Beyond the Black Box

Interpreting ML models with SHAP

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About Me

- Staff Data Scientist at Intuit
- Editor at PyOpenSci
- Engineering + Data Science
- Love PS5 + Steam Deck
- Soccer + Tennis
- Driving is therapy!

Agenda

1. Why does explainability matter?
2. SHAP theory and intuition
3. Case Study 1: Decision Trees
4. Case Study 2: Deep Neural Networks
5. Limitations

Explainable AI

Why does it matter?

- ML models are not just used to classify cats vs dogs
- Used in very crucial industries / use-cases
  - *Resume screening for a job application*
  - *Medical image diagnosis*
  - *Credit risk for analysis for loan application*
- Ethical concerns

Shapley Values

Concept

<u>Example</u>

- 3 friends start a business and bring in $20k profit
- Alice alone: $5k profit
- Bob alone: $3k profit
- Charlie alone: $4k profit

How can they fairly split the $20k profit?

Shapley Values

Concept

- Originates from game theory
- Fairly distribute rewards among “players” in a cooperative “game”
- In machine learning terms
  - Player == Feature
  - Game == ML Task
  - ML task can be classification, regression, etc.

SHAP

SHapley Additive exPlanations

- Specific implementation of Shapley values
- Explain ML predictions
- Model Agnostic
  - Decision Trees
  - Neural Networks
  - Any kind of model really
- Linear model of feature contributions

SHAP

Mathematical intuition

$$f(x) = E[f(X)] + \sum_{i=1}^{M} \phi_i(x)$$

- $f(x)$ is the prediction of a single instance
- $E[f(X)]$ is mean prediction of the dataset or background data
- $\phi_i(x)$ is the SHAP value for feature i for input x

How do we calculate SHAP?

The actual calculation is
$O(2^M)$

For 3 features, we need to test all 8 combinatons!

SHAP calculation is exponential

Example

<u>Question</u>

How much does each feature contribute to the loan application?

- Age

- Income

- Credit Score

<u>Approach</u>

Try all combination of features.

1. {} - no features
2. {Age}
3. {Income}
4. {Credit}
5. {Age, Income}
6. {Age, Credit}
7. {Income, Credit}
8. {Age, Income, Credit}

SHAP calculates how much each feature helps on average across all combinations!

SHAP

Approximation methods

<u>Kernel SHAP</u>

- Applicable to any model type
- Slow for large datasets

<u>Tree SHAP</u>

- Optimized for tree-based models
- Exploits the hierarchical structure

<u>Deep SHAP</u>

- Estimation for deep neural networks
- Leverage backpropagation

Now let’s see how all this plays out!

Case Study I: Decision Trees

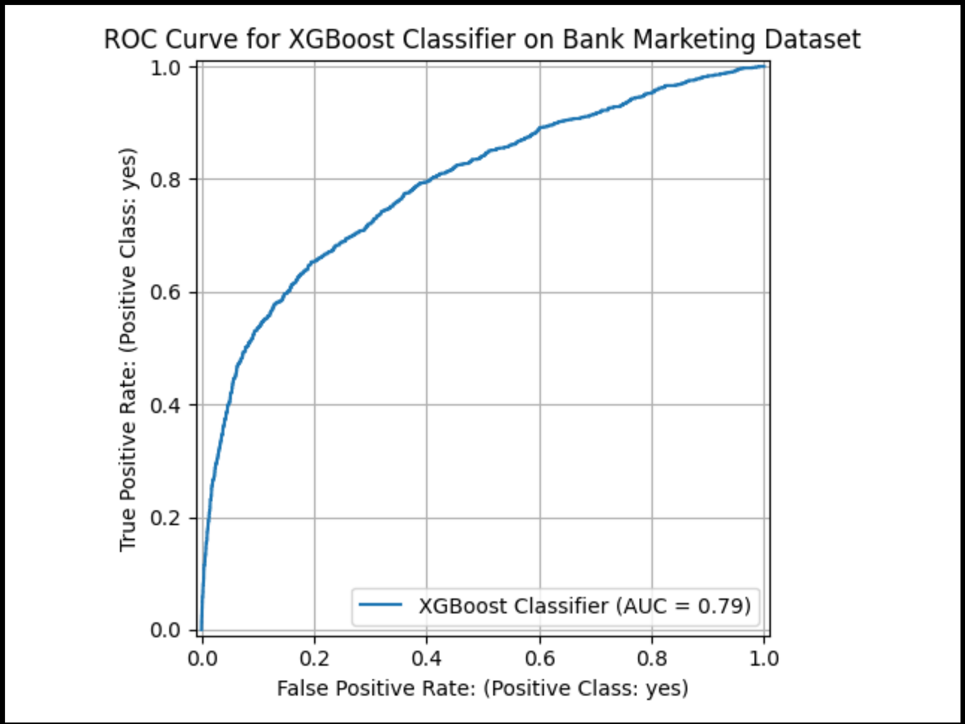
Business Problem

A Portuguese bank wants to predict which customers will subscribe to a term deposit based on direct marketing campaigns, i.e. phone calls

SHAP for Decision Trees

Bank Marketing Dataset

- Tabular data
- Features include
  - Customer demographics
  - Financial details
  - Previous interaction history
- Classes: 2 (yes, no)
- Number of total samples: 45,211
- Model used: XGBoost Classifier



SHAP for Decision rees

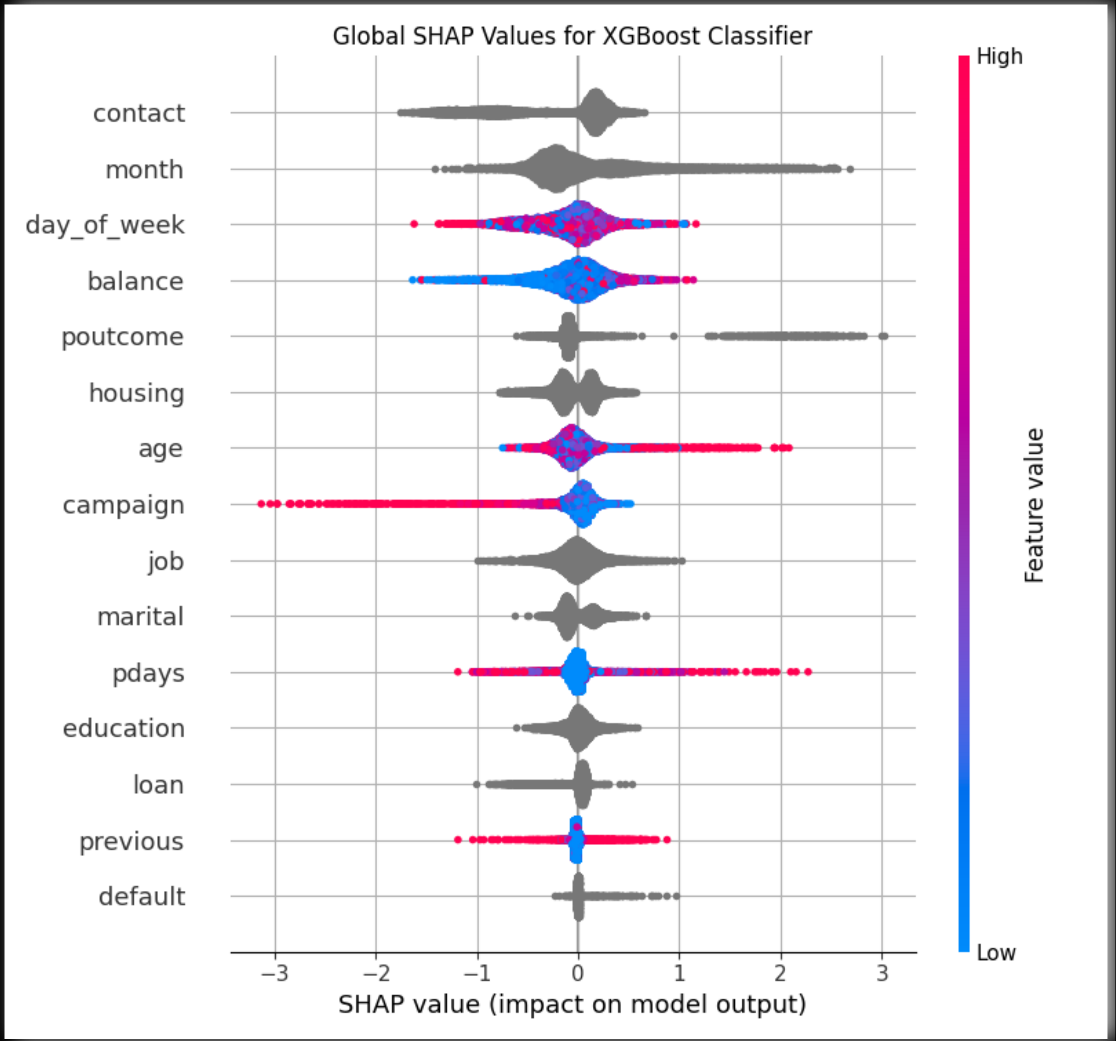
Calculation

```
import shap

# xgb is the trained XGBoost classifier
# x_test is the test dataset of shape (9043, 15)

# Setup TreeSHAP explainer
explainer = shap.TreeExplainer(xgb)
shap_values = explainer.shap_values(x_test)

# shap_values shape: (9043, 15)
```

SHAP for Decision Trees

Global explanations with beeswarm plot

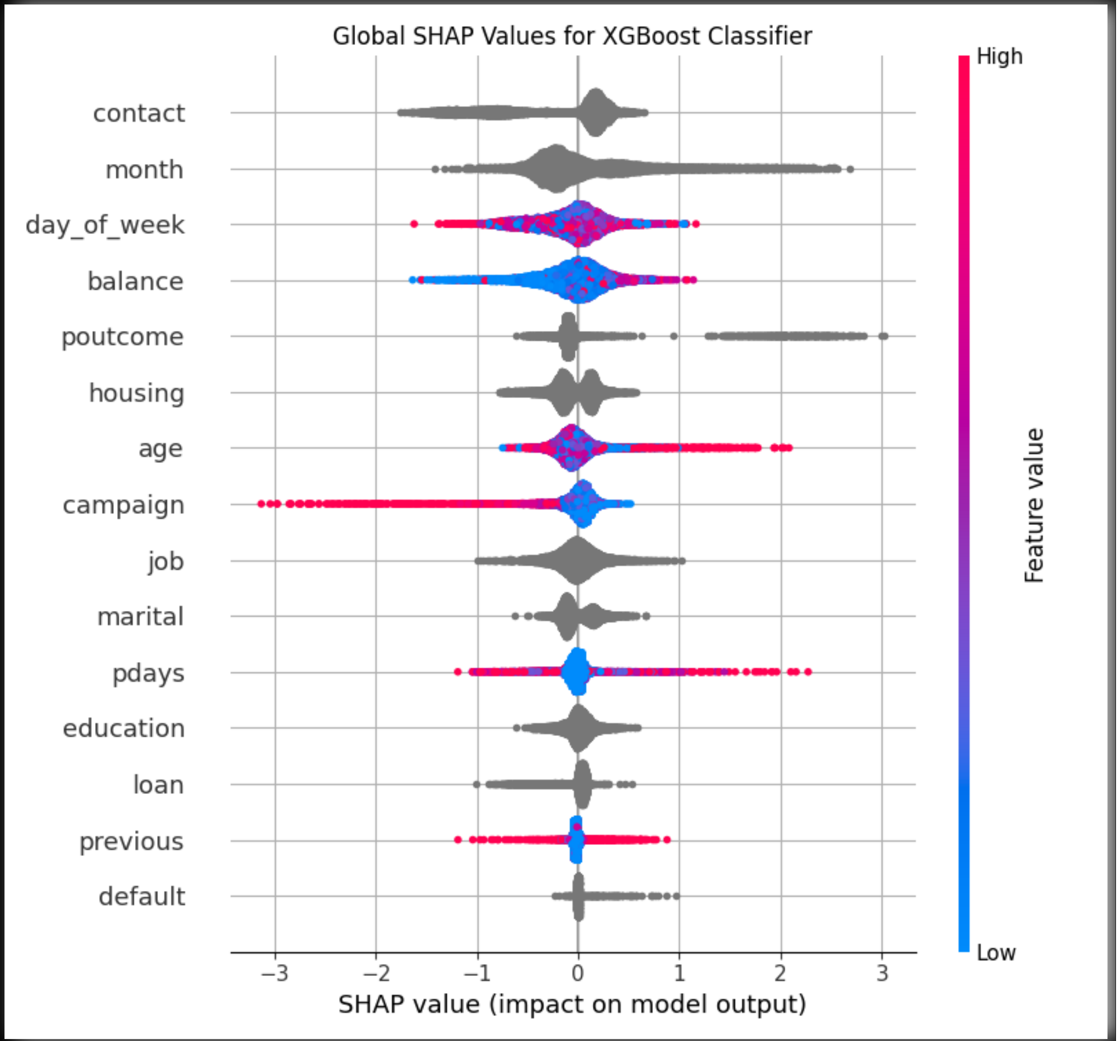
- High-level summary of the model's behavior
- Useful for understanding the overall impact of each feature
- Features are ordered by importance



SHAP for Decision Trees

Global explanations with beeswarm plot

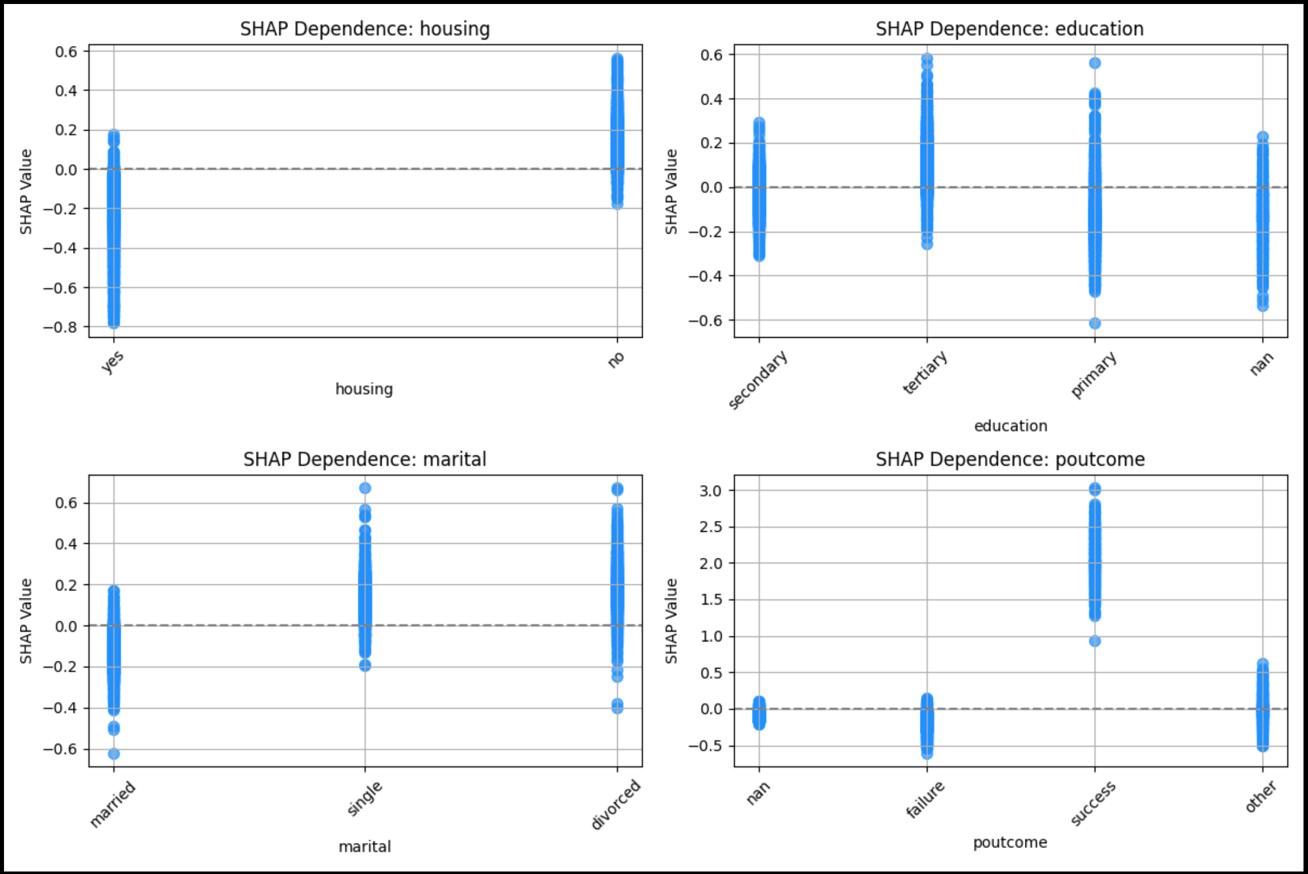
- SHAP values represent the impact each feature has on the model's predictions
- Positive SHAP values indicate that the feature pushes the model prediction higher, i.e. towards the "yes" class
- The distance from the center (zero) indicates magnitude
- Categorical variables are displayed in gray



SHAP for Decision Trees

Dependency plots

- Deeper analysis for a single feature and its effect on model predictions
- Especially useful for categorical features



⚙️ Tabular data 📊 to Timeseries 📈

Case Study II: Neural Networks

SHAP for Convolutional Neural Networks

Human Activity Recognition dataset

- Time series sensor data collected from a smartphone
- A smartphone is attached to the waist of the individual
- Data collected from 30 individuals within the 19-48 years age group

Six Activities

1. *Walking*
2. *Walking Upstairs*
3. *Walking Downstairs*
4. *Sitting*
5. *Standing*
6. *Laying*

SHAP for Convolutional Neural Networks

Problem formulation

Dataset

- Multivariate time series
- 560+ features (all numeric)
- 6 classes
- Objective: Multiclass classification

Model

- 1D CNN using PyTorch
- Normalize the data [0, 1]
- Convert into window sequences

SHAP for CNN

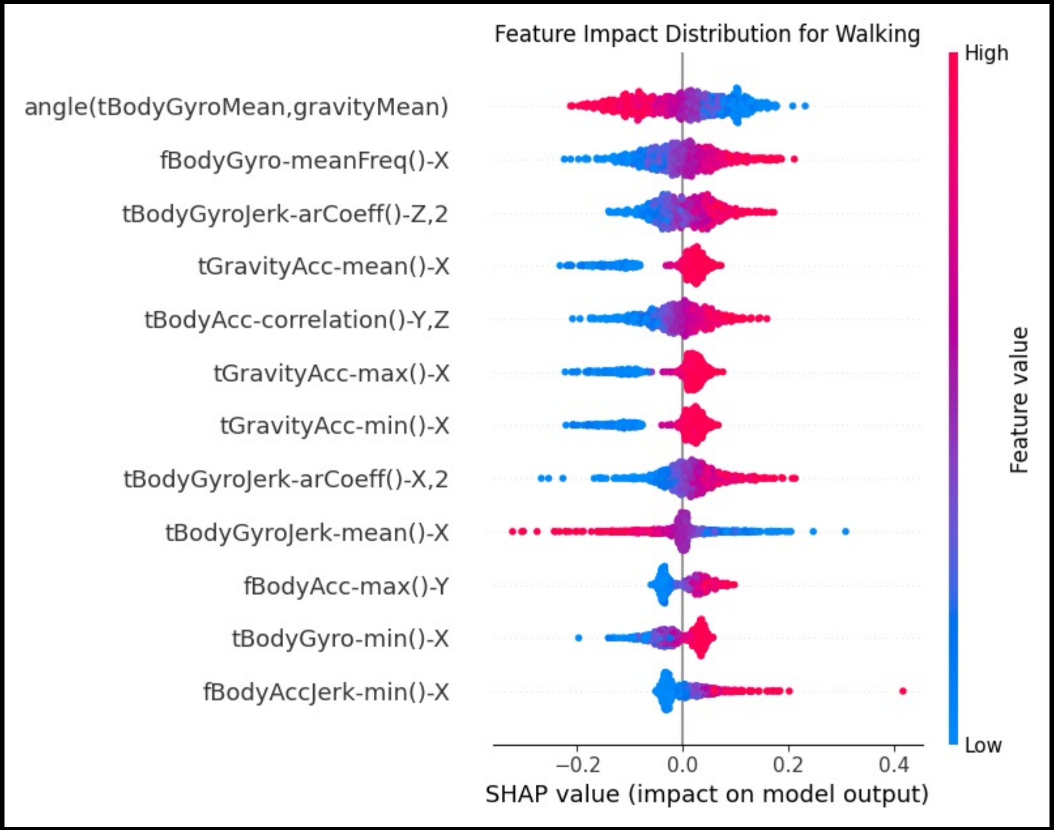
Calculation

```
import shap

# Create balanced background dataset (20 samples per class)
background_data = create_balanced_background(
    x_train_seq, y_train_seq, n_per_class=20
)

# Setup DeepSHAP explainer
explainer = shap.DeepExplainer(model, background_data)
shap_values = explainer.shap_values(x_test_seq[:1000])
# shap_values shape: (1000, 561, 64, 6)

# Extract feature importance and visualize
feature_importances = shap_values[:, :, -1, :]  # Last time step
shap.plots.beeswarm(feature_importances[:, :, 0])  # Walking class
```

SHAP for CNN

Global explanations

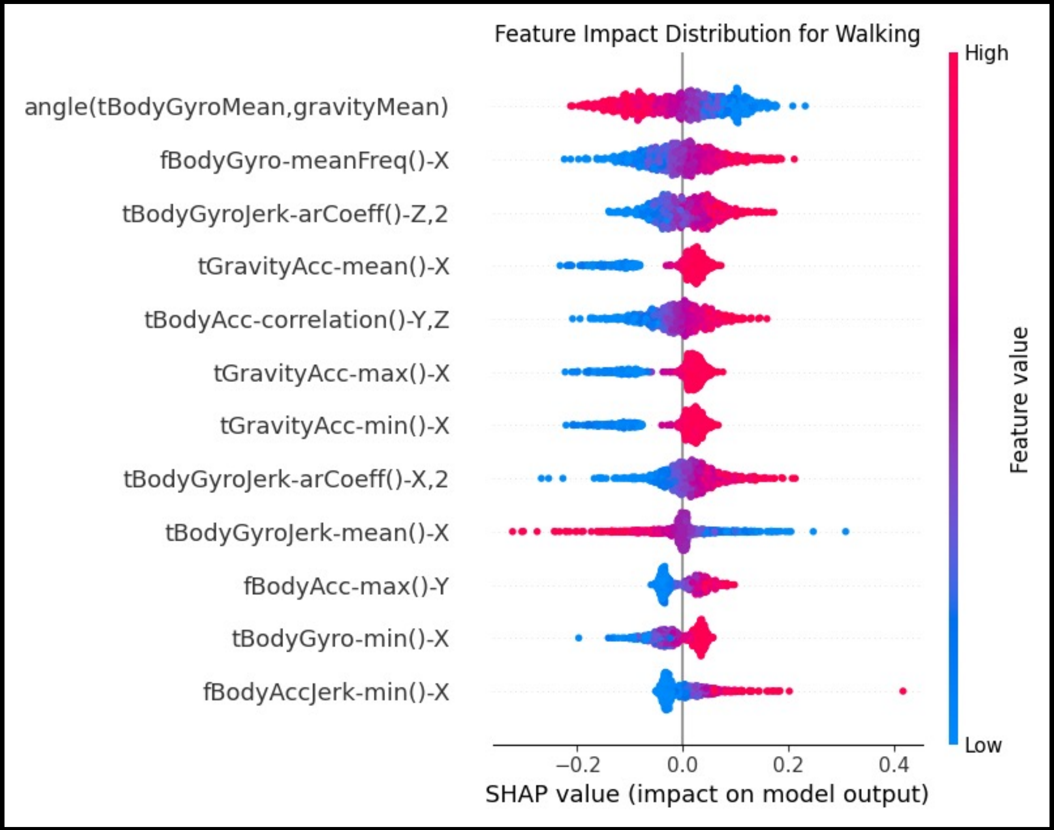
- In a multiclass setting, we have a set of shap values for every class in a one-vs-all fashion
- Positive SHAP values pushes the feature towards the positive class (Walking)
- Negative SHAP values reduces the model's prediction towards all the negative class (all other classes)



SHAP for CNN

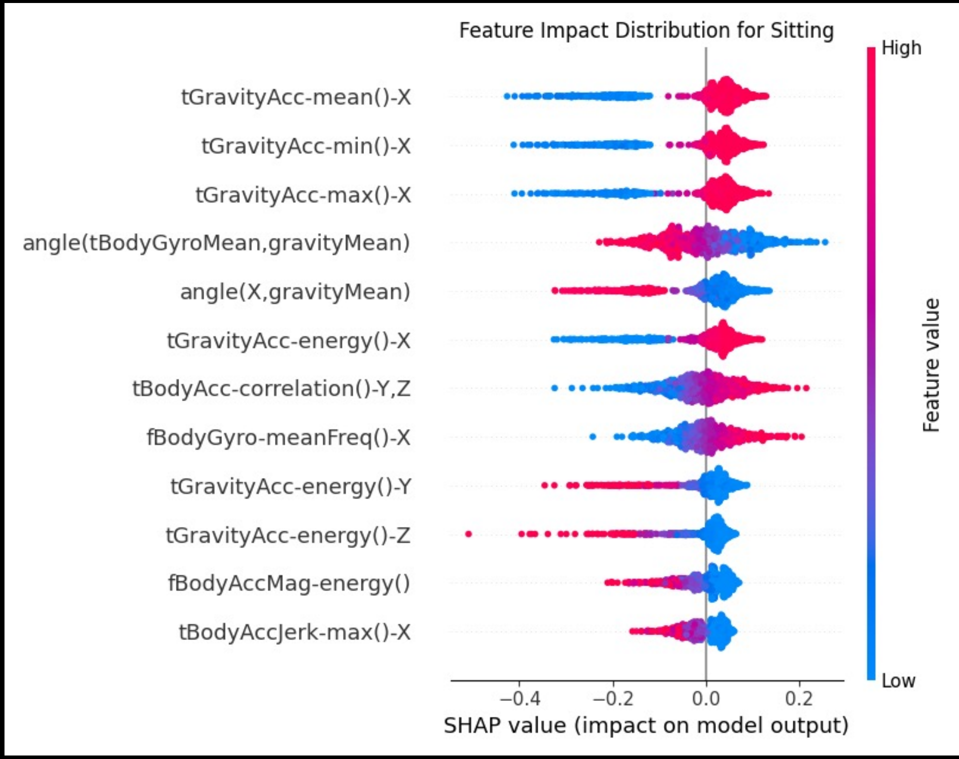
Global explanations: Walking

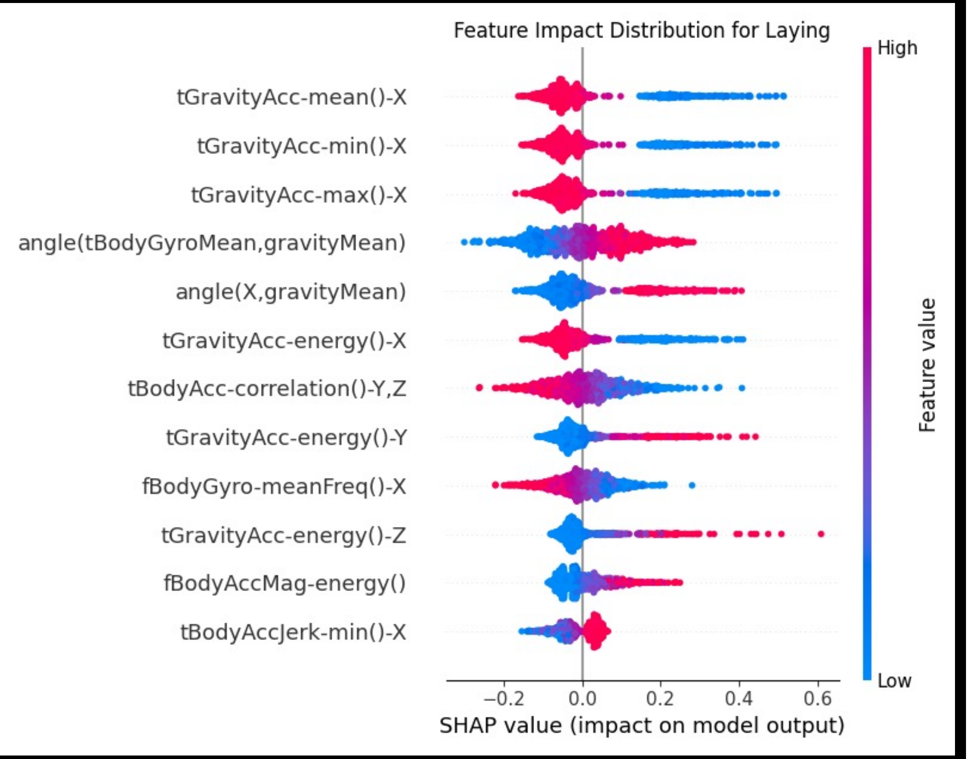
- When *Walking*, the angle between the mean gyroscope signal and the mean gravity signal is smaller
- Low values of gravitational acceleration along the X axis pushes the prediction away from the *Walking* class



SHAP for CNN

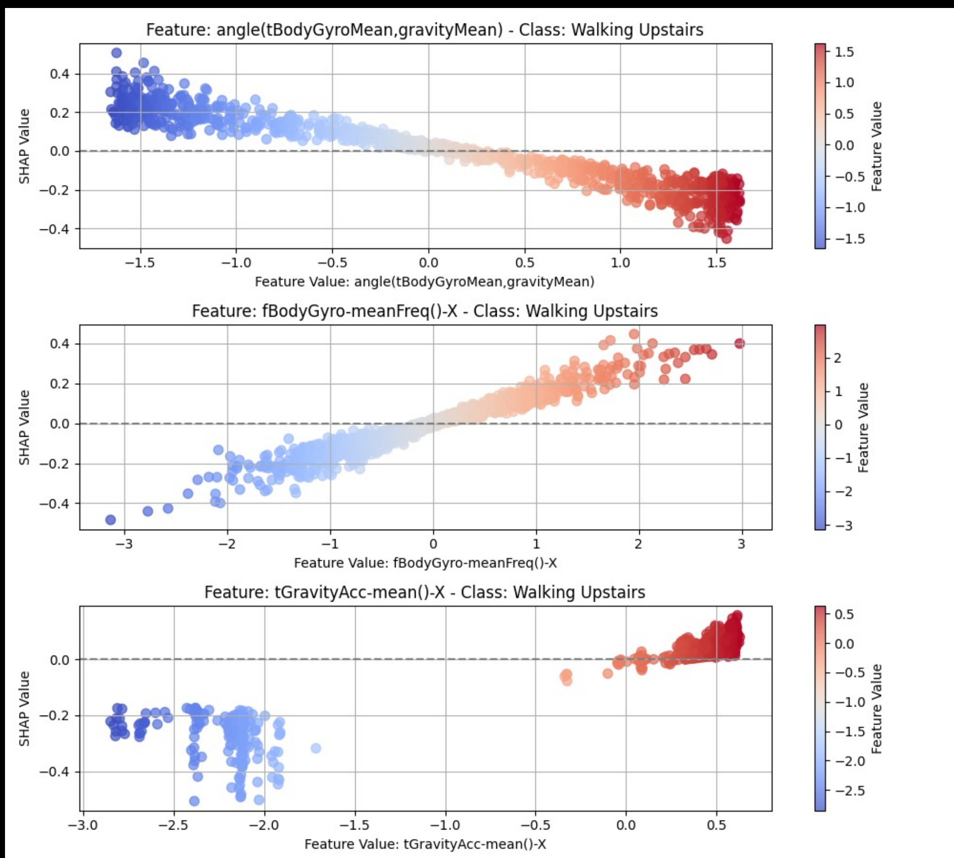
Global explanations: Sitting vs Laying

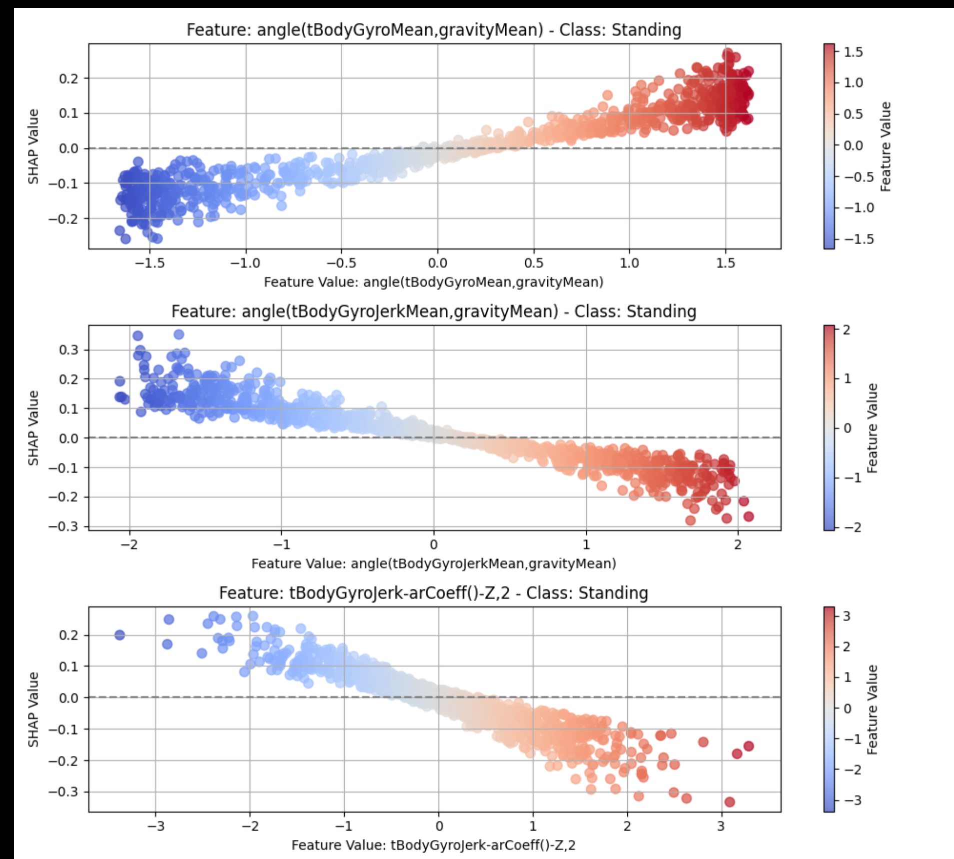




SHAP for CNN

Dependency plots

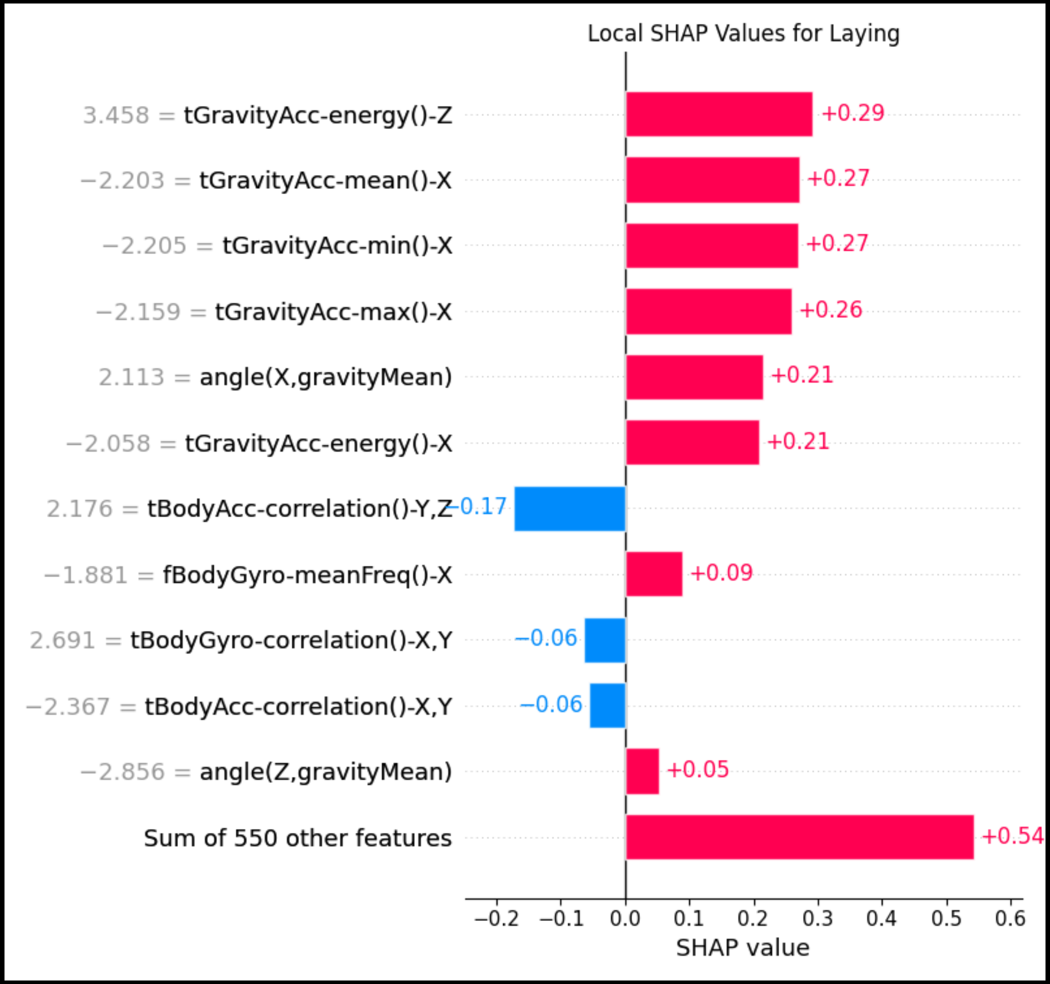




SHAP for CNN

Local explanations

- Helps understand factors influencing individual predictions
- Positive SHAP values in red push the prediction towards the "*Laying*" class
- Negative SHAP values in blue push the prediction away from the "*Laying*" class



Things to look out for!

Limitations

- Explains the Model, not Reality!
- For large datasets, the calculation is very resource-intensive
- SHAP values can be misleading when features are highly correlated
- SHAP values show feature contributions, NOT causal effects
- Results depend on the choice of background dataset

Thank You! 🙏

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