Explainable Machine Learning

SLIDES BY:

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Outline

Motivation: Why Explainable ML matters?

Big Picture: Taxonomy

State-of-the-art Techniques

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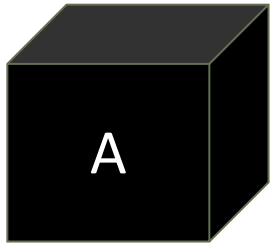
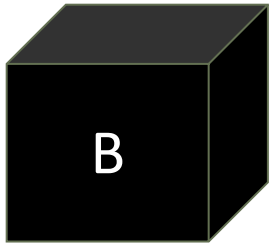
Evaluation



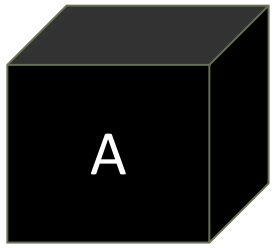
Bird: 99.0%



Bird: 99.9%

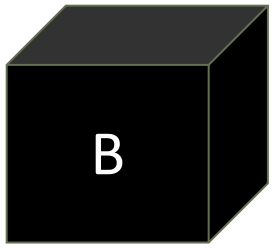
Which model are you going to choose?

Evaluation



Because it has wings and a beak

Bird: 99.0%



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.

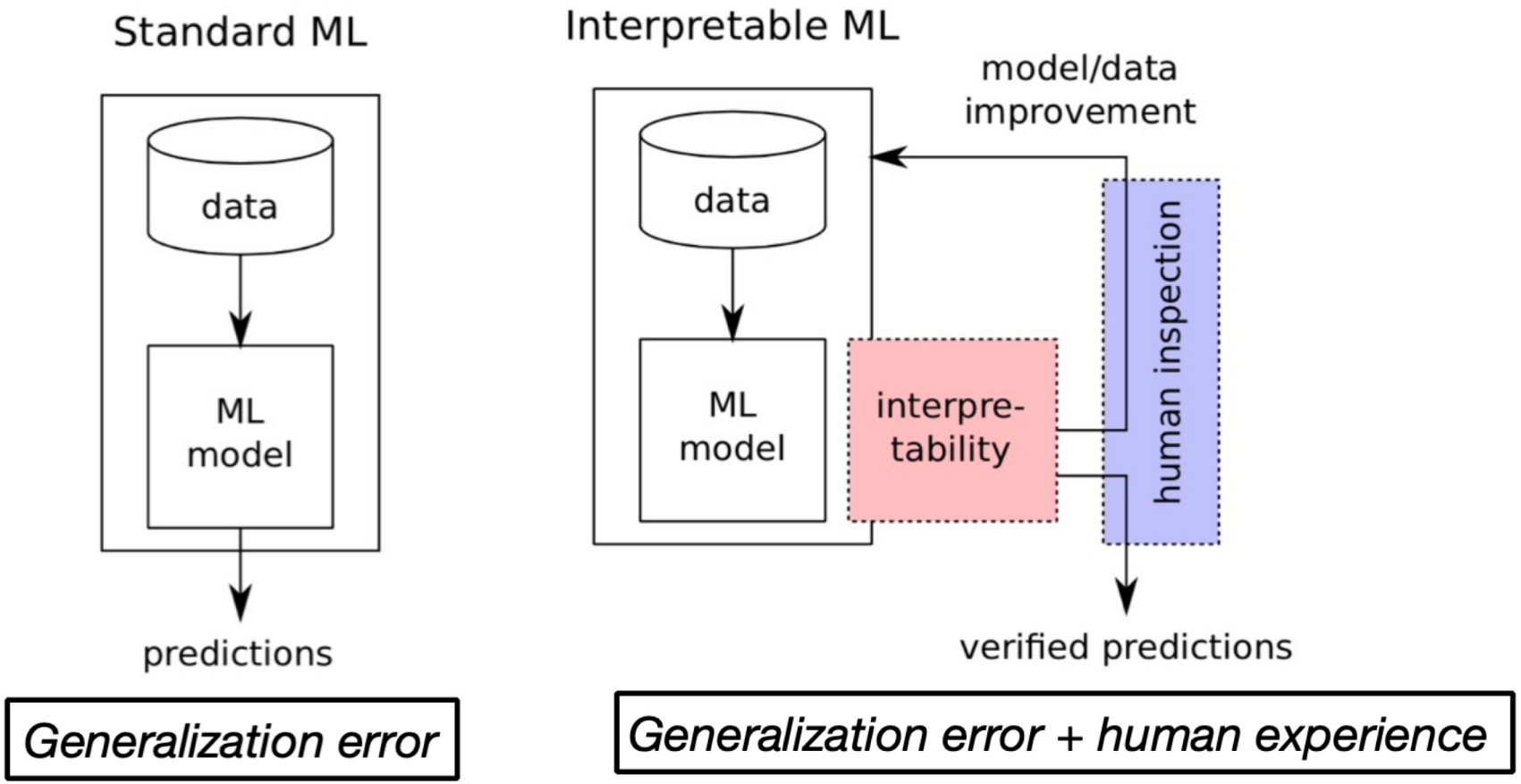
Debugging

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

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

General Data Protection Regulation

Art. 22 GDPR

Automated individual decision-making, including profiling

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Motivation: Why Explainable ML matters?

Big Picture: Taxonomy

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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…

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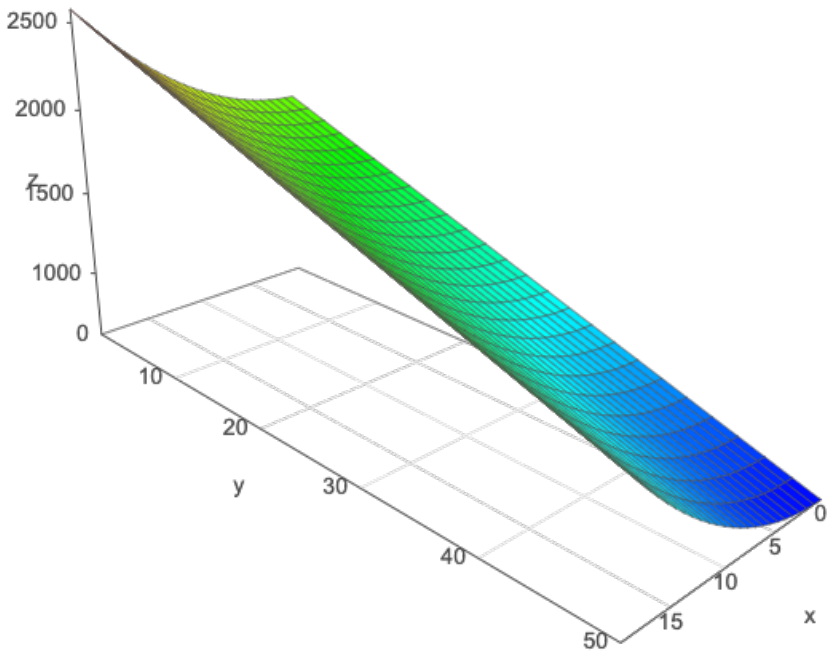
Linear Regression

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

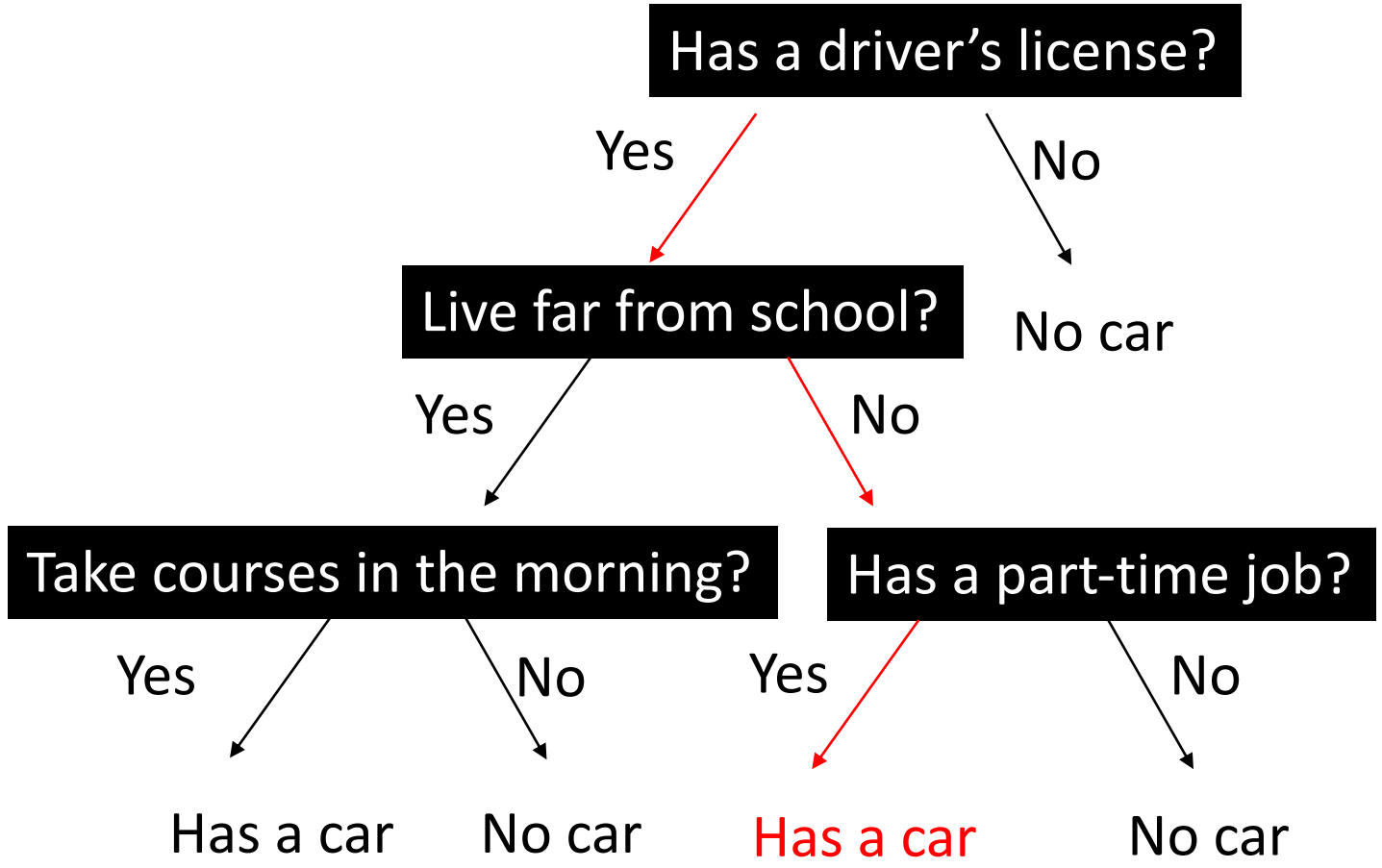
$$z = 2.1x - 2.4y + 1800$$



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 …
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Permutations

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

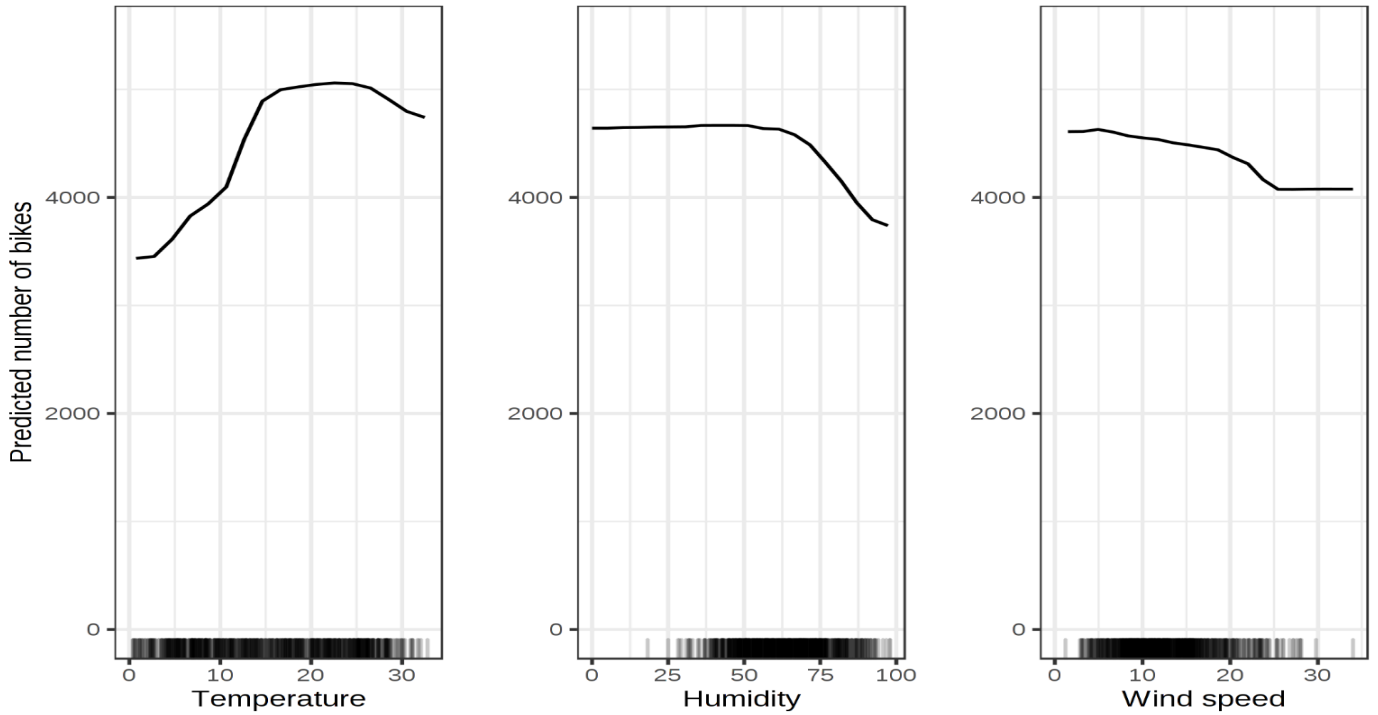
ID	Distance from SFU	# bathroom	Area	Closest bus stop	…
1	5.0km	1	$670ft^2$	0.30km	…
2	8.2km	2	$920ft^2$	0.12km	…
3	2.3km	2	$880ft^2$	1.20km	…
…	…	…	…	…	…
9999	10km	1	$680ft^2$	0.05km	…
10000	7.8km	1	$730ft^2$	0.23km	…

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



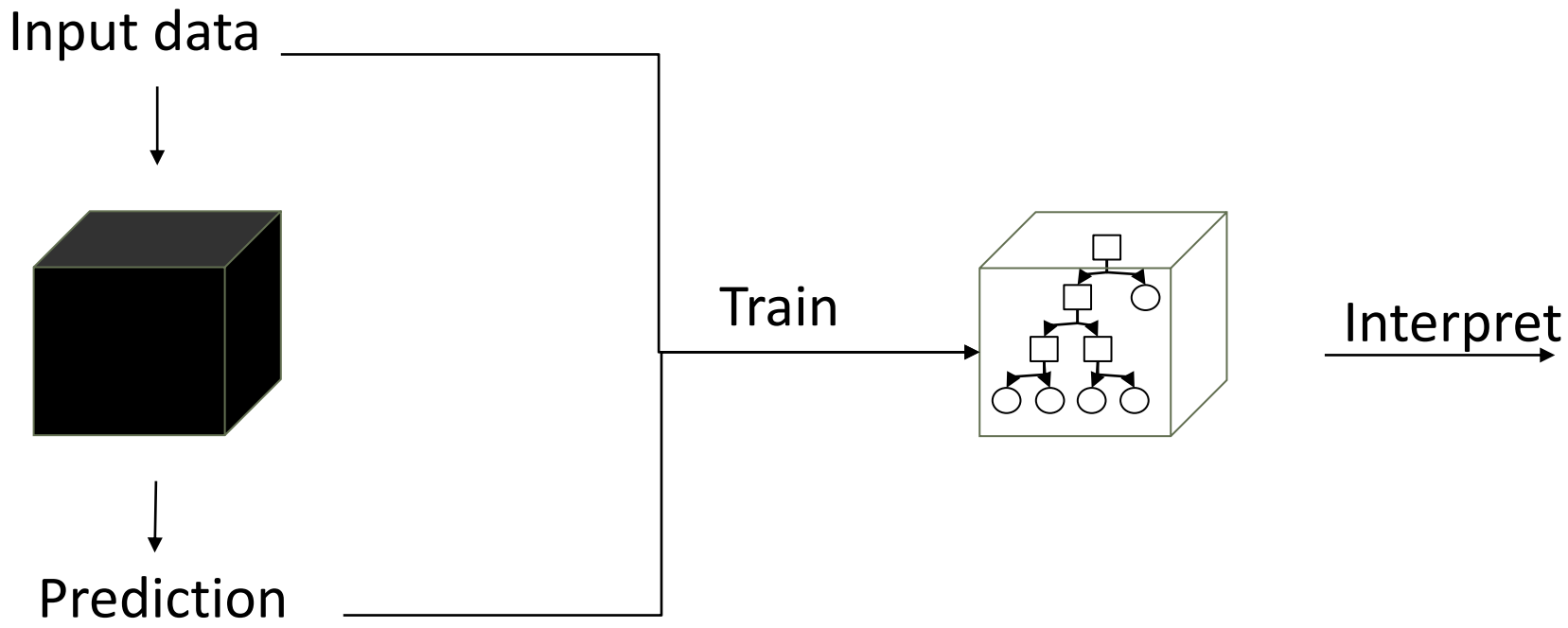
Partial Dependence Plots

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

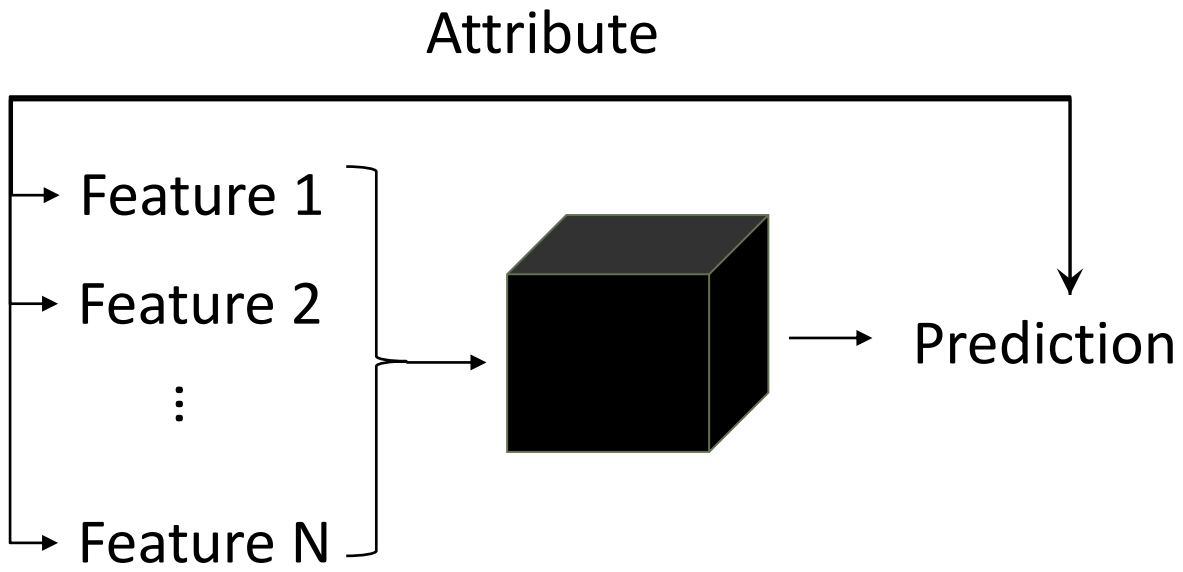
Transparent Models — Linear regression, Decision tree, KNN, Bayesian Network…

Post-hoc Explanation

- **Global Model Explanation** — Permutations, Partial dependence plots, Global surrogate …
- **Individual Prediction Explanation** — Attribution, Influential instances, Local surrogate …

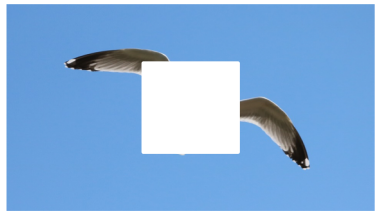
Attribution

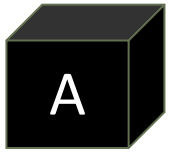
- **Main idea:**
  - Attribute a model's prediction on a sample to its input features
- **Approaches:**
  - Ablation
  - Shapely value
  - …



Attribution (Ablation)

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

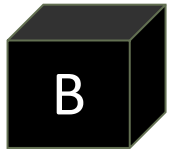




Bird (99%)

Bird (20%)

Bird (96%)



Bird (99%)

Bird (98%)

Bird (35%)

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 $val_x(S) =$

    $\int \hat{f}(x_1, x_2, \dots, x_p) dP_{x \notin S} - E(\hat{f}(X))$
- Marginal contribution of a feature i to a subset of other features: $val_x(S \cup \{x_i\}) - val_x(S)$

Attribution (Shapely Value)

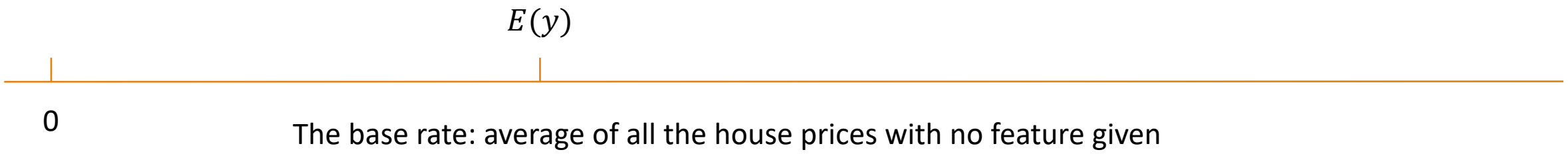
- Shapely value of a feature i on sample x: weighted aggregation of its marginal contribution over all possible combinations of subsets of other features

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

- 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.

Attribution (Shapely Value)

Explaining the house price prediction $\hat{y}$ based on x_1: distance from SFU, x_2: is pet allowed, x_3: nearest bus stop



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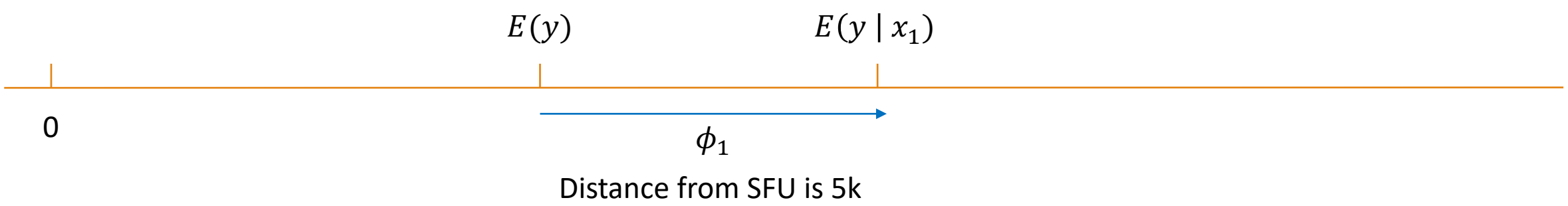

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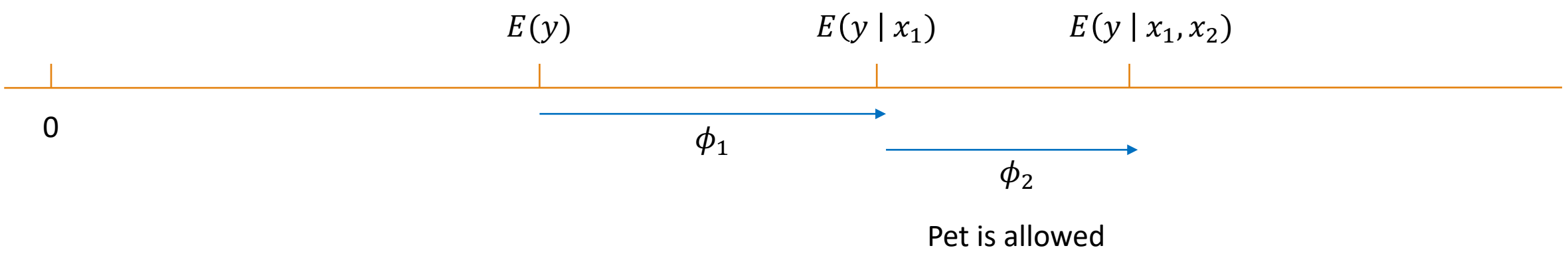

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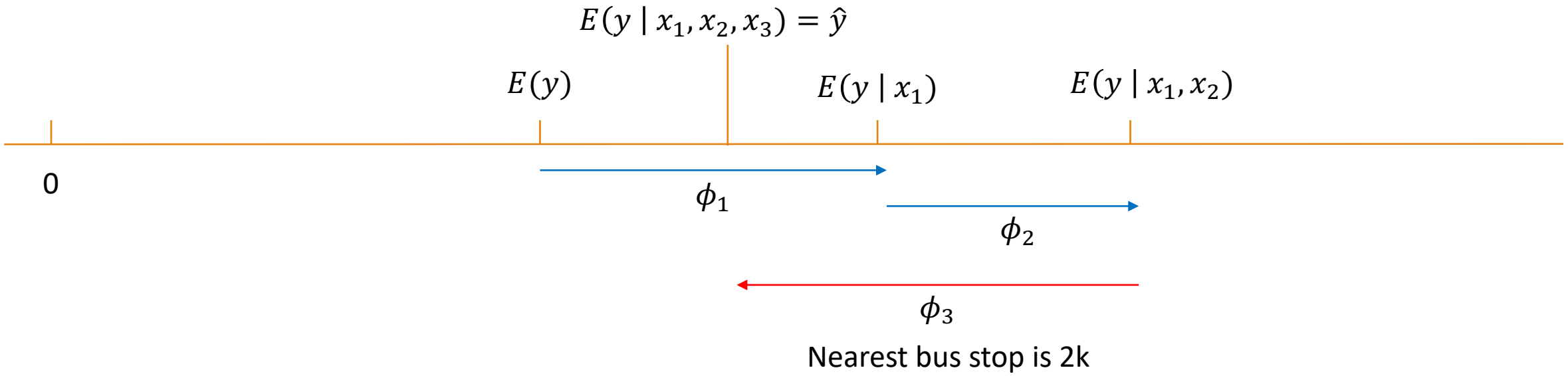
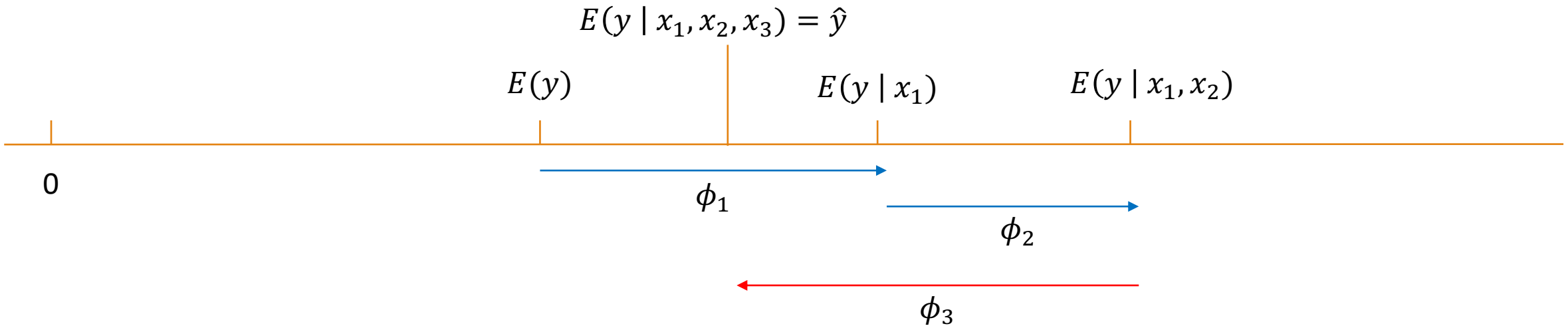


Attribution (Shapely Value)

Explaining the house price prediction $\hat{y}$ based on x_1: distance from SFU, x_2: is pet allowed, x_3: nearest bus stop

The order Matters! Need to average on all the permutations!



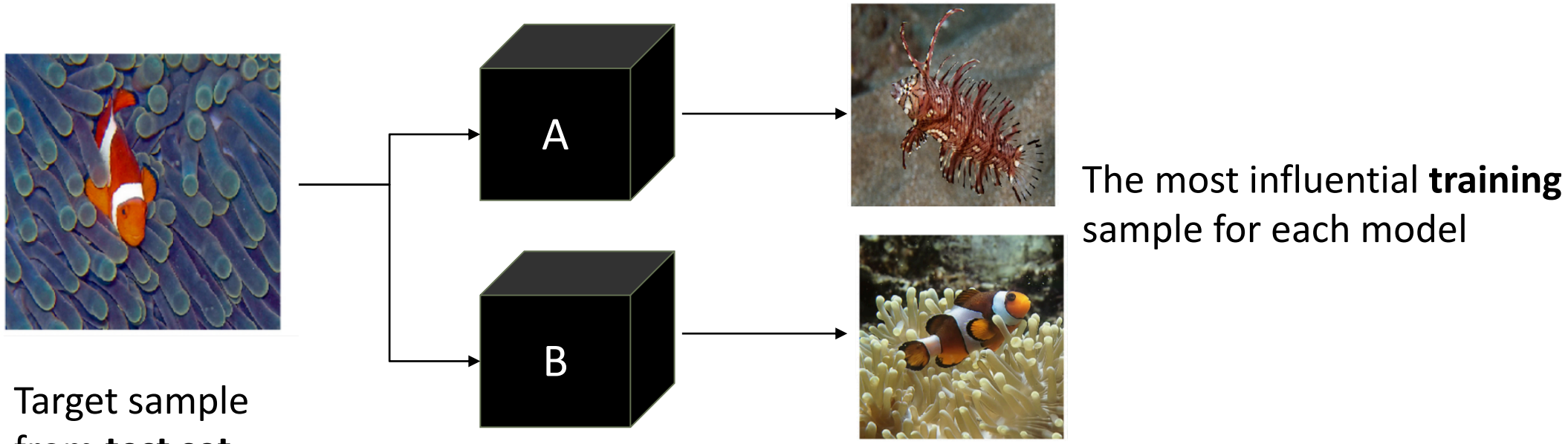
Attribution (Shapely Value)

- 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 deletion from training data considerably changes the model's prediction)



Target sample from **test set**

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

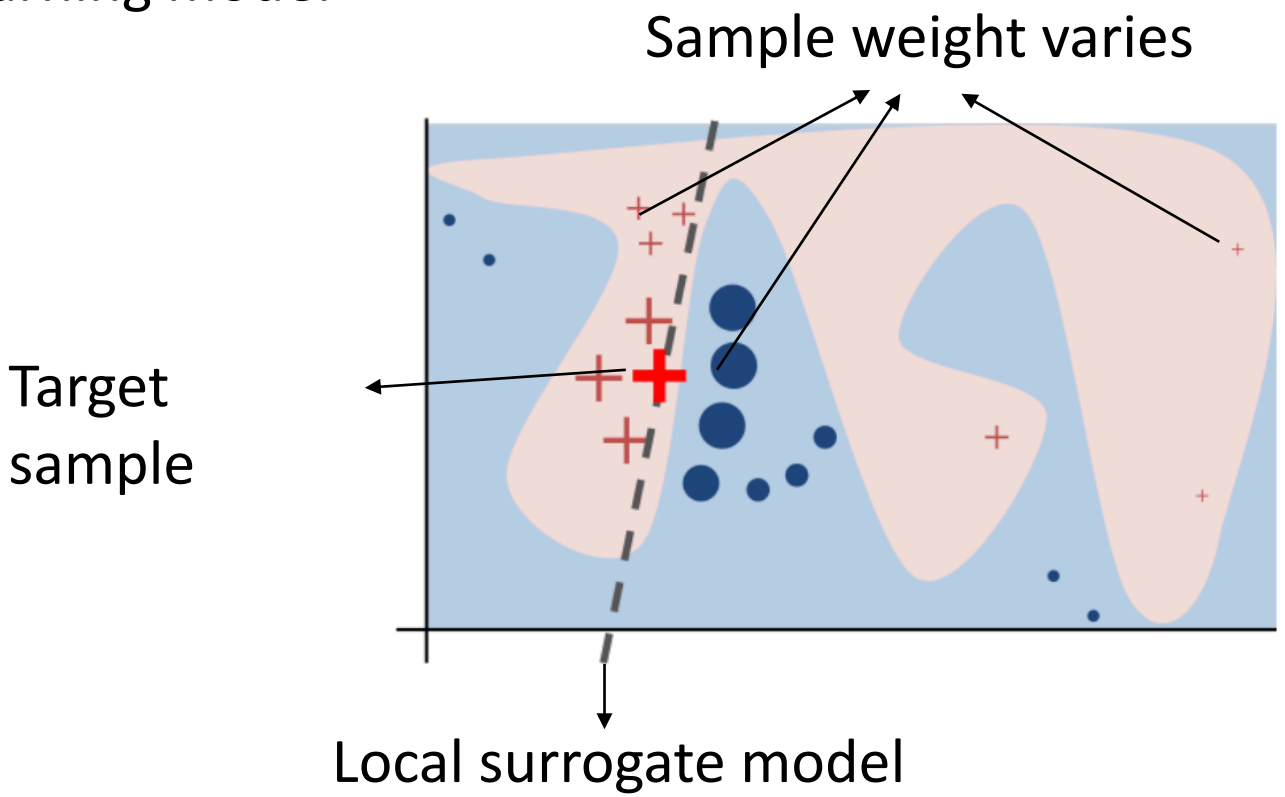
KOH, PANG WEI, AND PERCY LIANG. "UNDERSTANDING BLACK-BOX PREDICTIONS VIA INFLUENCE FUNCTIONS." PROCEEDINGS OF THE 34TH INTERNATIONAL CONFERENCE ON MACHINE LEARNING-VOLUME 70. JMLR. ORG, 2017

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)

Local Surrogate (LIME)

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



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

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

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- Anon. KDD'19 Explainable AI Tutorial. Retrieved September 13, 2019 from https://sites.google.com/view/kdd19-explainable-ai-tutorial
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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 …