Explainable Machine Learning

SLIDES BY:

XIAOYING WANG & JIANNAN WANG

https://www.cs.sfu.ca/~jnwang/

Outline

Motivation: Why Explainable ML matters?

Big Picture: Taxonomy

State-of-the-art Techniques

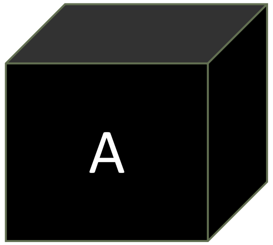
Outline

Motivation: Why Explainable ML matters?

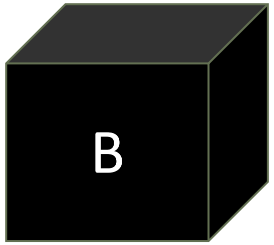
Big Picture: Taxonomy

State-of-the-art Techniques

Evaluation



Bird: 99.0%



Bird: 99.9%

Which model are you going to choose?

Evaluation

A

Because it has wings and a beak

Bird: 99.0%

B

Because it is white and the background is blue

Bird: 99.9%

Which model are you going to choose?

Debugging

What’s wrong?

Q: How symmetrical are the white bricks on either side of the building?

A: very

Q: How asymmetrical are the white bricks on either side of the building?

A: very

Q: How fast are the bricks speaking on either side of the building?

A: very

MUDRAKARTA, P.K., TALY, A., SUNDARARAJAN, M. AND DHAMDHERE, K., 2018. DID THE MODEL UNDERSTAND THE QUESTION?. ARXIV PREPRINT ARXIV:1805.05492.

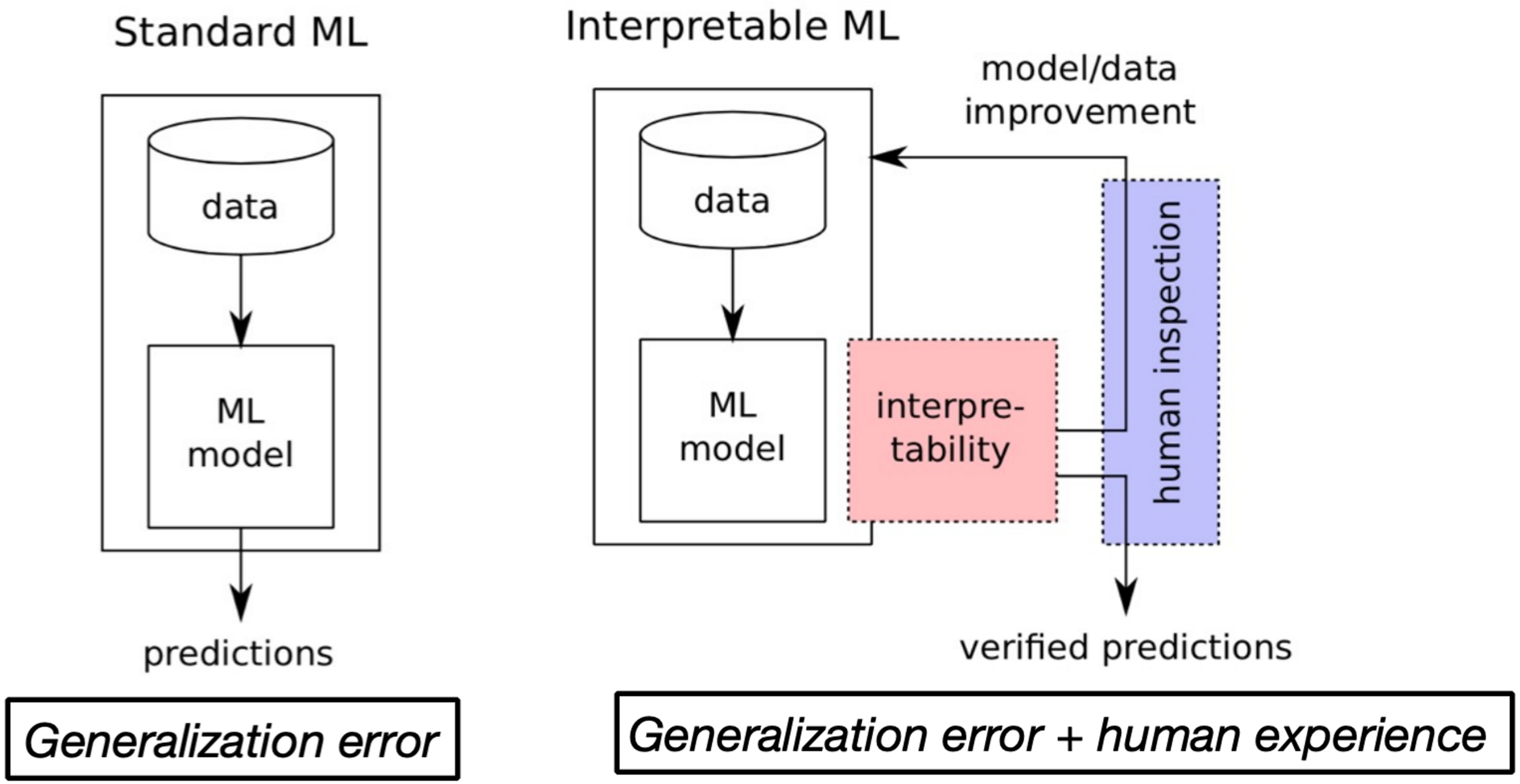
Debugging

How symmetrical are the white bricks on either side of the building?

red: high attribution
blue: negative attribution
gray: near-zero attribution

MUDRAKARTA, P.K., TALY, A., SUNDARARAJAN, M. AND DHAMDHERE, K., 2018. DID THE MODEL UNDERSTAND THE QUESTION?. ARXIV PREPRINT ARXIV:1805.05492.

Improvement



Learning insights

"It's not a human move. I've never seen a human play this move"

"So beautiful."

- Fan Hui

CADE METZ. 2017. THE SADNESS AND BEAUTY OF WATCHING GOOGLE'S AI PLAY GO. (JUNE 2017). RETRIEVED SEPTEMBER 20, 2019 FROM HTTPS://WWW.WIRED.COM/2016/03/SADNESS-BEAUTY-WATCHING-GOOGLES-AI-PLAY-GO/

Legal Concerns

SR 11-7: Guidance on Model Risk Management

BOARD OF GOVERNORS
OF THE FEDERAL RESERVE SYSTEM
WASHINGTON, D.C. 20551

DIVISION OF BANKING
SUPERVISION AND REGULATION

SR 11-7
April 4, 2011

TO THE OFFICER IN CHARGE OF SUPERVISION AND APPROPRIATE SUPERVISORY AND EXAMINATION STAFF AT EACH FEDERAL RESERVE BANK

SUBJECT: Guidance on Model Risk Management

Art. 22 GDPR

Automated individual decision-making, including profiling

Outline

Motivation: Why Explainable ML matters?

Big Picture: Taxonomy

State-of-the-art Techniques

Taxonomy

Transparent Models Linear Regression, Decision Tree, KNN, Bayesian Network…

Post-hoc Explanation

- **Global Model Explanation** Permutations, Partial Dependence Plots, Global Surrogate …
- **Individual Prediction Explanation** Attribution, Influential Instances, Local Surrogate …

Taxonomy

Transparent Models Linear Regression, Decision Tree, KNN, Bayesian Network…

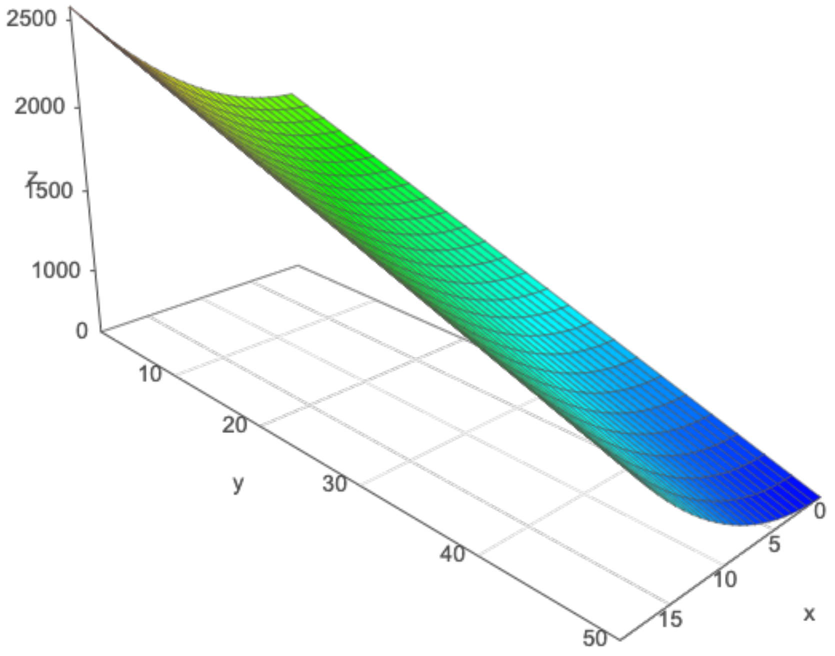
Post-hoc Explanation

- **Global Model Explanation** Permutations, Partial Dependence plots, Global Surrogate …
- **Individual Prediction Explanation** Attribution, Influential Instances, Local Surrogate …

Linear Regression

House rent (z) with respect to its area (x) and distance from SFU (y)

$$z = 2.1x - 2.4y + 1800$$

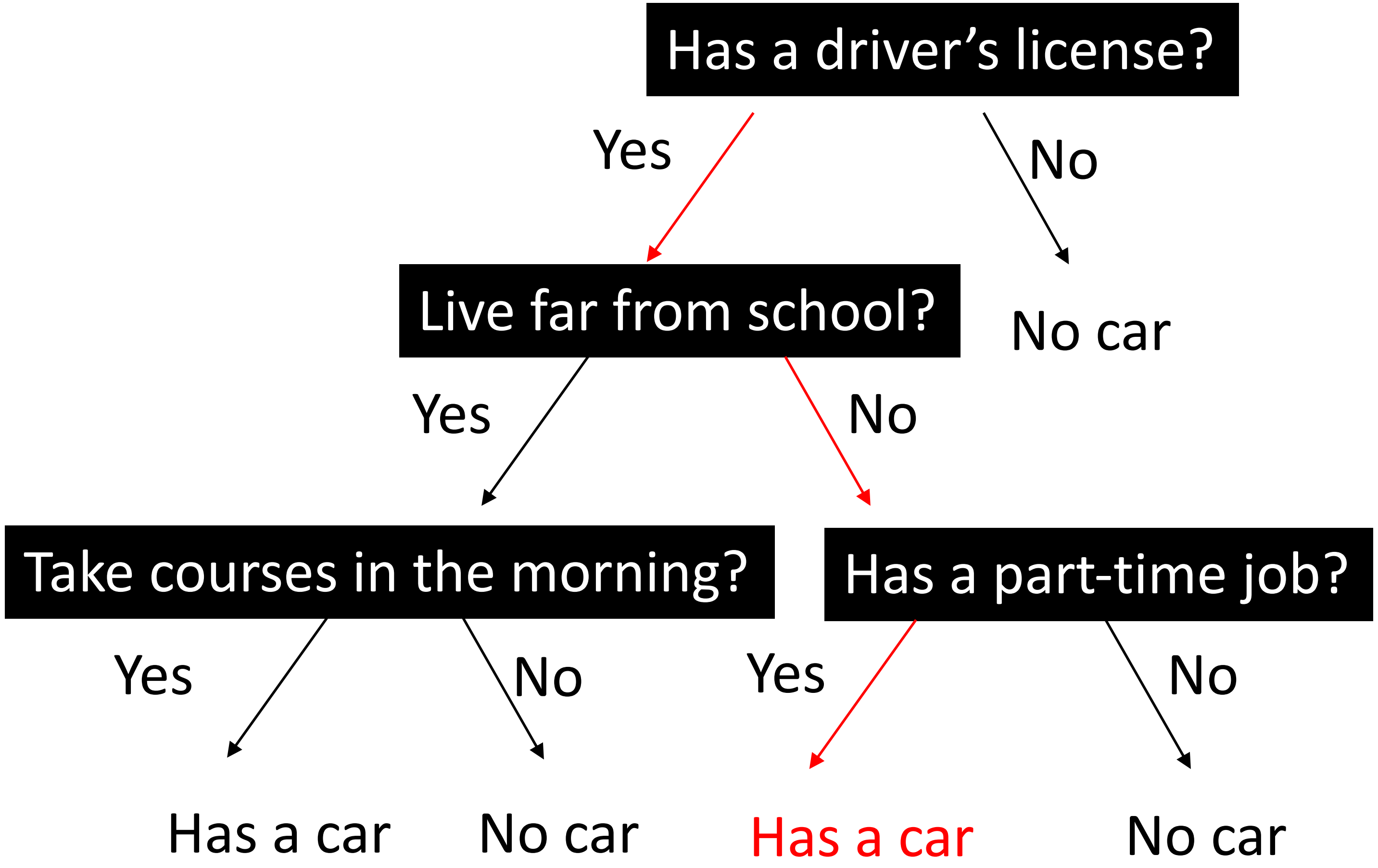


How do area and distance affect the house rent?

Decision Tree

Does a student own a car?

Why does the model predict student A has a car ?



Taxonomy

Transparent Models Linear Regression, Decision Tree, KNN, Bayesian Network…

Post-hoc Explanation

- **Global Model Explanation** Permutations, Partial Dependence Plots, Global Surrogate …
- **Individual Prediction Explanation** Attribution, Influential Instances, Local Surrogate …

Permutations

Main idea: measure the importance of a feature by calculating the increase in the model's prediction error after permuting the feature

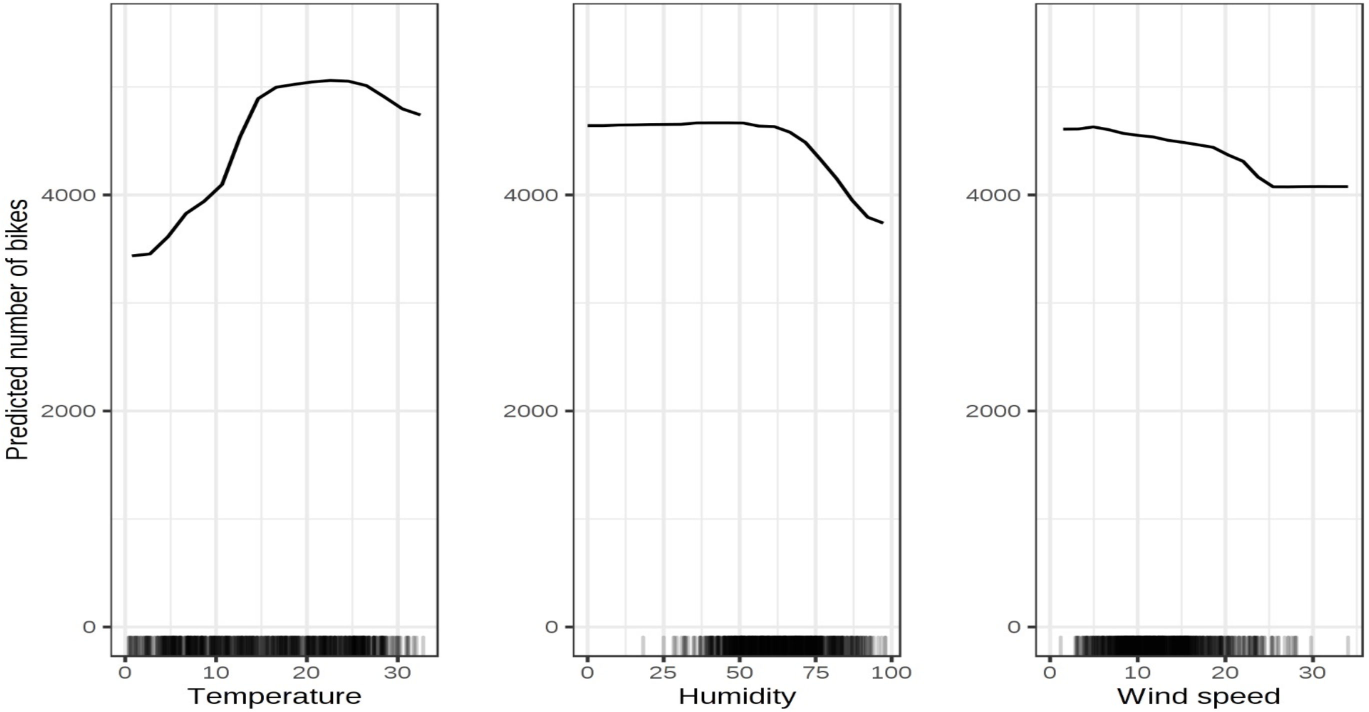
ID	Distance from SFU	# bathroom	Area	Closest bus stop	…
1	5.0km	1	$670ft^2$	0.30km	…
2	8.2km	2	$920ft^2$	0.12km	…
3	2.3km	2	$880ft^2$	1.20km	…
…	…	…	…	…	…
9999	10km	1	$680ft^2$	0.05km	…
10000	7.8km	1	$730ft^2$	0.23km	…

Permutations

- Input: trained model and labeled dataset for evaluation
- Output: relative importance for each feature
- Method:
  - Apply the model on original dataset and get an estimation error E
  - For each feature:
    - Permute feature and apply the model again on the permuted data to get a new estimation error E’
    - The feature importance can be measured by E’-E or E’/E

Partial Dependence Plots

Main idea: show the marginal effect one or two features have on the predicted outcome of a machine learning model



ID	Temperature	Humidity	Wind Speed	Rental#
1	20	30	20	3000
2	25	35	10	2500
3	22	25	15	3300
4	30	20	18	2000
..	..	…	…	…

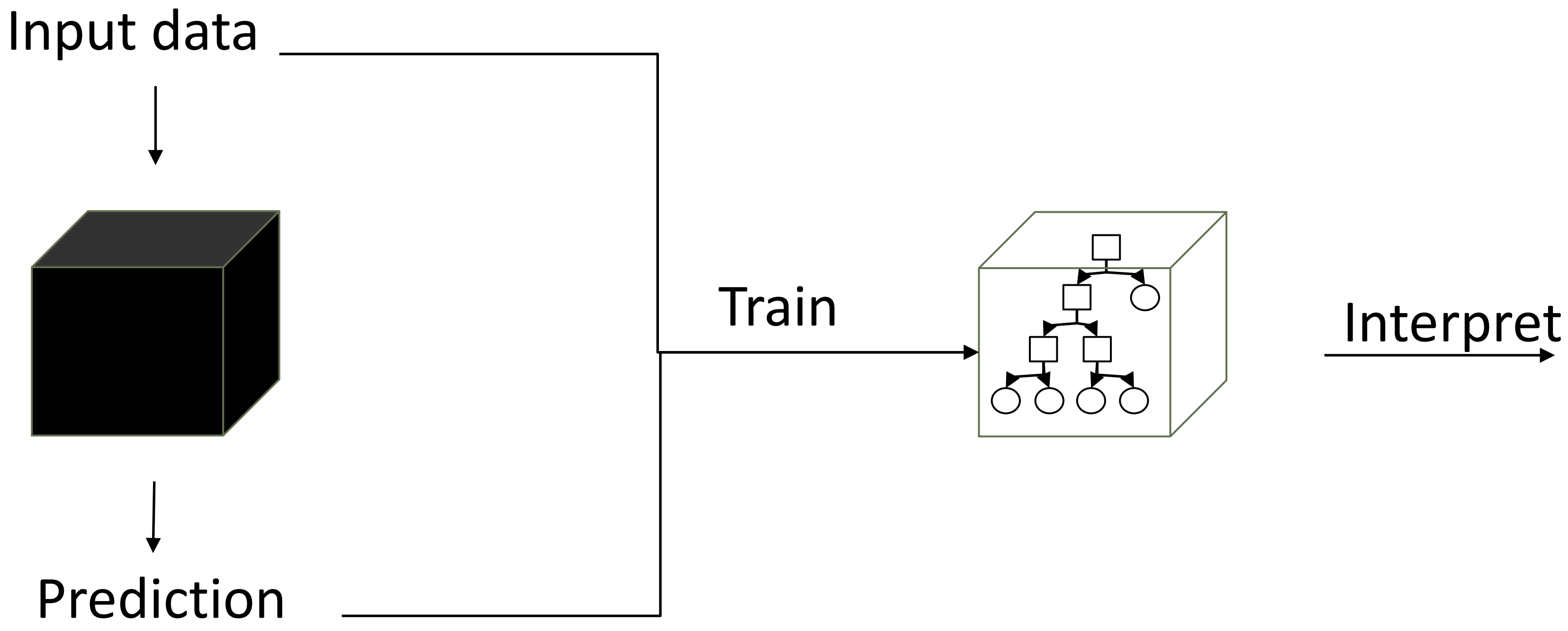
Partial Dependence Plots

Let x_S is the features set ($|x_S| \in \{1,2\}$) we want to examine, and x_C be the rest of the features used in the model $\hat{f}$:

- Partial dependence function: $\hat{f}_{x_S}(x_C) = E_{x_C}\left[\hat{f}(x_S, x_C)\right] = \int \hat{f}(x_S, x_C)dP(x_C)$
- Can be estimated by: $\hat{f}_{x_S}(x_C) = \frac{1}{n}\sum_{i=1}^{n} \hat{f}\,(x_S, x_C^{(i)})$

Global Surrogate

Main idea: train a transparent model to approximate the predictions of a black box model



Global Surrogate

Let $\hat{y}^{(i)}$ and $\hat{y}_*^{(i)}$ be the target model and surrogate model's prediction for the ith input data, we can use R-squared measure we can evaluate how good the surrogate model is in approximating the target model:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}\left(\hat{y}_*^{(i)} - \hat{y}^{(i)}\right)^2}{\sum_{i=1}^{n}\left(\hat{y}^{(i)} - \hat{y}_{avg}\right)^2}$$

Taxonomy

Transparent Models Linear regression, Decision tree, KNN, Bayesian Network…

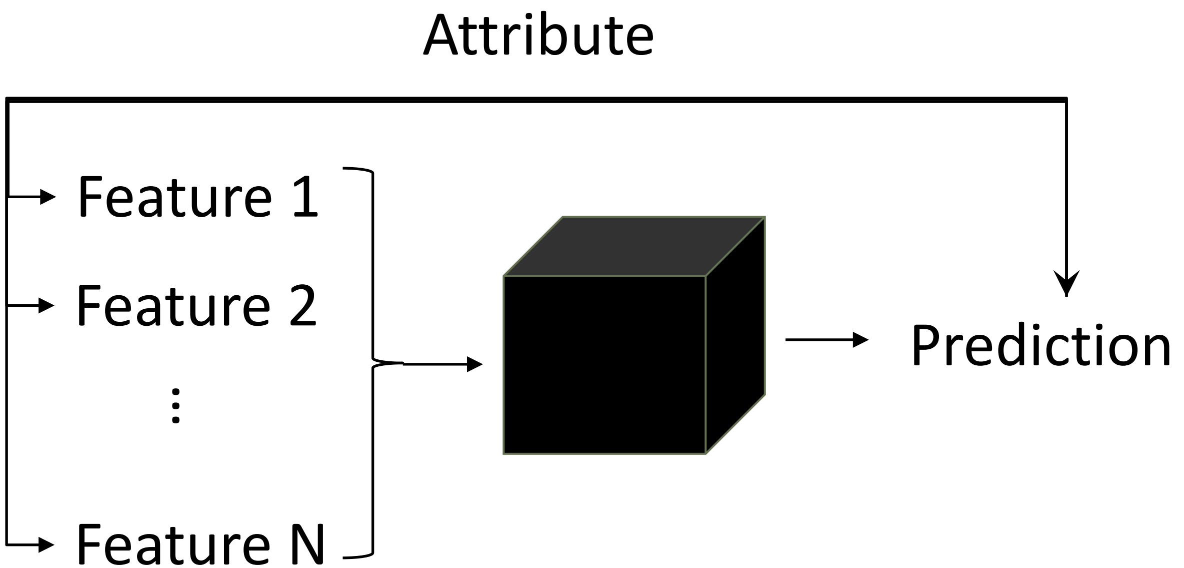
Post-hoc Explanation

Global Model Explanation Permutations, Partial dependence plots, Global surrogate …

Individual Prediction Explanation Attribution, Influential instances, Local surrogate …

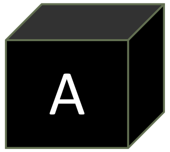
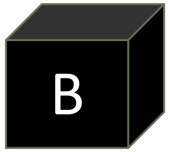
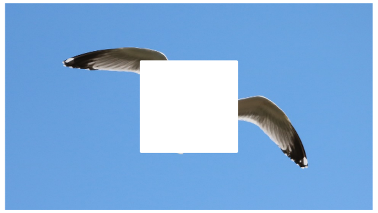
Attribution

- **Main idea:**
  - Attribute a model's prediction on a sample to its input features
- **Approaches:**
  - Ablation
  - Shapely value
  - …



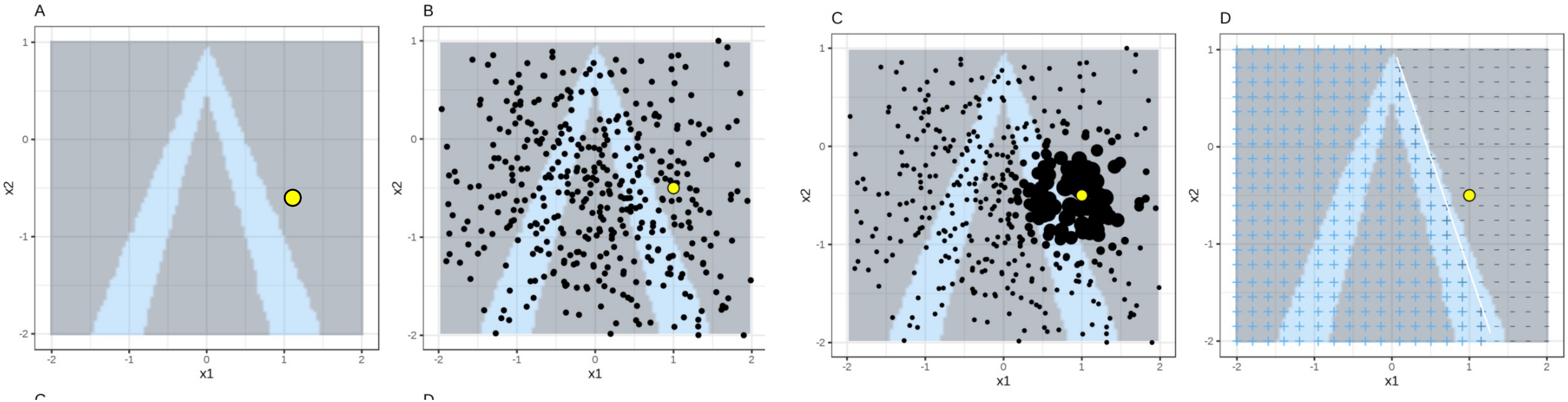
Attribution (Ablation)

Ablation: drop each feature and attribute the change in prediction to the feature

		
	Bird (99%)	Bird (99%)
	Bird (20%)	Bird (98%)
	Bird (96%)	Bird (35%)

Local Surrogate (LIME)

Main idea: Test what happens to the prediction when give variations of data into the machine learning model



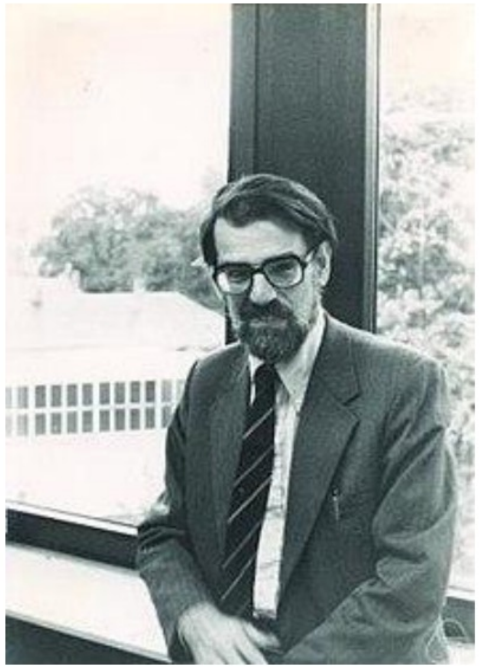
RIBEIRO, MARCO TULIO, SAMEER SINGH, AND CARLOS GUESTRIN. "WHY SHOULD I TRUST YOU?: EXPLAINING THE PREDICTIONS OF ANY CLASSIFIER." PROCEEDINGS OF THE 22ND ACM SIGKDD INTERNATIONAL CONFERENCE ON KNOWLEDGE DISCOVERY AND DATA MINING. ACM (2016)

Local Surrogate (LIME)

- The local surrogate model is obtained by: $argmin_{g \in G}\ L(f, g, \pi_x) + \Omega(g)$
  - f: target model, g: surrogate model, G: family of all possible g, π_x: neighborhood of target sample
  - L: measure fidelity, how the surrogate model approximate the target model
  - Ω: measure complexity of the surrogate model
- Get variation of data:
  - Text and image: turn single word or super-pixels on and off
  - Tabular data: create new samples by perturbing each feature individually

Shapley Value

- Classic result in game theory on distributing the total gain from a **cooperative game**
- Introduced by **Lloyd Shapley** in 1953 , who later won the **Nobel Prize in Economics** in the 2012
- Popular tool in studying cost-sharing, market analytics, voting power, and most recently **explaining ML models**



Lloyd Shapley in 1980

"A Value for n-person Games". Contributions to the Theory of Games 2.28 (1953): 307-317

Attribution (Shapely Value)

- Shapely value: derive from game theory on distributing gain in a coalition game
- Coalition game: players collaborating to generate some gain, function $val(S)$ represents the gain for any subset S of players
  - Game: prediction task
  - Players: input features
  - Gain: marginalized actual prediction minus average prediction $val_x(S) = \int \hat{f}(x_1, x_2, \ldots, x_p) dP_{x \notin S} - E(\hat{f}(X))$
- Marginal contribution of a feature i to a subset of other features: $val_x(S \cup \{x_i\}) - val_x(S)$

Attribution (Shapely Value)

- Shapely value of a feature i on sample x: weighted aggregation of its marginal contribution over all possible combinations of subsets of other features

$$\sum_{S \subseteq \{x_1, x_2, \ldots, x_p\} \setminus \{x_i\}} \frac{|S|!\,(p - |S| - 1)!}{p!} \left(val_x(S \cup \{x_i\}) - val_x(S)\right)$$

- Intuition: The feature values enter a room in random order. All feature values in the room participate in the game (= contribute to the prediction). The Shapley value of a feature value is the average change in the prediction that the coalition already in the room receives when the feature value joins them.

Example

- A company with two employees **Alice** and **Bob**
  - No employees, **0** profit
  - Alice alone makes **20** units of profit
  - Bob alone makes **10** units of profit
  - Alice and Bob make total **50** units of of profit
- What should be the bonuses be?

All Possible Orders	Marginal for Alice	Marginal for Bob
Alice, Bob	20	30
Bob, Alice	40	10
Shapley Value	30	20

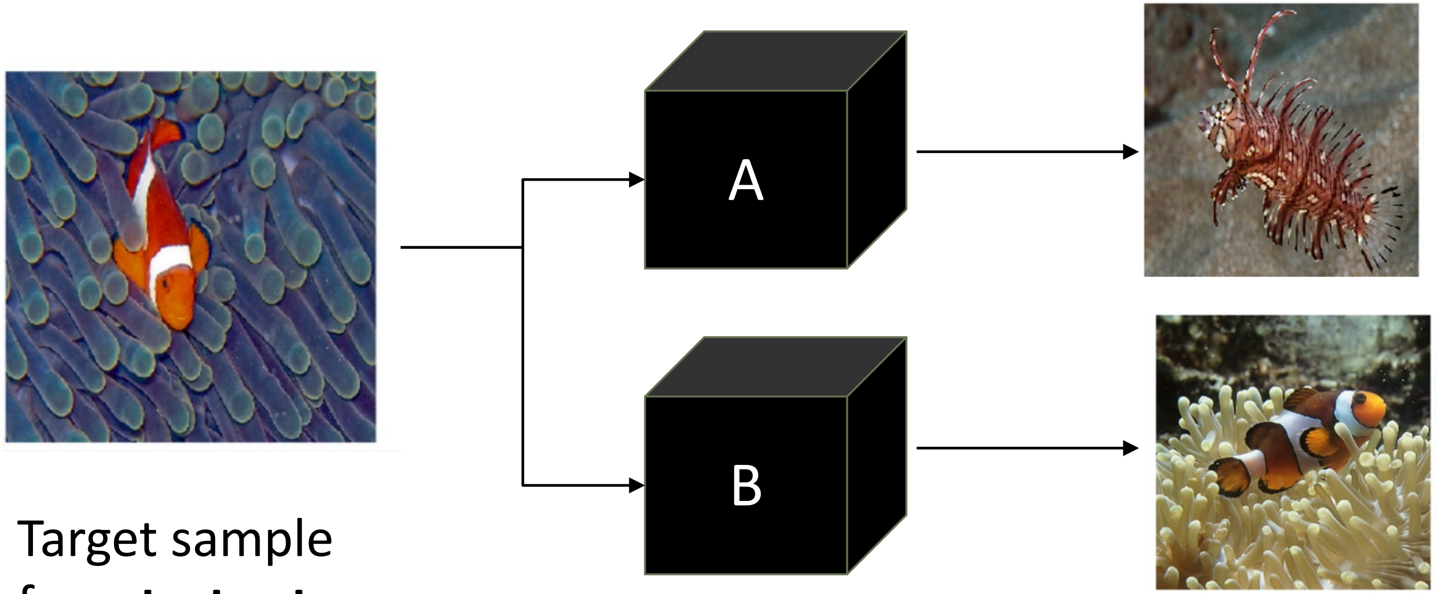
Attribution (Shapely Value)

- Two challenges when computing shapely value:
  - Exponential time since the permutation
  - Cannot inference on models when some features are not provided
- SHAP (SHapley Additive exPlanations) provide solutions for these two challenges:
  - KernelSHAP: an approximation solution for all models:
    - Sample a subset of feature orders
    - Filling missing features with background dataset provided by user

LUNDBERG, SCOTT M., AND SU-IN LEE. “A UNIFIED APPROACH TO INTERPRETING MODEL PREDICTIONS.” ADVANCES IN NEURAL INFORMATION PROCESSING SYSTEMS. 2017.

Influential Instances

Main idea: debug machine learning model by identifying influential training instances (a training instance is influential when its <u>deletion</u> from training data considerably changes the model's prediction)



The most influential **training** sample for each model

Target sample from **test set**

KOH, PANG WEI, AND PERCY LIANG. "UNDERSTANDING BLACK-BOX PREDICTIONS VIA INFLUENCE FUNCTIONS." PROCEEDINGS OF THE 34TH INTERNATIONAL CONFERENCE ON MACHINE LEARNING-VOLUME 70. JMLR. ORG, 2017

Influential Instances

- **Naïve approach: deletion diagnostics**
  - Train a model on all data instances, predict on test data and choose a target sample, for example: an incorrectly predicted sample with high confidence
  - For each training data, remove the data and retrain a model, predict on target sample and calculate the differences between the prediction and original prediction
  - Get the most influential top K instances (very likely to be mislabeled in this scenario)
  - Train a transparent model to find out what distinguishes the influential instances from the non-influential instances by analyzing their features (optional, for better understand the model)

Evaluation

- **Human review:** which method that human can get more insight of the model?
- **Fidelity:** how well does the method approximate the black box model?
- **Stability:** how much does an explanation differ for similar instances?
- **Complexity:** computational complexity of the method
- **Coverage:** the types of models that the method can explain
- ...

Available Tools

- LIME https://github.com/ankurtaly/Integrated-Gradients
- SHAP implementation in Python https://github.com/slundberg/shap
- Captum: PyTorch model interpretability tool https://github.com/pytorch/captum
- Skater: a Python Library for Model Interpretation/Explanations
  https://oracle.github.io/Skater/overview.html
- ELI5: a library for debugging/inspecting machine learning classifiers and explaining their predictions
  https://eli5.readthedocs.io/en/latest/
- Influence function implementation in Python https://github.com/kohpangwei/influence-release

References

- Molnar, Christoph. "Interpretable machine learning. A Guide for Making Black Box Models Explainable", 2021. https://christophm.github.io/interpretable-ml-book/.
- Anon. KDD'19 Explainable AI Tutorial. Retrieved September 13, 2019 from https://sites.google.com/view/kdd19-explainable-ai-tutorial
- Anon. ICCV'19 Tutorial on Interpretable Machine Learning in Computer Vision. Retrieved September 20, 2019 from https://interpretablevision.github.io/

Summary

Transparent Models Linear Regression, Decision Tree, KNN, Bayesian Network…

Post-hoc Explanation

- **Global Model Explanation** Permutations, Partial Dependence Plots, Global Surrogate …
- **Individual Prediction Explanation** Attribution, Influential Instances, Local Surrogate …