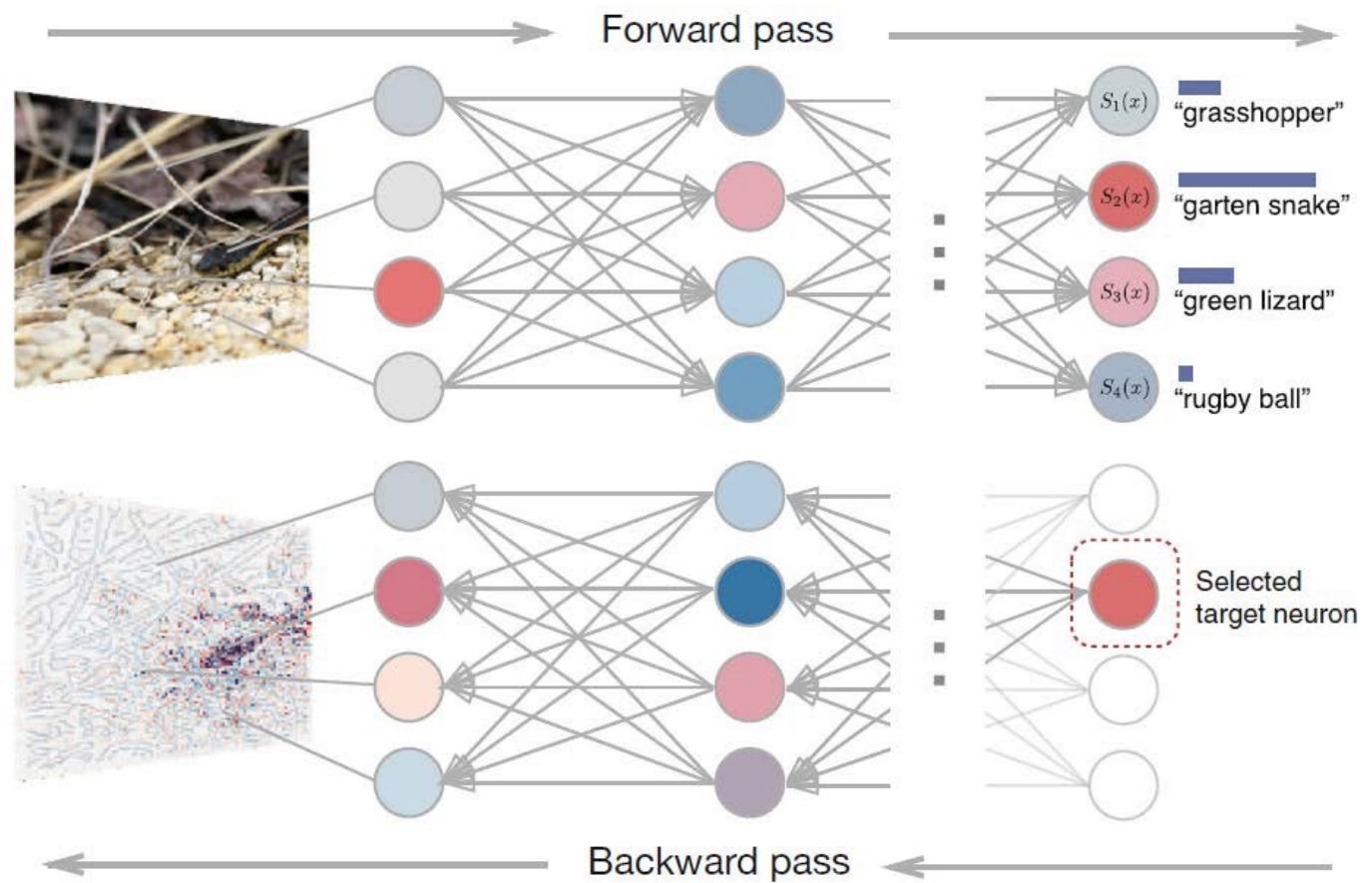


Differences in the methodology

- ❑ Employ the partial derivatives on inputs or change input data
- ❑ Gradient-based Explanations
 - Combine network activations and gradients
- ❑ Perturbation-based Explanations
 - Change the input and observe the effect on the output

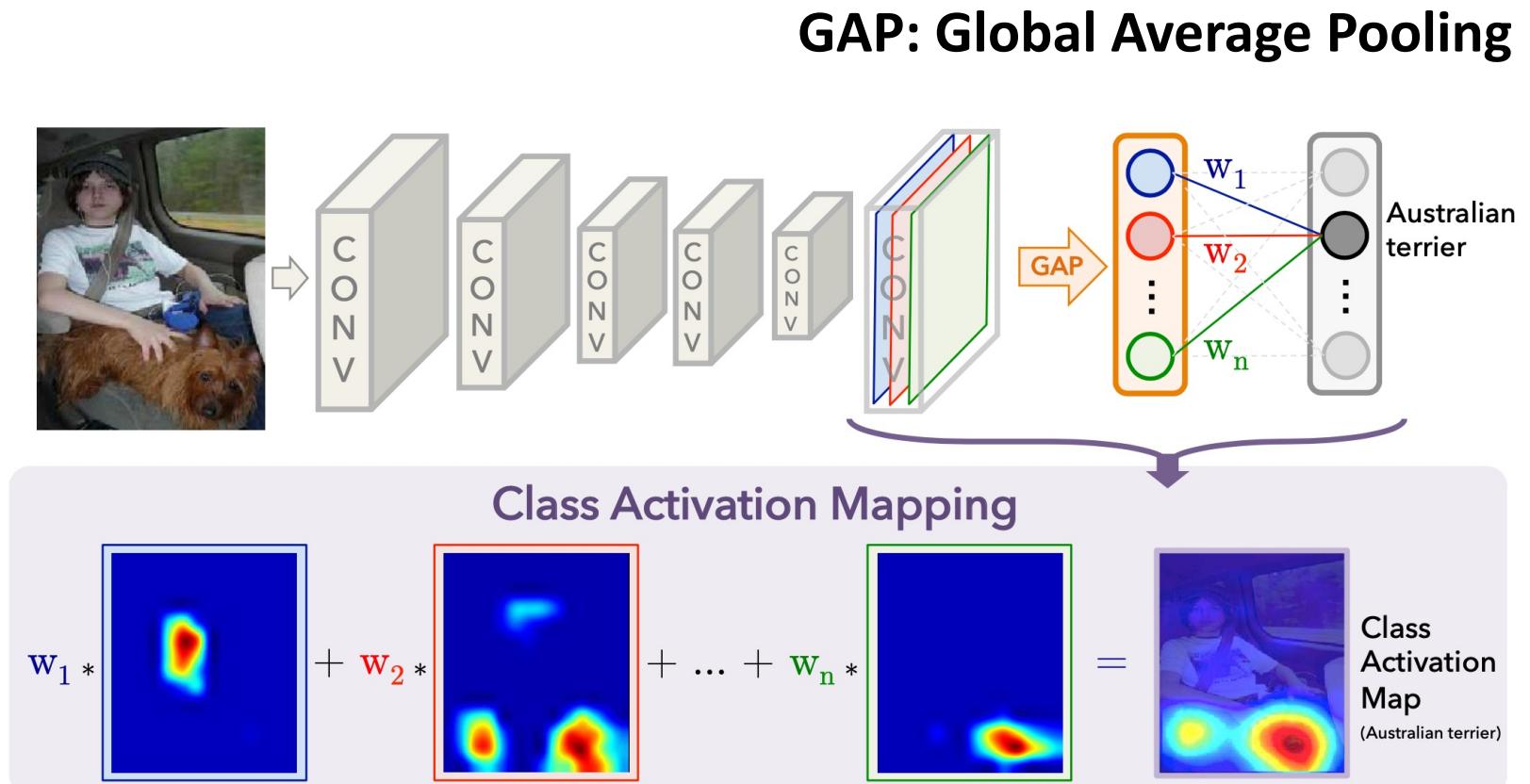
Methodology: Gradient-based Explanations

- Forward pass and back-propagation
 - Class activation mapping (CAM), Grad-GAM



Methodology: Gradient-based Explanations

- ❑ Forward pass and back-propagation
 - Class activation mapping (CAM), Grad-GAM



Methodology: Gradient-based Explanations

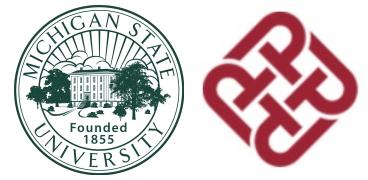
- Forward pass and back-propagation
 - Class activation mapping (CAM), Grad-GAM



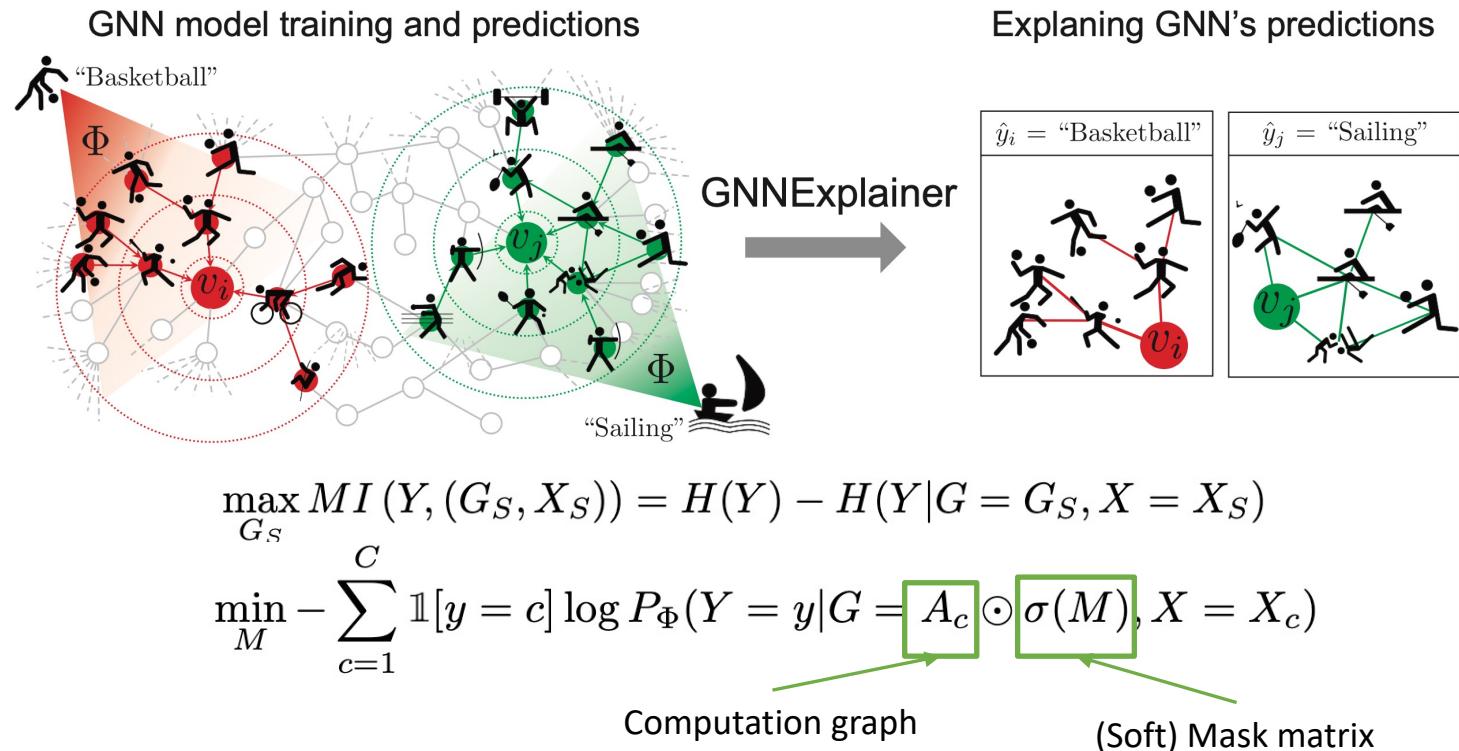
Zhou, Bolei, et al. "Learning deep features for discriminative localization.", 2016.

Selvaraju, Ramprasaath R., et al. "Grad-cam: Visual explanations from deep networks via gradient-based localization.", 2017.

Methodology: Perturbation-based Explanations



- ❑ Change the input and observe the effect on the output
 - GNNExplainer on Graphs
 - A **small subgraph** of the input graph that are most influential for target prediction



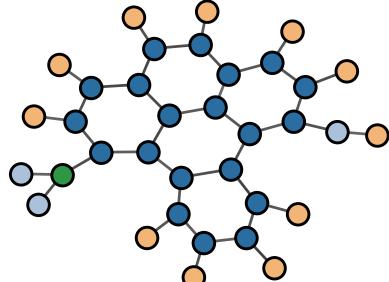
Methodology: Perturbation-based Explanations

- Change the input and observe the effect on the output

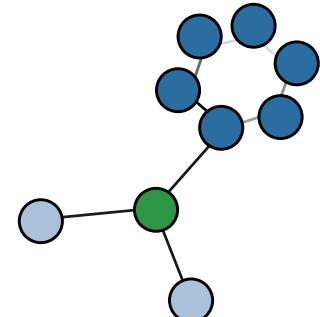
- GNNExplainer on Graphs
 - A small subgraph of the input graph that are most influential for target prediction

Molecular (atoms: hydrogen/carbon and bonds)

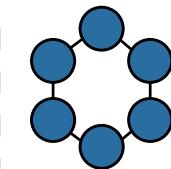
Computation graph



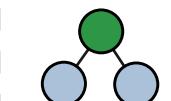
GNNExplainer



Ground Truth



Ring
structure



NO₂ group



Scope of Explanation

- ❑ Provide an explanation only for a specific instance or for the whole model
- ❑ Local Explanations
 - Explain a specific instance
- ❑ Global Explanations
 - Explain the whole model or a class

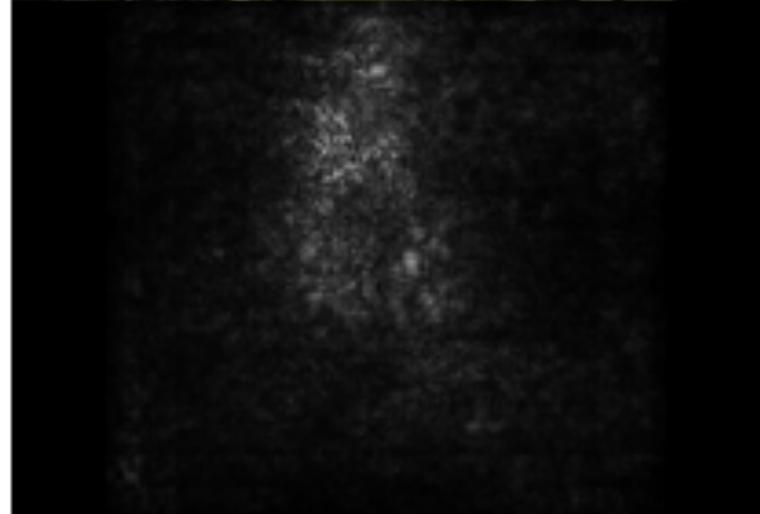
Scope: Local Explanations

- Explain a specific instance
 - Image-Specific Saliency Map

$$\text{SaliencyMap} = \text{gradient} = \frac{\partial \text{class score}}{\partial \text{input image}}$$

$$I^* = \text{argmax}_I S_y(I) - R(I)$$

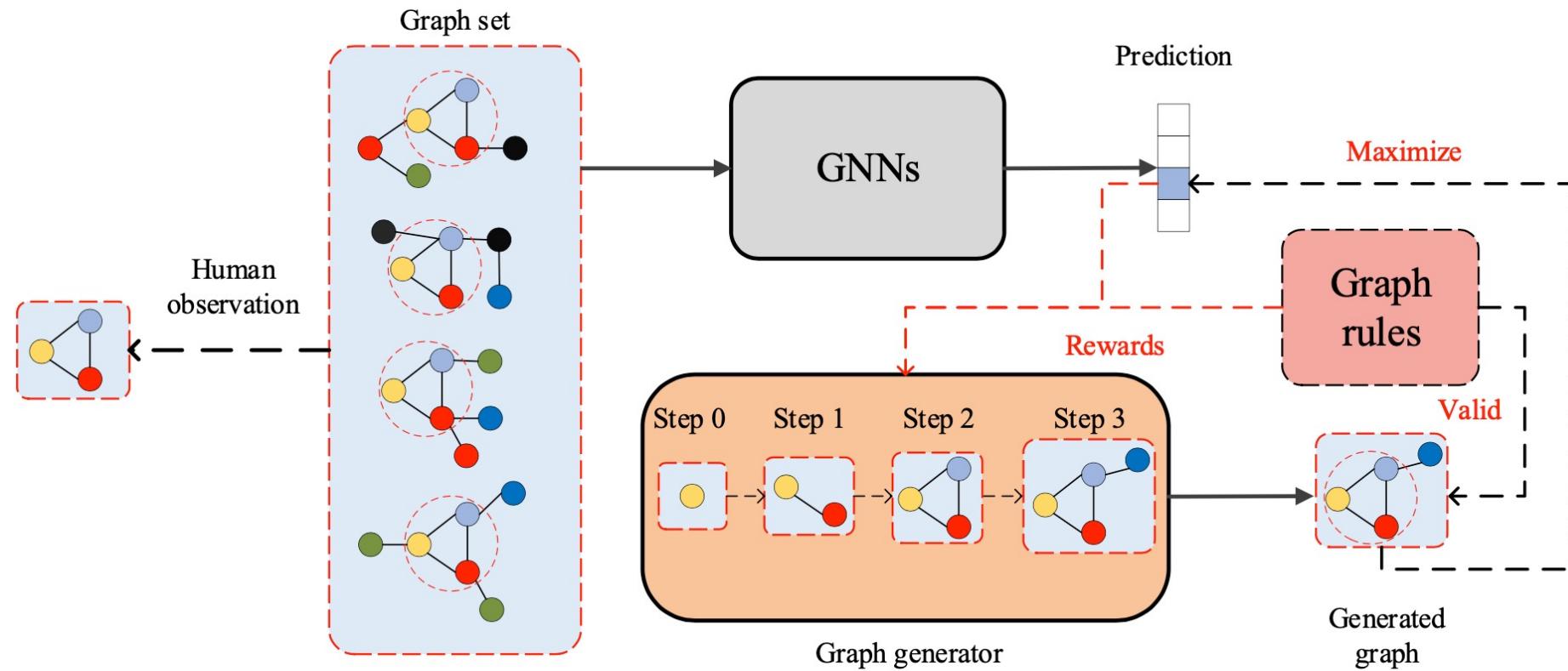
“Why is a given image classified as a monkey?”



Scope: Global Explanations

❑ Explain the whole model or a class

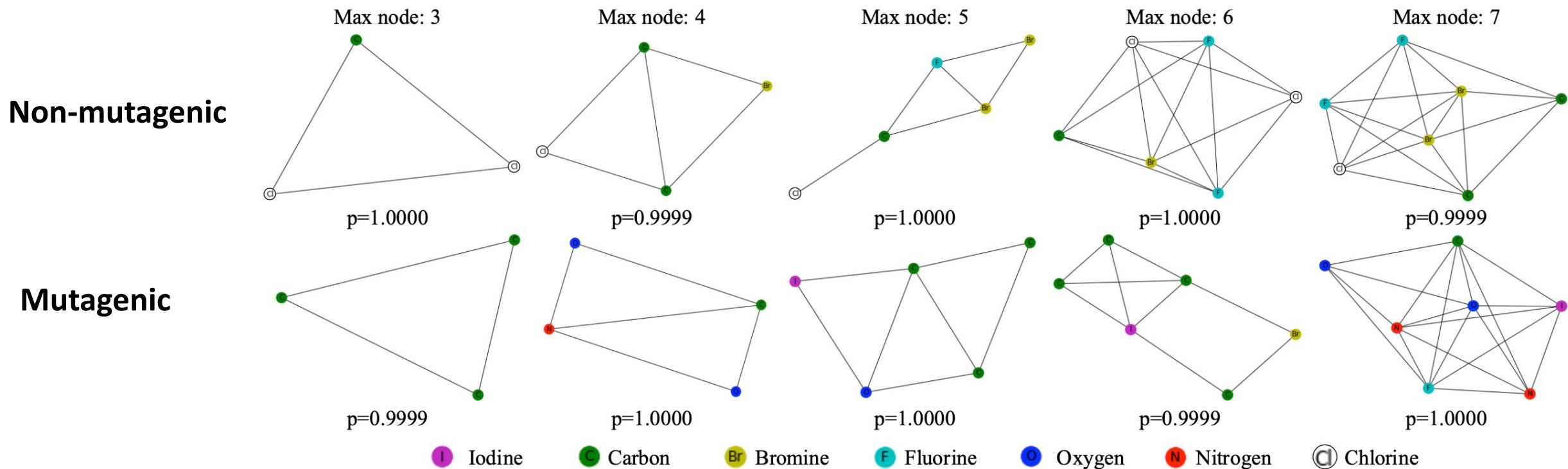
- XGNN: Model/Global-level Explanations on Graphs
 - Explain what **graph patterns** lead to a certain prediction (e.g., motifs)



Scope: Global Explanations

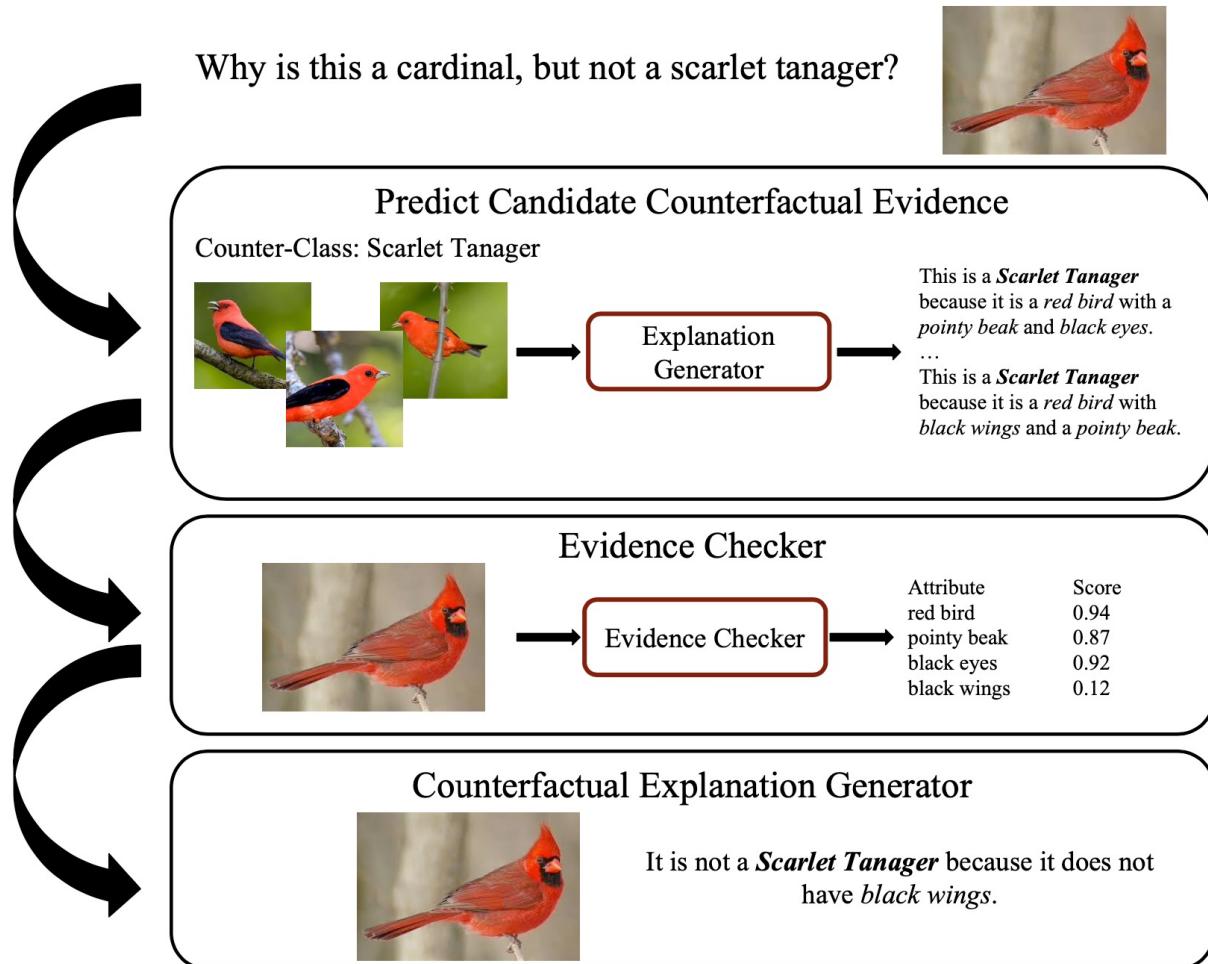
XGNN: Model/Global-level Explanations on Graphs

MUTAG (molecular: atoms/bonds)



Counterfactual Explanations

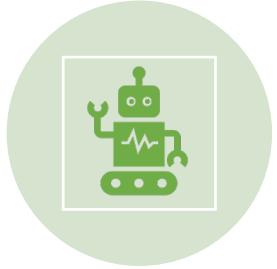
- Causal situation: “If X had not occurred, Y would not have occurred”.



Outline



CONCEPTS AND TAXONOMY



TECHNIQUES FOR
EXPLAINABILITY IN AI
(XAI)



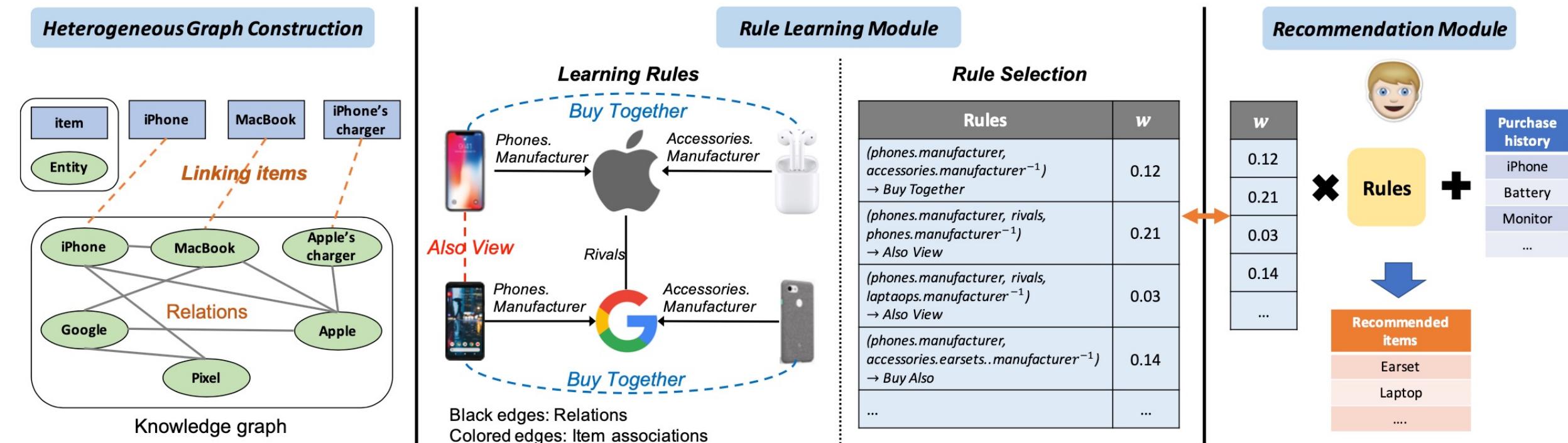
APPLICATIONS IN REAL
SYSTEMS



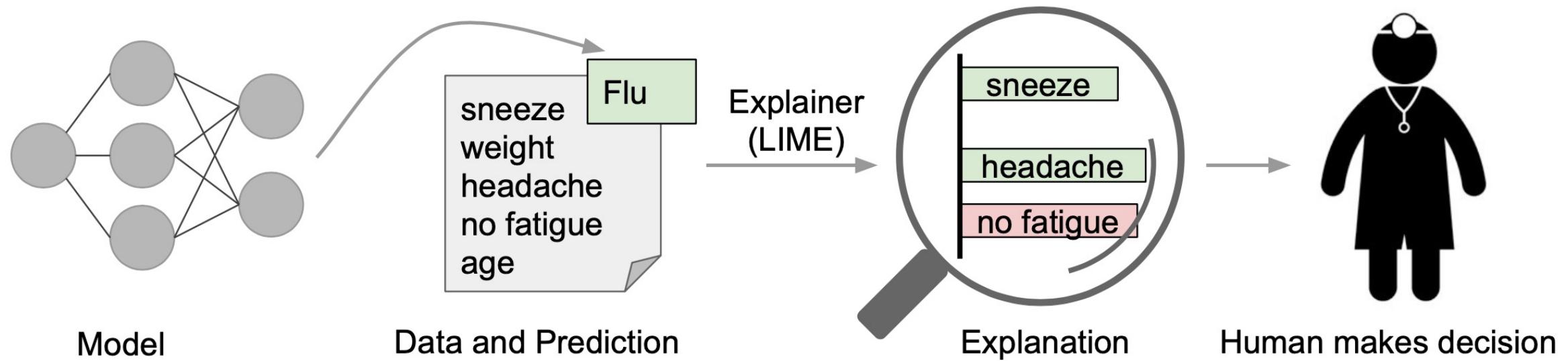
SURVEYS AND TOOLS

Recommender Systems

Explanations: Frequently Buy together, Also view, Buy after view, and Also buy, etc.



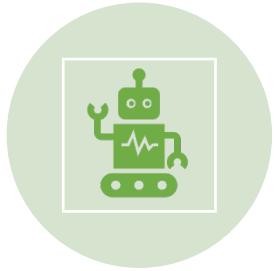
Natural Language Processing (NLP)



Outline



CONCEPTS AND TAXONOMY



TECHNIQUES FOR
EXPLAINABILITY IN AI
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APPLICATIONS IN REAL
SYSTEMS



SURVEYS AND TOOLS



Surveys

- Doshi-Velez, Finale, et al. "Towards a rigorous science of interpretable machine learning.", 2017.
- Guidotti, Riccardo, et al. "A survey of methods for explaining black box models.", 2018.
- Du, Mengnan, et al. "Techniques for interpretable machine learning.", 2019.
- Belle, Vaishak, et al. "Principles and practice of explainable machine learning.", 2020
- Miller, Tim. "Explanation in artificial intelligence: Insights from the social sciences.", 2019
- Molnar, Christoph. "Interpretable machine learning.", 2020
- Yuan, Hao, et al. "Explainability in Graph Neural Networks: A Taxonomic Survey.", 2020
- Arrieta, Alejandro Barredo, et al. "Explainable Artificial Intelligence (XAI): Concepts, taxonomies, opportunities and challenges toward responsible AI.", 2020
- Linardatos, Pantelis, et al. "Explainable ai: A review of machine learning interpretability methods.", 2021
- ...



Tools

AIX360

- <https://aix360.mybluemix.net>

InterpretML

- <https://github.com/interpretml/interpret>

DeepExplain

- <https://github.com/marcoancona/DeepExplain>

DIG for graph deep learning research

- <https://github.com/divelab/DIG>



Future Directions

- ❑ Security of explainable AI
- ❑ Evaluation methodologies
- ❑ Knowledge to target model: from white-box to black-box