



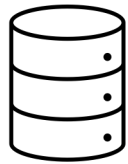
Explaining by removing

Explainable and Trustworthy AI

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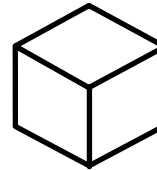
Stages of Explainability

- Explainability involves the entire AI development pipeline



Pre-modelling explainability

- Before building the model
- Data exploration
 - Data selection
 - Feature engineering



Explainable modeling

- Build inherently interpretable models
- Manage the accuracy and interpretability trade-off

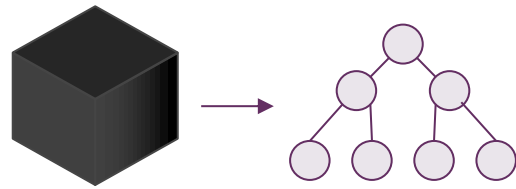


Post-modelling explainability

- After model development
- Explaining predictions and behavior of trained models

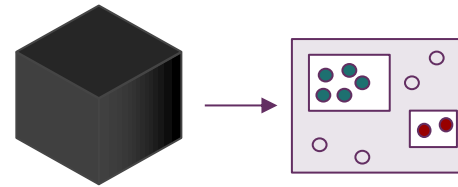
Scope of Explainability

- *What do we explain?*



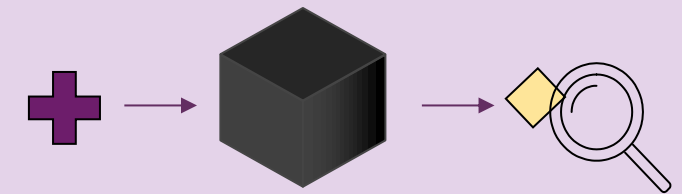
Global

How the model globally works



Subgroup

How the model behaves in data subgroups



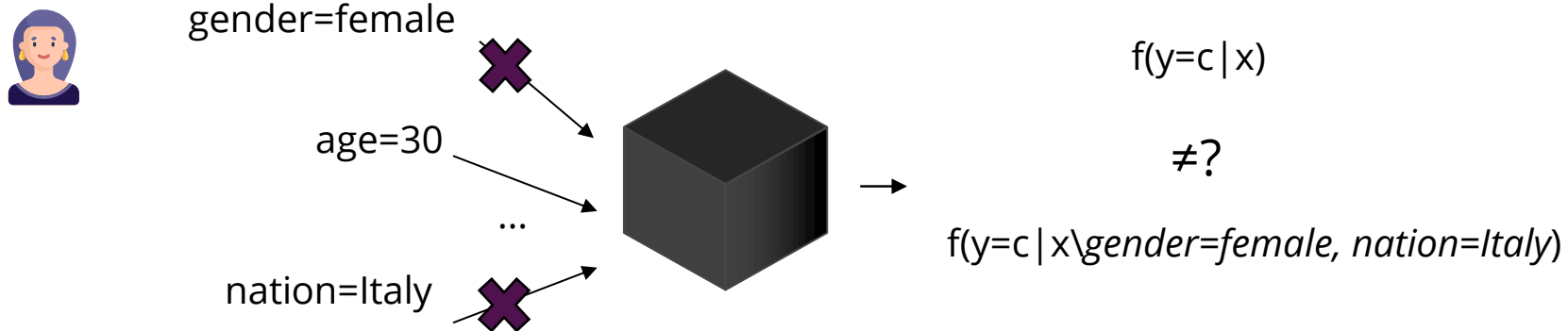
Individual/local

Explaining the reasons behind individual predictions

Explaining by removing

Also known as *occlusion-based* or *perturbation-based* since often the occlusion is performed via perturbations

The idea is to remove one or more input feature (or simulate the removal) to quantify the feature influence



Explaining by removing - Approaches

- PredDiff – base approach
- IME – Explaining with Shapley Values
- SHAP
- LIME*

*LIME indeed use perturbations!

PredDiff – Prediction Difference

Let f the model and let be x the instance to explain.

The importance of attribute A_i is:

$$\text{predDiff}_i(x) = f(x) - f(x \setminus A_i)$$

Where $x \setminus A_i$ is the instance x without the information of A_i .

PredDiff – Prediction Difference

Evaluation of the difference → Solution a) Difference in probability

A possibility is to directly evaluate the **difference between probabilities** for class c

$$\mathit{predDiff}_i(x) = p(y = c|x) - p(y = c|x \setminus A_i)$$

Where c is typically the predicted class, as we want to explain why the model made a particular decision

PredDiff – Prediction Difference

Evaluation of the difference → Solution b) Information difference

Another possibility is to compute the information difference

$$\text{infoDiff}_i(x) = \log_2 p(y = c|x) - \log_2 p(y = c|x \setminus A_i)$$

Where c is typically the predicted class, as we want to explain why the model made a particular decision

PredDiff

How to model the removal of information $f(x \setminus A_i)$?

The approach was proposed for tabular data.

Simulate it with an 'average value'

$$p(y|x \setminus A_i) = \sum_{s=1}^{m_i} p(A_i = a_s) p(y|x \leftarrow A_i = a_s)$$

Categorical attributes.

Replace the value $A_i = a_k$ in x with all possible values of A_i (m_i is the number of values of the attribute A_i) and weight each prediction by the prior probability of the value.

The $p(y|x \leftarrow A_i = a_s)$ represents the probability for y when in x we replace the value of A_i with a_s

PredDiff

How to model the removal of information $f(x \setminus A_i)$?

The approach was proposed for tabular data.

Simulate it with an 'average value'

$$p(y|x \setminus A_i) = \sum_{s=i}^{s=m_i} p(A_i = a_s) p(y|x \leftarrow A_i = a_s)$$

Numerical attributes.

First discretize and split the values of A_i into sub-intervals. The middle points of these sub-intervals are the representative values for a_s

Use probabilities of the sub-intervals for weighting the predictions

PredDiff

We obtain a **feature importance** for each feature

The higher the magnitude \rightarrow the more the attribute values impact the prediction

Positive contribution \rightarrow the attribute values pushes toward the prediction for class c

Negative contribution \rightarrow the attribute values pushes against the prediction for class c

Advantages of PredDiff

- Model agnostic
- Local explanations
- Provides feature attributions
- Direct interpretation of the result

Limitations of PredDiff

- Defined for structured data
- Perturbations/info removals may create unrealistic data
- Need access data to compute $x \setminus A_i$
 - Replace the attribute with values from (training) instances $p(y|x \leftarrow A_i = a_s)$
- Does not consider interaction between features for the removal

Explaining by removing – consider interactions

Consider the **contribution of multiple features** at the time,
i.e., removing feature A_i and removing features A_i and A_j

Research question.

How can we **aggregate** such importance scores into a single attributions?

- i.e., the contribution of A_i , considering the interactions with other attributes

A possibility → Shapley values

Shapley value

Concept for game theory to assign a **relevance score to each player of a team**, assuming that they collaborate

Team



Player 1



Player 2



Player 3



Player 4

Total score of Team

Goal. Compute the contribution of each player ϕ_i ?



Shapley value

- N players
- v is a function maps subsets of players to the real numbers: $v: 2^N \rightarrow \mathbb{R}$, with $v(\emptyset) = 0$
- S = coalition of players
- $v(S)$ is the total expected sum of payoffs the player in S can obtain by cooperating

Contribution of player i $\phi_i(v)$

$$\phi_i(v) = \sum_{S \subseteq N} \frac{(|N| - |S|)! (|S| - 1)!}{|N|!} (v(S) - v(S \setminus \{i\}))$$

Marginal contribution

Shapley value

$$\phi_i(v) = \sum_{S \subseteq N} \frac{(|N| - |S|)! (|S| - 1)!}{|N|!} (v(S) - v(S \setminus \{i\}))$$

- Players A, B, C
- $\phi_A(v)$?

Terms to sum:

- $\frac{2}{6} (v(A) - v(\emptyset))$
- $\frac{1}{6} ((v(\{A, B\}) - v(B))$
- $\frac{1}{6} (v(\{A, C\}) - v(C))$
- $\frac{2}{6} (v(\{A, B, C\}) - v(\{B, C\}))$
- Coalition considered: 2^3

Properties of Shapley Value (1/2)

- **Efficiency**

The sum of the Shapley values of all players is equal to the value of the entire team

$$\sum_{i \in N} \phi_i(v) = v(N)$$

- **Simmetry**

Players with the same marginal contributions have the same contribution ϕ

If $v(S \cup \{i\}) = v(S \cup \{j\})$ for all $S \subseteq N \setminus \{i, j\}$, then $\phi_i(v) = \phi_j(v)$

Properties of Shapley Value (2/2)

- **Linearity**

If two games described by functions v and w are combined, then the distributed contribution correspond to sum of the contribution from v and the contribution from w

- $\phi_i(v + w) = \phi_i(v) + \phi_i(w)$
- $\phi_i(\alpha \cdot v) = \alpha \cdot \phi_i(v)$

- **Null player**

A player with marginal contribution equal to 0 will have 0 as contribution ϕ

$$v(S \cup i) = v(S) \forall S \rightarrow \phi_i(v) = 0$$

Shapley value is the **only** assignment that satisfy the Efficiency, Symmetry, Linearity and Null player properties

Use Shapley value for XAI

Players \rightarrow feature values

Total score $v(N)$ \rightarrow difference in probability with the average prediction (prior)

S \rightarrow instance when feature values $N \setminus S$ are omitted

$v(S)$ \rightarrow (a) prediction probability for instance S with only feature values S are available compared to average prediction / (b) prediction

ϕ \rightarrow feature attributions

- How much has each feature value contributed to the prediction compared to the average prediction?

$$\phi_i(v) = \sum_{S \subseteq N} \frac{(|N| - |S|)! (|S| - 1)!}{|N|!} (v(S) - v(S \setminus \{i\}))$$

Function v

- How much has each feature value contributed to the prediction compared to the average prediction?

$$v(S) = f(S) - E[f(X)]$$

where $f(S)$ is the model prediction marginalizing over the feature not in S

This interpretation is in line with the interpretation of some interpretable model such as linear regression

- Contribution of the feature value respect to the average/prior behavior

Following this line, $v(N)$ (i.e., for the instance to explain x , all players) is the prediction probability for an instance minus the average prediction for all instances ,

$$v(N) = v(x) = f(x) - E[f(X)]$$

Computation of $v(S)$ and $v(S \setminus \{i\})$

How to model the removal of information?

- As for PredDiff: simulate it with an 'average value' substituting with possible values
 - Less adopted
- **Random**
 - Replace the feature values of features that are not in a coalition with random feature values from the dataset
 - Consider multiple replacement and provide the average value v

Example of coalitions to evaluate

Example. Gender=F, age=30, nationality=IT, income=20k

- To compute the contribution of gender=F, we need to evaluate the following coalitions (2^4)
 - {} | gender=F
 - age=30 | gender=F
 - nationality=IT | gender=F
 - income=20k | gender=F
 - age=30, nationality=IT | gender=F
 - age=30, income=20k | gender=F
 - nationality=IT, income=20k | gender=F
 - age=30, nationality=IT, income=20k | gender=F

Shapley value

- Contribution of player i $\phi_i(v)$

$$\phi_i(v) = \sum_{S \subseteq N} \frac{(|N| - |S|)! (|S| - 1)!}{|N|!} (v(S) - v(S \setminus \{i\}))$$

- Alternative form

$$\phi_i(v) = \sum_{S \subseteq N \setminus \{i\}} \frac{(|N| - |S| - 1)! (|S|)!}{|N|!} (v(S \cup \{i\}) - v(S))$$

Advantages of using the Shapley Values for XAI

- Model agnostic & Local explanations & Provides feature attributions & Direct interpretation of the result
- Consider interaction among features
- Efficiency Property of Shapley Values
 - The difference between prediction for instance x and average prediction is distributed among feature values.
 - $\sum_{i=1}^p \phi_i(f) = f(x) - E[f(X)]$
Where p is the number of attributes and f is the model to explain
- Solid Theoretical Foundation
 - Axioms: efficiency, symmetry, linearity, null player

Limitations of using the Shapley Values for XAI

- Computation time is exponential in the number of players/feature values
 - Exact computation is computationally expensive.
 - For N players, 2^K coalitions of the feature values
- Need access data to compute $v(S)$ and $v(S \setminus \{i\})$
- Perturbations/info removals may create unrealistic data
- The absence of a feature to compute $v(S)$ and $v(S \setminus \{i\})$ is simulated by drawing random instances \rightarrow variance for the estimate of the Shapley value

Problem of exact computation

Exact computation → **exponential** in the number of players/feature and feature values

- To compute $\phi_i(v)$ we have to evaluate all possible coalitions of feature values with and without the feature A_i

The **exact solution** to this problem becomes **problematic** as the number of possible coalitions exponentially increases as more features are considered

Proposed solution: approximation with Monte-Carlo sampling

Shapley Approximation - Random coalition

- Take a random instance z from the dataset
- x_{+j} is an instance where a **random** number of **feature values** are **replaced by feature values from the random data point z** . The value for feature j is as in the original feature x
 - The random features that are replaced are the features not in the coalition
- x_{-j} is as x_{+j} where **also the value of j is replaced** by the value of the sampled z .

Example of random coalition

- Input instance x : Gender=F, age=30, nationality=IT, income=20k
- Random instance z : Gender=M, age=35, nationality=IT, income=40k

- Random features values: age=30, income=20k

To compute $\phi_{j=gender=Female}(v)$ we consider

- x_{+j} - Gender=F, age=35, nationality=IT, income=40k
- x_{-j} - Gender=M, age=35, nationality=IT, income=40k

Note that the considered coalition S in this case is nationality=IT

Approximated Shapley estimation

M = number of iterations

- For m in $1, \dots, M$:
 - Sample a random instance z from the dataset
 - Randomly select a permutation of the feature values O
 - Compute x_{+j} and x_{-j}
 - x_{+j} = take values from x preceding j -th in O + j + take values from z succeeding j -th in O
 - x_{-j} = take values from x preceding j -th in O + take values from z succeeding j -th-1 in O (i.e., j -th included)
 - Compute the marginal contribution $\phi_j^m = f(x_{+j}) - f(x_{-j})$
- Compute the Shapley values as the average over the M iterations $\phi_j(x) = \frac{1}{M} \sum_{m=1}^M \phi_j^m$

Example of random coalition (2) – use permutations

- Input instance x : Gender=F, age=30, nationality=IT, income=20k
- Random instance z : Gender=M, age=35, nationality=IT, income=40k

- Random permutation at iteration m : nationality, **gender**, age, income

To compute $\phi_{j=gender=Female}^m(v)$ we consider

- x_{+j} - nationality=IT, **Gender=F**, age=35, income=40k
- x_{-j} - nationality=IT, **Gender=M**, age=35, income=40k

Note that the considered coalition S in this case is nationality=IT

Advantages and limitations of the approximation

Advantages

- Same as exact Shapley
- +
- Reduced computational complexity

Limitations

- Same as exact Shapley except for exponential computation
- +
- It is an approximation
- Variance for the estimate of the Shapley value depends on the number of iterations M
 - Decreasing M reduces computation time but increases the variance of the Shapley value

SHAP

- SHAP = SHapley Additive exPlanations
- Local, model agnostic explanation method based on Shapley values
- SHAP proposes two approaches for estimating the Shapley values
 - KernelSHAP - kernel-based estimation approach
 - Model agnostic
 - TreeSHAP - efficient estimation approach for tree-based models
 - Not model agnostic
- It also propose to aggregate local explanation to provide global insights

SHAP

- Idea of SHAP brings is to represent the Shapley value explanation as an additive feature attribution method, a linear model
- Use the notion of surrogate model

$$g(x') = \sum_{i=1}^p \phi_i$$

SHAP

- f : the original model to explain
- g : simpler explanation model, **interpretable approximation** of the original model
- x : instance to explain. We want to explain $f(x)$

- x' : simplified input of x , such that $x = h_x(x')$ where h_x is a mapping function
 - As the interpretable representation of LIME

SHAP target defying a g such that: $g(z') \approx f(h_x(z'))$ for $z' \approx x'$

SHAP - SHapley Additive exPlanations

- M : number of simplified features
- $z' \in \{0,1\}^M$: defined as binary feature
 - As the interpretable representation of LIME
- Definition of **additive feature attribution method**

$$g(z') = \phi_0 + \sum_{i=1}^M \phi_i z'_i$$

SHAP - SHapley Additive exPlanations

- Recall the interpretable representation of LIME for tabular data

Welcome	to	the	Explainable	and	Trustworthy	AI	Course
1	1	0	0	1	0	0	1

- We use $z' \in \{0,1\}^M$ to model the coalitions of players!
 - An entry of 1 means that the corresponding feature value is “present” and 0 that it is “absent”
 - In the example, the player are the tokens/words ‘Welcome’, ‘to’, ‘and’ and ‘Course’. The other words are omitted/removed
 - Recall that to compute Shapley values, we simulate that only some feature values are playing (“present”) and some are not (“absent”).

Properties of additive feature attributions

- **Local accuracy**

- The explanation model $g(x')$ matches the original model $f(x)$ when $x = h_x(x')$

$$f(x) = g(x') = \phi_0 + \sum_{i=1}^M \phi_i x'_i$$

If we define $\phi_0 = E[f(X)]$

$$f(x) = \phi_0 + \sum_{i=1}^M \phi_i x'_i = E[f(X)] + \sum_{i=1}^M \phi_i x'_i$$

Properties of additive feature attributions

- **Missingness**

- Simplified input x model the presence and absence of feature
- Missingness requires that features missing have no impact, i.e., get an attribution 0

- $x'_i = 0 \implies \phi_i = 0$

Properties of additive feature attributions

- **Consistency**

- If a model changes so that the marginal contribution of a simplified input increases or stays the same regardless of the other feature, the attribution of that feature should not decrease (hence, it should increase or stay the same as well)

Let $f_x(z') = f(h_x(z'))$ and $z' \setminus i$ indicate that $z'_i = 0$ (i.e., feature i is absent/removed).

For any two models f and f' , if

$$f'_x(z') - f'_x(z' \setminus i) \geq f_x(z') - f_x(z' \setminus i)$$

For all $z' \in \{0,1\}^M$, then $\phi_i(f', x) \geq \phi_i(f, x)$

SHAP

- The Shapley value is the only one possible explanation model g that follows the definition of 'Additive feature attribution methods' and the three Properties

$$\phi_i(f, x) = \sum_{z' \subseteq x'} \frac{(|M| - |z'| - 1)|z'|!}{|M|!} (f_x(z') - f_x(z' \setminus \{i\}))$$

Where $|z'|$ is the number of non-zero values in z' and $z' \subseteq x'$ indicates all z' where non-zero entries are a subset of the non-zero entries in x'

SHAP - $f_x(z')$

- $f_x(z') = f(h_x(z')) = E[f(z)|z_S]$

where

- S : set of non-zero values in z'
- z_S : instance that has **missing** values for features **not in S**
 - i.e., non-zero just the ones in S
- We approximate $f(z_S)$ with $E[f(z)|z_S]$ by marginalizing the features not in S

SHAP - $f_x(z')$ - Estimation

$$f_x(z') = f(h_x(z')) = E[f(z)|z_S] =$$

$$= E_{z_{\bar{S}}|z_S}[f(z)]$$

expectation over $z_{\bar{S}}|z_S$

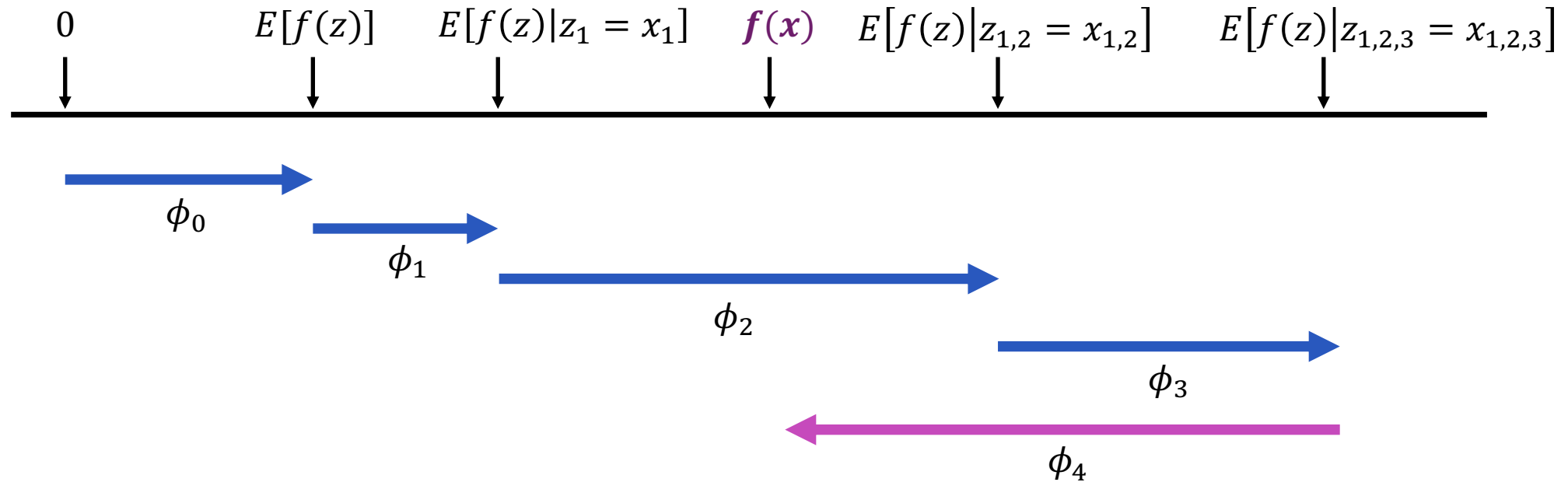
where \bar{S} is the complement of S (i.e., features not in S)

$$\approx E_{z_{\bar{S}}}[f(z)]$$

assume feature independence

$$\approx f([z_S, E[z_{\bar{S}}]])$$

SHAP - ϕ_i interpretation



- $E[f(z)]$ is the base value, when we did not know any features
- The diagram shows a single ordering (1 then 2 then 3)
 - The weights takes into account the multiple ordering --> weighted average t

Kernel SHAP

- The exact computation of the Shapley values is expensive
 - Exponential in the number of players

KernelSHAP is a technique to estimate for an instance x the contributions of each feature value to the prediction as an approximation of the Shapley value - ϕ_i

It uses the intuition of **local interpretable models**

From LIME to Kernel SHAP

Recall the objective of LIME

$$\text{explanation}(x) = \underset{g \in G}{\operatorname{argmin}} L(f, g, \pi_x) + \Omega(g)$$

The explanation for instance x is the model g that minimizes loss L :

- $L(f, g, \pi_x)$ – how unfaithful g is to f in the locality given by π_x - **Local**

$$L(f, g, \pi_x) = \sum_{z, z' \in \mathcal{Z}} \pi_x(z) (f(z) - g(z'))^2$$

Ridge regression - Linear least squares with l2 regularization in the code

- $\Omega(g)$ – i.e., the complexity of g - how the model is interpretable is kept low – **Interpretable**

Shapley Kernel

- Interpretability term

$$\Omega(g) = 0$$

- Locality term

$$L(f, g, \pi_x) = \sum_{z' \in \mathcal{Z}} \pi_{x'}(z') (f(h_x(z')) - g(z'))^2$$

- Where $\pi_{x'}(z')$ is computed as follows

$$\pi_{x'}(z') = \frac{M - 1}{\binom{M}{|z'|} |z'| (M - |z'|)}$$

$|z'|$ is the number of non-zero elements in z and M is the maximum coalition size (i.e., the number of interpretable features)

- $h_x(z')$ is the function to go from the interpretable feature space of z' to the original feature space to compute $f(h_x(z'))$ as model f operates on the original space

Kernel SHAP - Pseudocode

- Sample K coalitions $z'_k \in \{0,1\}^M$, $k \in \{1, \dots, K\}$
 - $z'_{k,j}$ has value 1 if the feature j is present in the coalition, 0 if it is absent
- Compute $f(h_x(z'_k))$, i.e., the prediction of model f first converting the instance z'_k to the original feature space with function h_x

- Compute the weight for each coalition z'_k with SHAP kernel

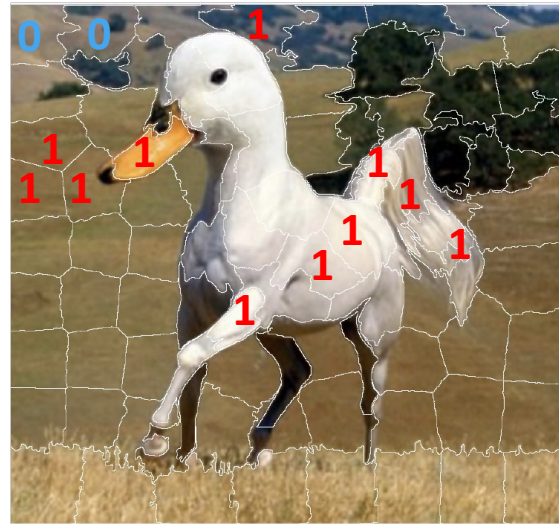
$$\pi_{x'}(z'_k) = \frac{M - 1}{\binom{M}{|z'_k|} |z'_k| (M - |z'_k|)}$$

- Fit weighted linear model

$$L(f, g, \pi_x) = \sum_{z' \in \mathcal{Z}} \pi_{x'}(z') (f(h_x(z')) - g(z'))^2$$

- The coefficient of the linear model ϕ_i are the (approximated) Shapley values

Example of coalition sampling – image data



$$z'_k = [0, 0, 0, 1, 0, \dots, 0, 1, \dots]$$



$$h_x(z')$$

Example of coalition sampling - tabular

- x : Gender=F, age=30, nationality=IT, income=20k
- $z'_k = [1, 0, 1, 0]$
- $h_x(z')$ = Gender=F, age=55, nationality=IT, income=20k
 - $f([z_S, E[z_{\bar{S}}]])$
 - marginalizing, substituting the feature not in S (\bar{S}) with values for a random instance (actually done by marginalizing over multiple random instances, less variance)

Example of coalition sampling – text data

- x : Welcome to the Explainable and Trustworthy AI Course
- $z'_k = [1, 1, 0, 0, 1, 0, 0, 1]$

Welcome	to	the	Explainable	and	Trustworthy	AI	Course
1	1	0	0	1	0	0	1

- $h_x(z')$ = Welcome to [UNK] [UNK] and [UNK] [UNK] Course

Global insights – SHAP Feature importance

- **Global feature importance** as the average of absolute Shapley values per feature across the data

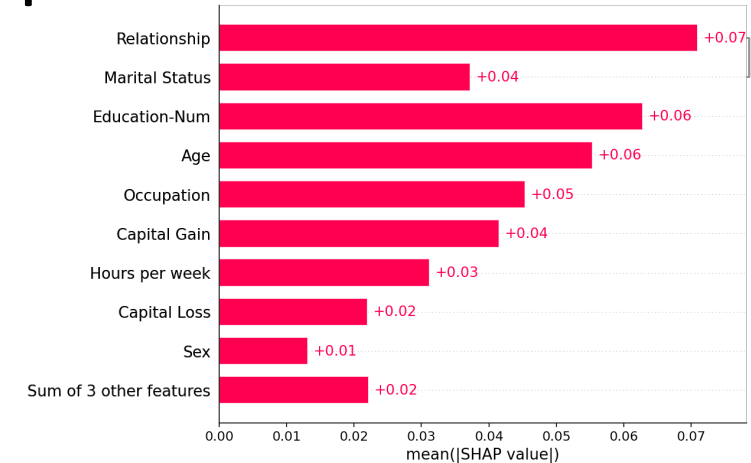
Steps

- Compute SHAP for each instance of the datasets
 - For each attribute, we have the importance of its value for explaining a specific instance
- Compute the average the absolute Shapley values per feature across the data:

$$I_j = \frac{1}{n} \sum_{i=1}^n |\phi_j^{(i)}|$$

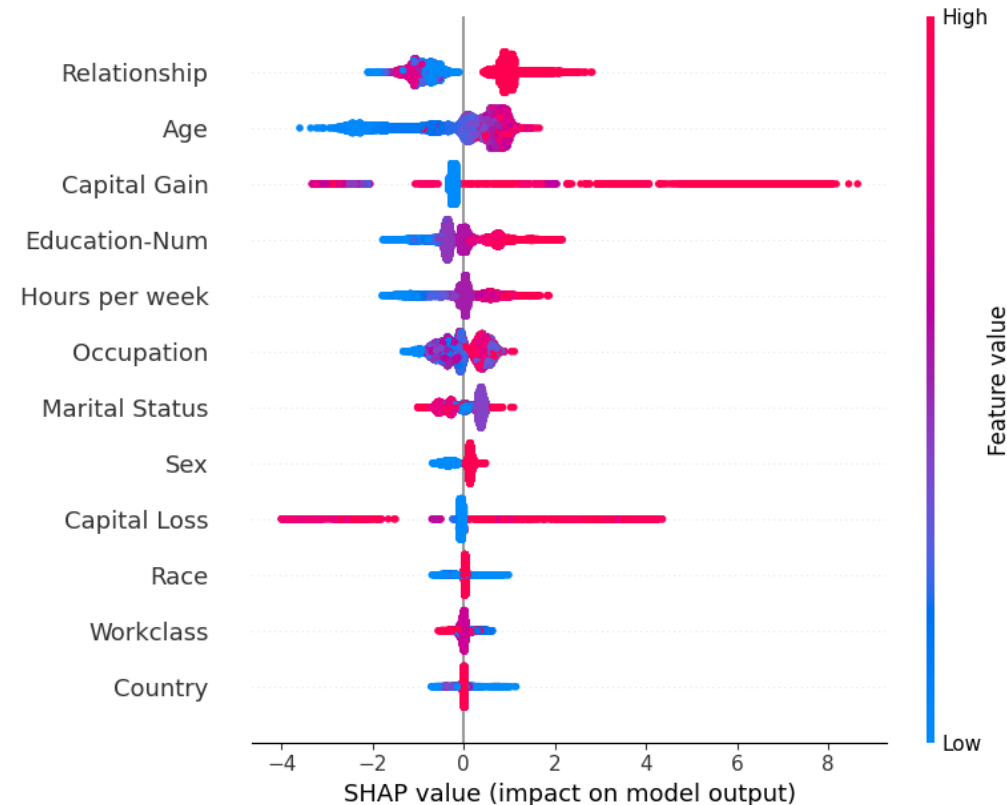
whew $\phi_j^{(i)}$ is the ϕ of the attribute j for the i -th instance and n is the number of instances

The higher the value of a feature, the more the features is important for model f



Global insights – SHAP Summary plot

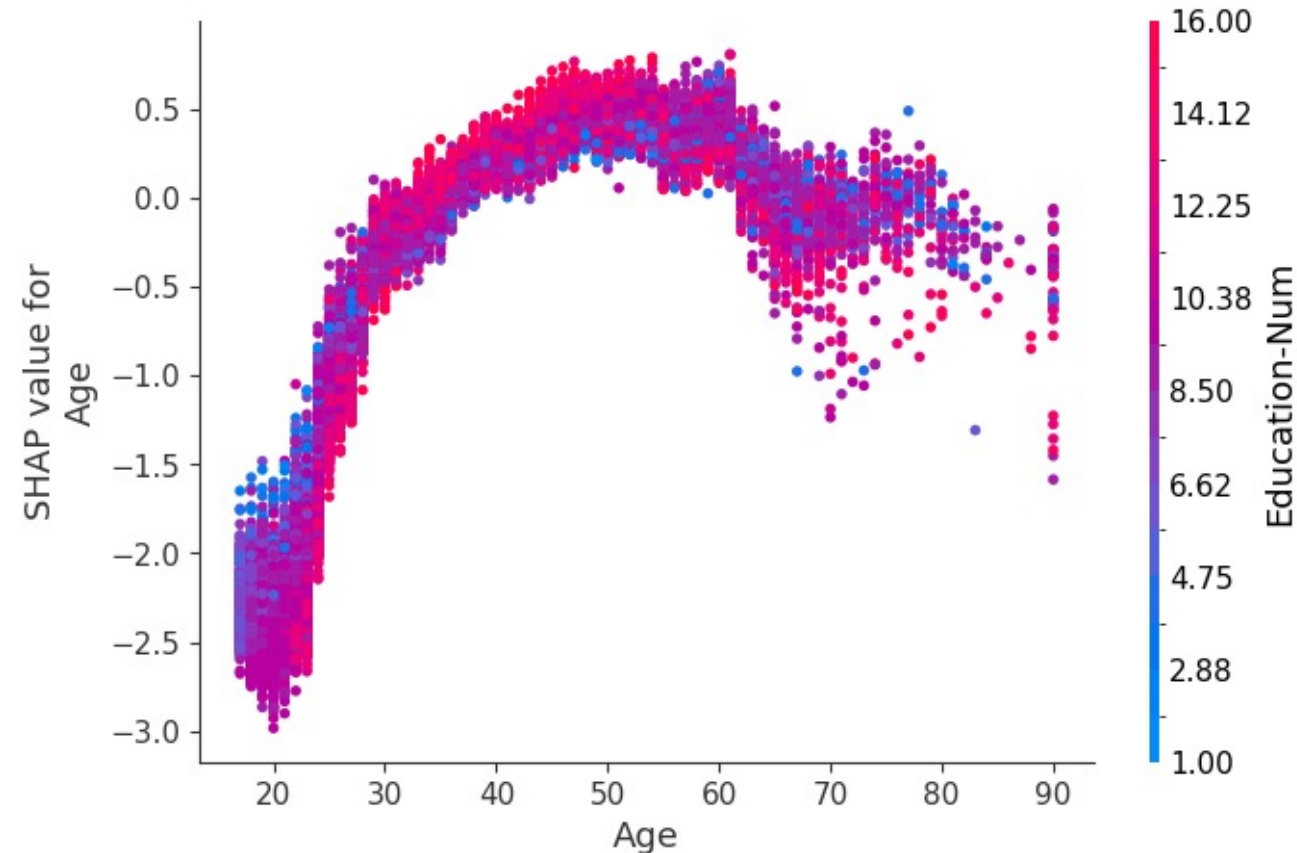
- **Density scatter plot**
- Each point is a Shapley value for a feature and an instance
 - We compute SHAP for all instances first
- x-axis - the Shapley value
- y-axis - the feature
- Features are sorted by the sum of the SHAP value magnitudes across all samples.



Global insights – SHAP Dependence Plot

Dependence Plot

- Given a feature j , for each data instance i we plot a $\{x_j^{(i)}, \phi_j^{(i)}\}$ with
 - the feature value on the x-axis
 - the corresponding Shapley value on the y-axis
- We can also color the point based on another feature k to highlight possible interactions with other features



Advantages of SHAP

- Same as exact Shapley
 - Model agnostic & Local explanations & Provides feature attributions & Direct interpretation
- Consider interaction among features
- Efficiency Property of Shapley Values
 - The difference between prediction for instance x and average prediction is distributed among feature values
- Solid Theoretical Foundation
 - Axioms: efficiency, symmetry, linearity, null player
- +
- **Reduced computational complexity**
- **Global model interpretations**
- **Nice and well documented library**

Limitations of SHAP

- Need access data to compute $f(h_x(z'))$
- Perturbations/info removals may create unrealistic data
 - Assumption feature independence
- The absence of a feature to compute $f(h_x(z'))$ is simulated by drawing random instances
→ variance on the estimation
- It is an approximation of Shapley values
- KernelSHAP is slow
 - But other faster approximation have been proposed and are available in the library

Unification of removal-based explanations

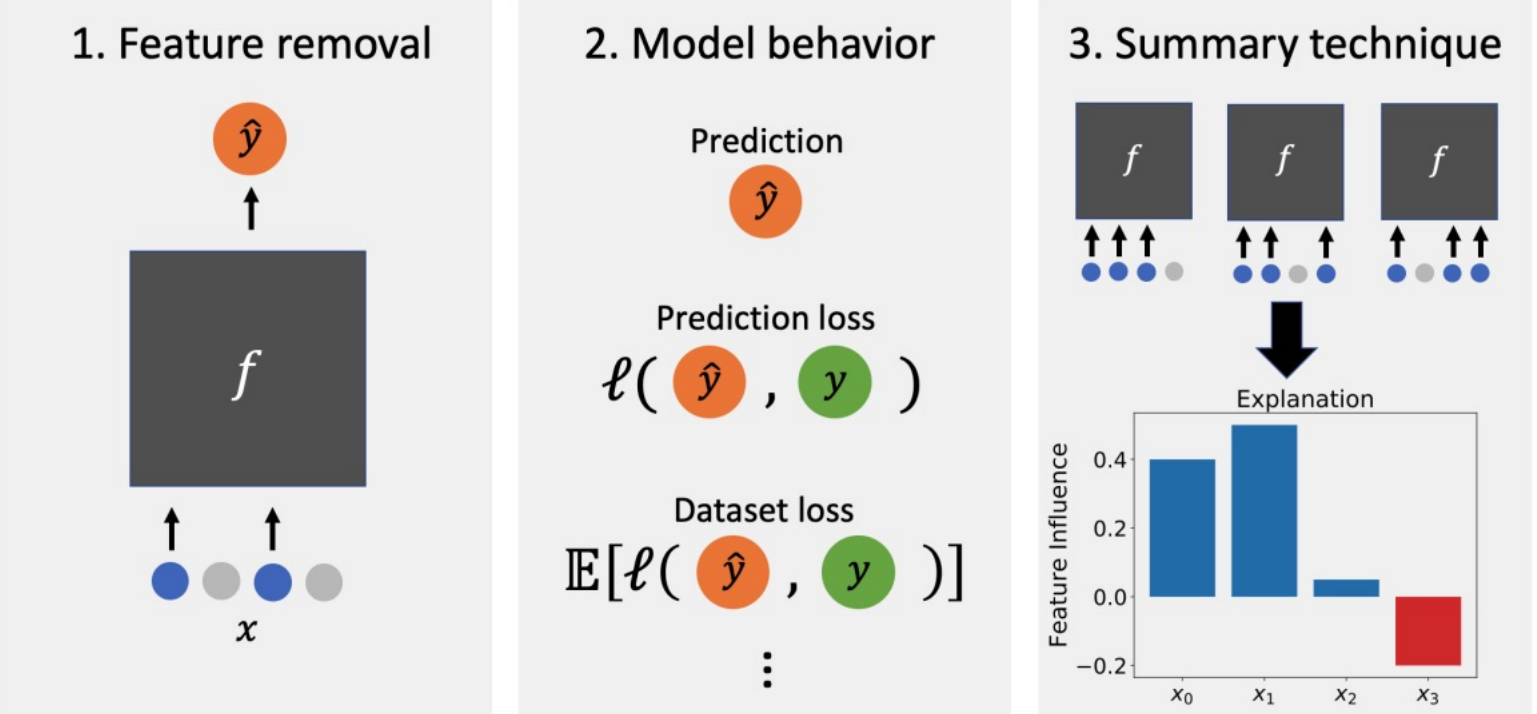
- Removal-based explanations are based on the principle of simulating feature removal to quantify the influence of each feature to the prediction
- We can characterize them according three dimensions
 - 1) Feature removal**

How the method removes features (e.g. by setting them to default values, or by marginalizing over a distribution of values)
 - 2) Model behavior**

What model behavior the method explains (e.g., the probability of the true class, or the model loss)
 - 3) Summary technique**

How the method summarizes each feature's influence (e.g., by removing a feature individually, or by calculating Shapley values)

Unification of removal-based explanations



1) Feature removal $f(x \setminus \bar{S})$ - examples

- **Zeroing**

- Remove features simply by setting them to zero:

$$f(x \setminus \bar{S}) = f(x_S, 0)$$

- **Default values**

- Remove features by setting them to user-defined default values such as gray pixels for images or a mean value (e.g., in LIME for image). Given default values $r \in X$, calculate:

$$f(x \setminus \bar{S}) = f(x_S, r_{\bar{S}})$$



1) Feature removal $f(x \setminus \bar{S})$ - examples

- **Blurring**

- Remove features from images by blurring them with a Gaussian kernel



- **Marginalize with marginal**

- Removes features by marginalizing them out using their joint marginal distribution (e.g., KernelSHAP):

$$f([z_S, E[z_{\bar{S}}]])$$

2) Model behavior - examples

- **Prediction probability**

$$f(\mathbf{x}) = p(y = c|\mathbf{x})$$

- **Prediction loss**

Consider the true label y for an input x and calculate the prediction loss using a loss function

- **Dataset loss**

Consider the expected loss across the entire dataset, i.e., quantify how much the model's performance degrades when different features are removed

3) Summarizing feature influence - examples

- **Remove individual**

Calculate the impact of removing a single feature from the model (e.g., PredDiff)

Note that this can be applied for interpretable representations (e.g., super-pixels)

- **Additive model**

Fit a regularized additive linear model to a dataset of perturbed examples (e.g., LIME). The learned coefficients represent the incremental value associated with including each feature.

- **Shapley value**

Calculate feature attributions using the Shapley value

Recap of the limitations of removal-based techniques

- Perturbations/info removals may create unrealistic data
- The absence of a feature is often simulated by drawing random instances → variance on the estimation
- The removal is often based on marginalization/mean values, thus requiring accessing to the data

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