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### Interpretability



## Welcome

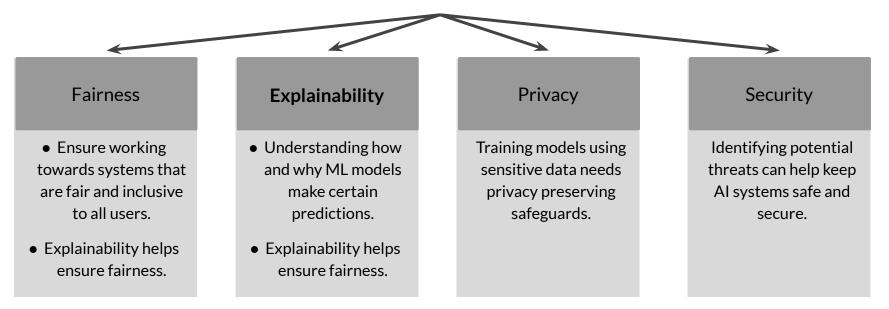
## Explainable AI



# Explainable AI

#### Responsible Al

- Development of AI is creating new opportunities to improve lives of people
- Also raises new questions about the best way to build the following into Al systems:



#### Explainable Artificial Intelligence (XAI)

The field of XAI allow ML system to be more transparent, providing explanations of their decisions in some level of detail.

These explanations are important:

To ensure algorithmic fairness.

Identify potential bias and problems in training data.

To ensure algorithms/models work as expected.

#### Need for Explainability in Al

- 1. Models with high sensitivity, including natural language networks, can generate wildly wrong results
- 2. Attacks
- 3. Fairness
- 4. Reputation and Branding
- 5. Legal and regulatory concerns
- 6. Customers and other stakeholders may question or challenge model decisions

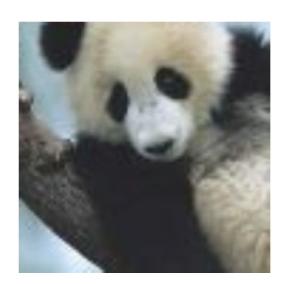
#### Deep Neural Networks (DNNs) can be fooled



DNNs can be fooled into misclassifying inputs with no resemblance to the true category.

#### Deep Neural Networks (DNNs) can be fooled

3+



"Panda" 57.7 % confidence



"Nematode" 8.2 % confidence



"Gibbon" 99.3 % confidence

### Interpretability



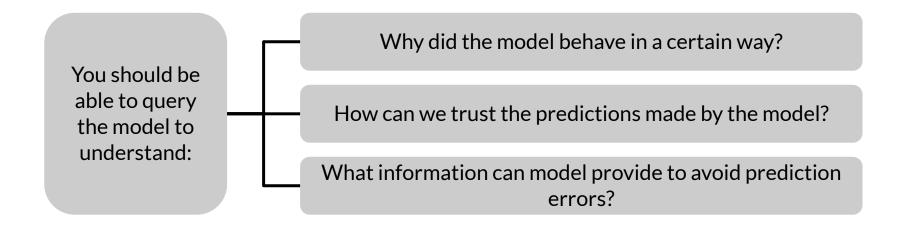
# Model Interpretation Methods

#### What is interpretability?

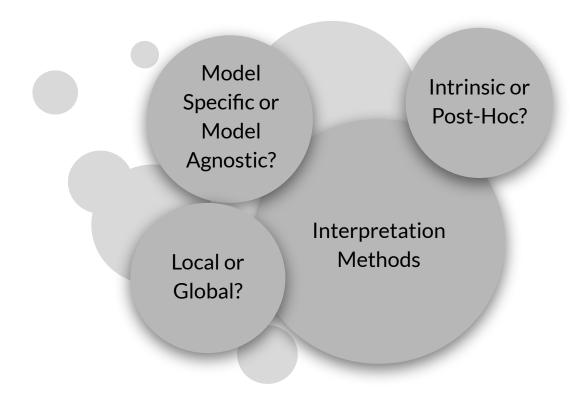
"(Models) are interpretable if their operations can be understood by a human, either through introspection or through a produced explanation."

"Explanation and justification in machine learning: A survey" - O. Biran, C. Cotton

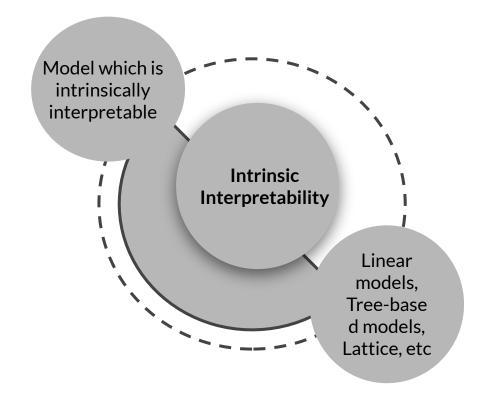
#### What are the requirements?



#### Categorizing Model Interpretation Methods



#### Intrinsic or Post-Hoc?



#### Intrinsic or Post-Hoc?

- Post-hoc methods treat models as black boxes
- Agnostic to model architecture
- Extracts relationships between features and model predictions, agnostic of model architecture
- Applied after training

#### Types of results produced by Interpretation Methods



Feature Summary
Statistics



Feature Summary Visualization



**Model Internals** 

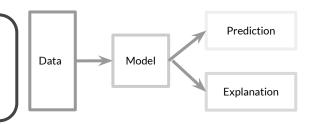


Data point

#### Model Specific or Model Agnostic

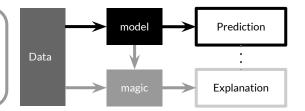
**Model Specific** 

- These tools are limited to specific model classes
- Example: Interpretation of regression weights in linear models
- Intrinsically interpretable model techniques are model specific
- Tools designed for particular model architectures

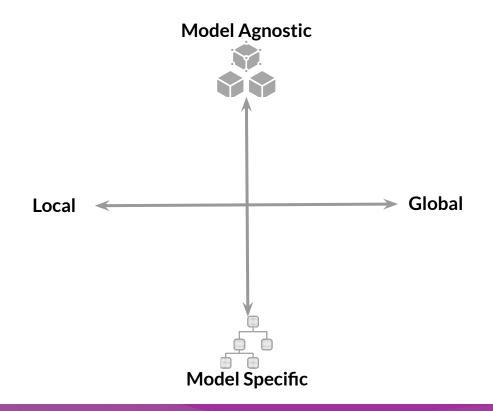


**Model Agnostic** 

- Applied to any model after it is trained
- Do not have access to the internals of the model
- Work by analyzing feature input and output pairs

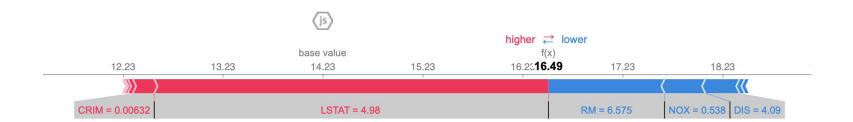


#### Interpretability of ML Models



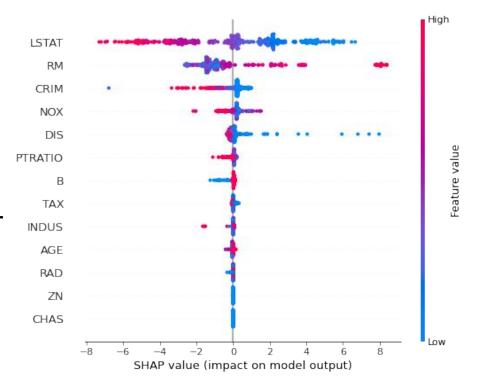
#### Local or Global?

- Local: interpretation method explains an individual prediction.
- Feature attribution is identification of relevant features as an explanation for a model.



#### Local or Global?

- Global: interpretation method explains entire model behaviour
- Feature attribution summary for the entire test data set



### Interpretability

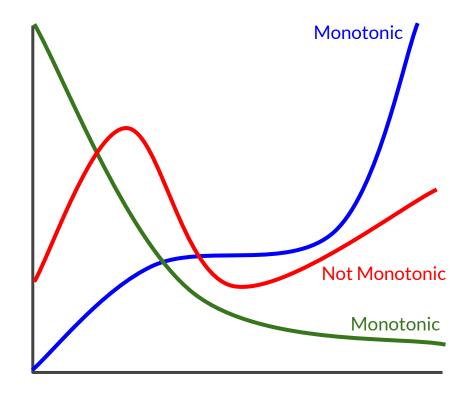


Intrinsically Interpretable Models

#### Intrinsically Interpretable Models

- How the model works is self evident
- Many classic models are highly interpretable
- Neural networks look like "black boxes"
- Newer architectures focus on designing for interpretability

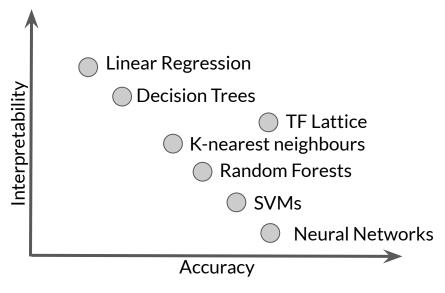
#### Monotonicity improves interpretability



### Interpretable Models

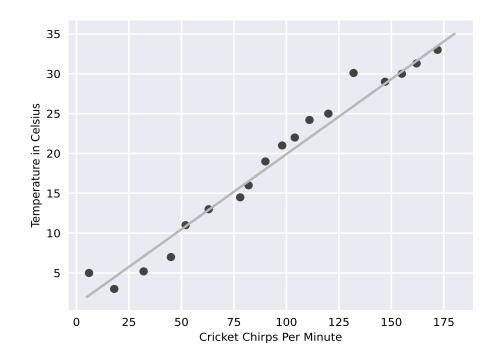
Algorithm	Linear	Monotonic	Feature Interaction	Task
Linear regression	Yes	Yes	No	regr
Logistic regression	No	Yes	No	class
Decision trees	No	Some	Yes	class, regr
RuleFit	Yes*	No	Yes	class, regr
K-nearest neighbors	No	No	No	class, regr
TF Lattice	Yes*	Yes	Yes	class, regr

#### Model Architecture Influence on Interpretability



Interpretability vs Accuracy Trade off

#### Classics: Linear Regression



#### Interpretation from Weights

Linear models have easy to understand interpretation from weights

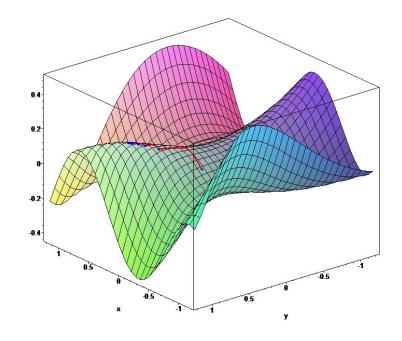
- Numerical features: Increase of one unit in a feature increases prediction by the value of corresponding weight.
- Binary features: Changing between 0 or 1 category changes the prediction by value of the feature's weight.
- Categorical features: one hot encoding affects only one weight.

#### Feature Importance

- Relevance of a given feature to generate model results
- Calculation is model dependent
- Example: linear regression model, t-statistic

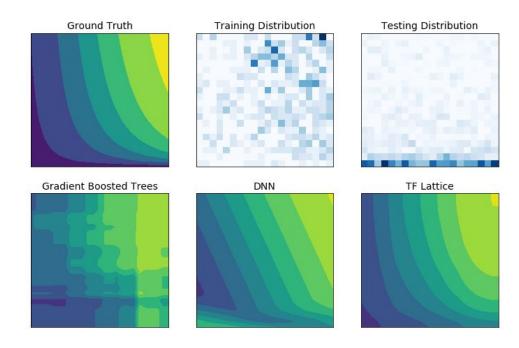
#### More advanced models: TensorFlow Lattice

- Overlaps a grid onto the feature space and learns values for the output at the vertices of the grid
- Linearly interpolates from the lattice values surrounding a point



#### More advanced models: TensorFlow Lattice

- Enables you to inject domain knowledge into the learning process through common-sense or policy-driven shape constraints
- Set constraints such as monotonicity, convexity, and how features interact



#### TensorFlow Lattice: Accuracy

#### Accuracy

- TensorFlow Lattice achieves accuracies comparable to neural networks
- TensorFlow Lattice provides greater interpretability



#### TensorFlow Lattice: Issues

#### **Dimensionality**

- The number of parameters of a lattice layer increases exponentially with the number of input features
- Very Rough Rule: Less than 20 features ok without ensembling

# Understanding Model Predictions



Model Agnostic Methods

#### Model Agnostic Methods

These methods separate explanations from the machine learning model.

#### Desired characteristics:

- Model flexibility
- Explanation flexibility
- Representation flexibility

#### Model Agnostic Methods

Partial Dependence Plots

**Individual Conditional Expectation** 

**Accumulated Local Effects** 

Permutation Feature Importance

Permutation Feature Importance

Global Surrogate

Local Surrogate (LIME)

**Shapley Values** 

**SHAP** 



# Understanding Model Predictions



# Partial Dependence Plots



#### Partial Dependence Plots (PDP)

A partial dependence plot shows:

- The marginal effect one or two features have on the model result
- Whether the relationship between the targets and the feature is linear, monotonic, or more complex

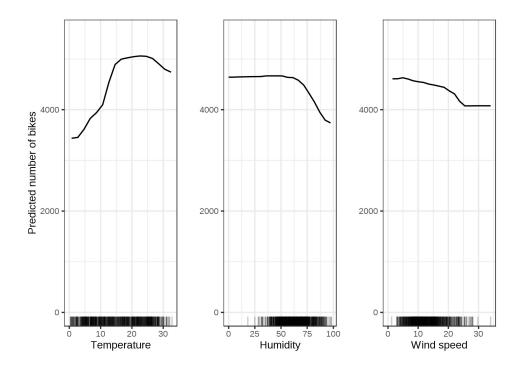
#### Partial Dependence Plots

The partial function  $f_{xs}$  is estimated by calculating averages in the training data:

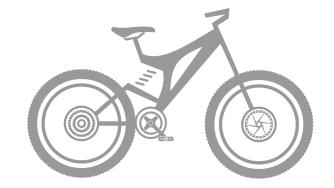


$$\hat{f}_{x_S}(x_S) = \frac{1}{n} \sum_{i=1}^n \hat{f}(x_S, x_C^{(i)})$$

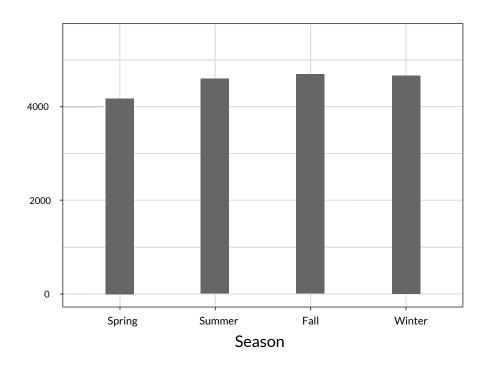
#### Partial Dependence Plots: Examples



PDP plots for a linear regression model trained on a bike rentals dataset to predict the number of bikes rented



#### PDP for Categorical Features



#### Advantages of PDP

- Computation is intuitive
- If the feature whose PDP is calculated has no feature correlations, PDP perfectly represents how feature influences the prediction on average
- Easy to implement

#### Disadvantages of PDP

- Realistic maximum number of features in PDP is 2
- PDP assumes that feature values have no interactions

### Understanding Model Predictions



# Permutation Feature Importance

#### Permutation Feature Importance

Feature importance measures the increase in prediction error after permuting the features

#### Feature is **important** if:

Shuffling its values increases model error

#### Feature is **unimportant** if:

Shuffling its values leaves model error unchanged



#### Permutation Feature Importance

- Estimate the original model error
- For each feature:
  - Permute the feature values in the data to break its association with the true outcome
  - Estimate error based on the predictions of the permuted data
  - Calculate permutation feature importance
  - Sort features by descending feature importance

#### Advantages of Permutation Feature Importance

- Nice interpretation: Shows the increase in model error when the feature's information is destroyed.
- Provides global insight to model's behaviour
- Does not require retraining of model

#### Disadvantages of Permutation Feature Importance

- It is unclear if testing or training data should be used for visualization
- Can be biased since it can create unlikely feature combinations in case of strongly correlated features
- You need access to the labeled data

### Understanding Model Predictions



### **Shapley Values**

#### Shapley Value

- The Shapley value is a method for assigning payouts to players depending on their contribution to the total
- Applying that to ML we define that:
  - Feature is a "player" in a game
  - Prediction is the "payout"
  - Shapley value tells us how the "payout" (feature contribution)
     can be distributed among features

#### Shapley Value: Example



Suppose you trained an ML model to predict apartment prices

You need to explain why the model predicts €300,000 for a certain apartment.

Average prediction of all apartments: €310,000.

#### Shapley Value

Term in Game Theory	Relation to ML	Relation to House Prices Example	
Game	Prediction task for single instance of dataset	Prediction of house prices for a single instance	
Gain	Actual prediction for instance - Average prediction for all instances	Prediction for house price (€300,000) - Average Prediction(€310,000) = -€10,000	
Players	Feature values that contribute to prediction	'Park=nearby', 'cat=banned', 'area=50m²', 'floor=2nd'	

#### **Shapley Value**

#### Goal:

Explain the difference between the actual prediction ( $\leq$ 300,000) and the average prediction ( $\leq$ 310,000): a difference of - $\leq$ 10,000.

Feature	Contribution
'park-nearby'	€30,000
size-50	€10,000
floor-2nd	€0
cat-banned	-€50,000
Total: -€10,000 (Final prediction - Average Prediction)	

One possible explanation

#### Advantages of Shapley Values

Based on solid theoretical foundation.
Satisfies Efficiency, Symmetry, Dummy, and Additivity properties

Value is fairly distributed among all features

Enables contrastive explanations

#### Disadvantages of Shapley Values

- Computationally expensive
- Can be easily misinterpreted
- Always uses all the features, so not good for explanations of only a few features.
- No prediction model. Can't be used for "what if" hypothesis testing.
- Does not work well when features are correlated

## Understanding Model Predictions

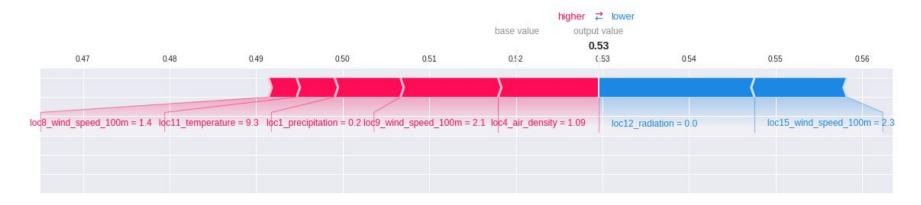


# SHAP (SHapley Additive exPlanations)

#### **SHAP**

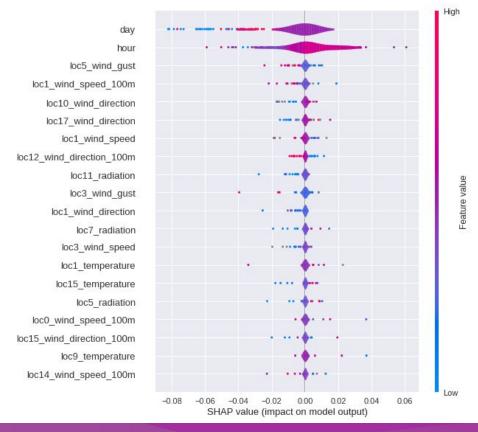
- SHAP (SHapley Additive exPlanations) is a framework for Shapley Values which assigns each feature an importance value for a particular prediction
- Includes extensions for:
  - TreeExplainer: high-speed exact algorithm for tree ensembles
  - DeepExplainer: high-speed approximation algorithm for SHAP values in deep learning models
  - GradientExplainer: combines ideas from Integrated Gradients, SHAP, and SmoothGrad into a single expected value equation
  - KernelExplainer: uses a specially-weighted local linear regression to estimate SHAP values for any model

#### **SHAP Explanation Force Plots**

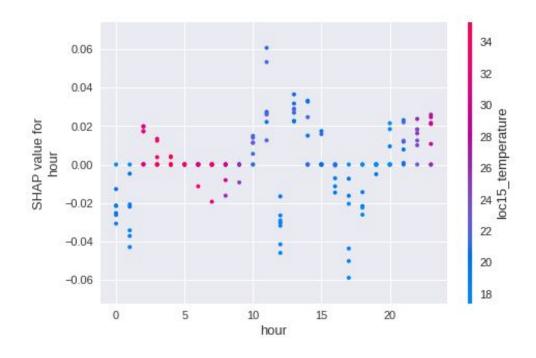


- Shapley Values can be visualized as forces
- Prediction starts from the baseline (Average of all predictions)
- Each feature value is a force that increases (red) or decreases (blue) the prediction

#### **SHAP Summary Plot**



#### SHAP Dependence Plot with Interaction



## Understanding Model Predictions



## Testing Concept Activation Vectors

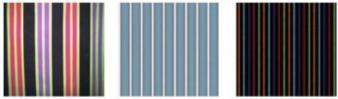
#### Testing Concept Activation Vectors (TCAV)

#### Concept Activation Vectors (CAVs)

- A neural network's internal state in terms of human-friendly concepts
- Defined using examples which show the concept

#### **Example Concepts**

CEO concept: most similar striped images



CEO concept: least similar striped images



Model Women concept: most similar necktie images







Model Women concept: least similar necktie images







## Understanding Model Predictions



### LIME

#### Local Interpretable Model-agnostic Explanations (LIME)

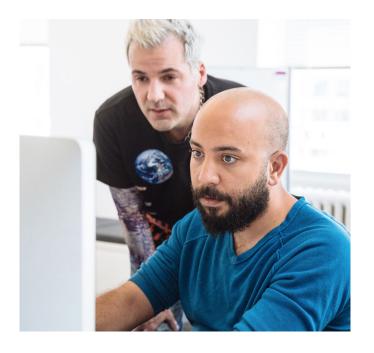
- Implements local surrogate models interpretable models that are used to explain individual predictions
- Using data points close to the individual prediction, LIME trains an interpretable model to approximate the predictions of the real model
- The new interpretable model is then used to interpret the real result

## Understanding Model Predictions



### Al Explanations

#### Google Cloud AI Explanations for AI Platform



**Explain** why an individual data point received that prediction

Debug odd behavior from a model

Refine a model or data collection process

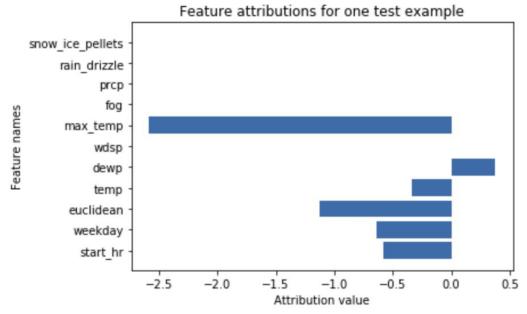
Verify that the model's behavior is acceptable

Present the gist of the model

#### Al Explanations: Feature Attributions

Predicted duration: 11.1651134 minutes

Actual duration: 10.0 minutes



**Tabular Data Example** 

#### Al Explanations: Feature Attributions





Image Data Examples

#### Al Explanations: Feature Attribution Methods

Predicted duration: 11.1651134 minutes
Actual duration: 10.0 minutes

Feature attributions for one test example

snow\_ice\_pellets
rain\_drizzle
prcp
fog
max\_temp
wdsp
temp
euclidean
wekday
start.hr
-2.5 -2.0 -1.5 -1.0 -0.5 0.0 0.5





Al Explanations: Integrated Gradients

A gradients-based method to efficiently compute feature attributions with the same axiomatic properties as Shapley values

### AI Explanations: XRAI (eXplanation with Ranked Area Integrals)

XRAI assesses overlapping regions of the image to create a saliency map

- Highlights relevant regions of the image rather than pixels
- Aggregates the pixel-level attribution within each segment and ranks the segments

### AI Explanations: XRAI (eXplanation with Ranked Area Integrals)

