Machine Learning in Bioinformatics

Explainability - XAI

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Introduction

- Machine learning studies the relationship between
  - independent or predictor variables X
  - dependent or response variables Y
- Machine learning and statistics may have multiple goals [Zhao and Hastie, 2021]:
  - *Prediction:* Predict the response variables Y as accurate at possible from X
  - *Science:* If $X \rightarrow Y$ is a causal relationship, we may want to understand the *laws of nature* that determine this relationship

Introduction

- Two opposing cultures of statistical analysis [Breiman, 2001]:
  - *Data modeling culture:* Assume a parametric function f such that $Y = f(X) + \epsilon$, where ϵ models the aleatoric uncertainty. The parameters of f are often easy to interpret and the model is used to understand the laws of nature
  - *Algorithmic modeling culture:* Use of *black-box* models that are very complex and optimized to maximize predictive accuracy. Black-box models are notoriously difficult to interpret and do barely allow to draw any conclusions about the laws of nature
- If we have a black-box model, how can we still gain some interpretation?

Outline I

- Assume we have a black-box machine learning model f
- Can we gain some *limited* understanding of the predictions of f?
- Understanding the predictions increases our *trust* in f

Outline II

- Given a fixed input x, what is the *contribution* of each feature to the prediction $y = f(x)$?
  (Attribution Map / Saliency Maps)
  - Occlusion
  - Layer-wise relevance propagation (LRP) / DeepLIFT
  - Integrated gradients
  - Shapley values
  - SHAP
- Given a fixed input x, is there an interpretable model that approximates f locally?

Outline III

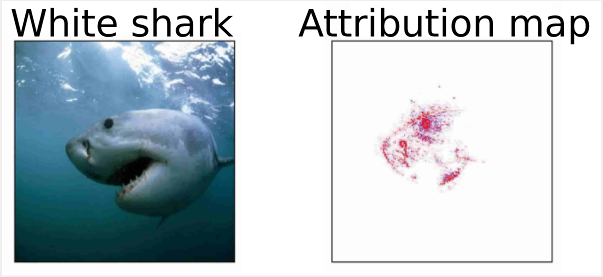
- Local interpretable model-agnostic explanations (LIME)
- Taylor approximations

- What would f predict if we vary one or more features?
  - Partial dependence plots (PDP)
  - Individual conditional expectation (ICE)
- What is the most likely input x for a given prediction $y = f(x)$?
  - Input optimization

Attribution maps

Attribution maps

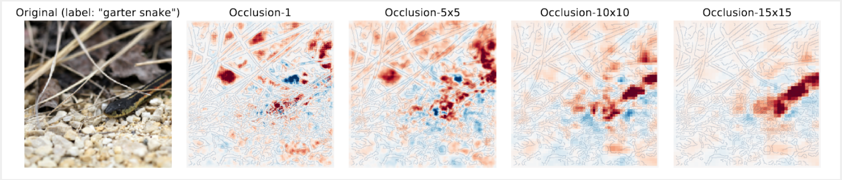
- Attribution maps are very popular with images, where the attribution of each pixel can be easily visualized
- Each input feature is assigned an attribution score (feature attribution)



[Kim et al., 2019]

Occlusion I

- Occlusion is a perturbation method that masks part of the input and measures the effect on the output of the network [Ancona et al., 2017]
- This method requires to evaluate the model for many perturbations
- The size of the mask is of particular importance

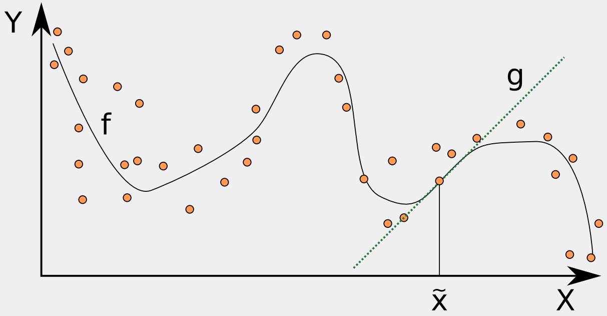


Occlusion II

- Assume we have a network that detects whether an image contains a cat
- If there are multiple cats in the image, occluding parts of the image with image patches (i.e. occluding at most one cat at a time) will not change the output of the network
- In this case, we would require masking multiple regions at the same time
- This leads to a combinatorial explosion

Gradient based explanations

Local explanations



Feature attribution

- Given a fixed input x and the corresponding output $y = f(x)$, what input features contribute most to the output value y?
- Note that for many applications (e.g. images) it is not very valuable to know which features (e.g. pixels) contribute most to the output of a neural network unless a specific input is considered
- The provided level of interpretability is hence limited to individual input data points

Gradient I

- Let f be a neural network or any other differentiable machine learning model

- Using the first-order Taylor expansion of f at an input $\tilde{x}$ we approximate f as a linear function

$$f(x) \approx f(\tilde{x}) + \nabla_x^\top f(\tilde{x})(x - \tilde{x})$$

  [Simonyan et al., 2013]

- With $w = \nabla_x f(\tilde{x})$ and $x' = x - \tilde{x}$ we obtain

$$f(x') \approx f(\tilde{x}) + w^\top x'$$

  where the gradient w can be easily interpreted as *feature importances*

Gradient × input I

- Using the gradient alone is problematic
- Let the network be defined as

$$f(x) = \max\{0, x - 10\}$$

  i.e. a single linear unit with ReLU activation

- The gradient is given by

$$\nabla_x f(x) = \begin{cases} 1 & \text{if } x > 10 \\ 0 & \text{otherwise} \end{cases}$$

- In this simple example, the larger x the larger the output $y = f(x)$ (assuming $x > 10$)

Gradient $\times$ input II

- However, for $f(20)$ we obtain the same attribution value as for $f(1000)$, i.e. 1 in both cases
- Multiplying the gradient with the input x seems to improve results [Shrikumar et al., 2016]
- For $f(20)$ we would obtain 20 as attribution value, whereas for $f(1000)$ the attribution is 1000

Integrated gradients I

- Integrated gradients (IG): Consider the gradient along an entire path from a baseline x_0 to an input $\tilde{x}$ [Sundararajan et al., 2017]

$$\mathrm{IG}_j(\tilde{x}) = (\tilde{x}^{(j)} - x_0^{(j)}) \int_{[0,1]} \frac{\partial f(\alpha \tilde{x} + (1-\alpha) x_0)}{\partial \tilde{x}^{(j)}} \mathrm{d}\alpha$$

- IG satisfies several convincing axioms that other methods violate

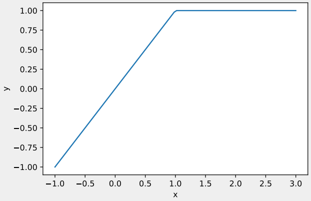
Integrated gradients II

Axiom 1: Sensitivity

Assume that x_0 and $\tilde{x}$ differ in at least one feature and that $f(x_0) \neq f(\tilde{x})$. Clearly the features that differ between x_0 and $\tilde{x}$ have some influence on the prediction. Hence, non-zero attribution should be given to these features

- Gradient and Gradient $\times$ input fail this axiom
- Consider the following example with just one feature

$$f(x) = 1 - \mathrm{ReLU}(1 - x)$$



Integrated gradients III

- For $x_0 = 0$ and $\tilde{x} = 2$ we obtain $f(x_0) = 0$ and $f(\tilde{x}) = 1$
- However, the gradient at $\tilde{x} = 2$ is zero
- The sensitivity axiom is the complement of the *dummy* property of Shapley values

Integrated gradients IV

Axiom 2: Implementation invariance

Let f and f' be two machine learning models. The two models are *functionally equivalent* if $f(x) = f'(x)$ for all x. Attributions should be identical for functionally equivalent models

- Gradients are invariant to implementations
- Several attribution methods fail this axiom, e.g. LRP and DeepLIFT

Integrated gradients V

Axiom 3: Linearity

Let f be a machine learning model such that

$$f(x) = af_1(x) + bf_2(x)$$

where a and b are weights. The attribution for f is the sum of attributions of f_1 and f_2 weighted by a and b

- Attribution methods should preserve any linearity in the machine learning models

Integrated gradients VI

Axiom 4: Completeness

Let f be a machine learning model. The attribution of all features at a point $\tilde{x}$ should sum up to

$$f(\tilde{x}) - f(x_0)$$

where x_0 is a baseline

- The completeness axiom corresponds to the efficiency property of Shapley values for $f(x_0) = \mathbb{E} f(X)$

Layer-wise relevance propagation (LRP)

Layer-wise relevance propagation (LRP) I

- Layer-wise relevance propagation (LRP) [Bach et al., 2015] exploints the layered structure of neural networks
- Let f be a neural network with L layers
- $R^{(l)} \in \mathbb{R}^{p_l}$ denotes a vector of relevance scores, one for each neuron in the l-th layer
- LRP satisfies the following law of conservation

$$f(x) = \cdots = \sum_{j=1}^{p_{l+1}} R_j^{(l+1)} = \sum_{j=1}^{p_l} R_j^{(l)} = \sum_{j=1}^{p_1} R_j^{(1)}$$

where $R_j^{(1)}$ are the relevances of the input features

Layer-wise relevance propagation (LRP) II

- The output of the neural network f for a given input x is the total relevance, which is distributed among neurons in previous layers
- More specifically, we call any relevance attribution method LRP if it satisfies

$$\begin{aligned} R_i^{(l)} &= \sum_{k:i\to k} R_{i\leftarrow k}^{(l,l+1)} \\ R_k^{(l+1)} &= \sum_{i:i\to k} R_{i\leftarrow k}^{(l,l+1)} \end{aligned}$$

where $R_{i\leftarrow k}^{(l,l+1)}$ is the relevance sent from neuron k to i between layers l and $l+1$

Layer-wise relevance propagation (LRP) III

- The relevances are in both the forward and backward direction sums of the relevances from connecting neurons

- Multiple solutions satisfy these constraints [Montavon et al., 2019], e.g.:
  - Basic rule (LRP-0)

$$R_{i\leftarrow k}^{(l,l+1)} = R_k^{(l+1)} \frac{a_i w_{ik}}{\sum_j a_j w_{jk}}$$

  - Epsilon rule (LRP-ϵ)

$$R_{i\leftarrow k}^{(l,l+1)} = R_k^{(l+1)} \frac{a_i w_{ik}}{\epsilon + \sum_j a_j w_{jk}}$$

  - a_i denotes the activation of neuron i (i.e. the output of a neuron before the non-linear activation is applied)

Layer-wise relevance propagation (LRP) IV

- DeepLIFT [Shrikumar et al., 2017] is an extension of LRP that backpropagates relevance values of

$$f(\tilde{x}) - f(x_0)$$

where x_0 is a user defined point that provides a baseline prediction (note that LRP uses $f(x_0) = 0$)

Local interpretable model-agnostic explanations (LIME)

LIME - Basic idea

- Local interpretable model-agnostic explanations (LIME)
- Model-agnostic: We can evaluate the model f but do not make any further assumptions about the model
- In particular, we do not require the model to be differentiable
- LIME locally approximates a machine learning model f using a simple interpretable model g at a specific point $\tilde{x}$ such that

  $$f(\tilde{x}) = g(\tilde{x})$$

  and $f(x) \approx g(x)$ whenever x is close to $\tilde{x}$
- g is typically a linear regression model

LIME - Basic idea

- Given a model class G, we determine a local interpretable model $\hat{g}$ by solving

$$\hat{g} = \arg\min_{g \in G} \mathcal{L}(f, g, \pi_{\tilde{x}}) + \Omega(g)$$

- G could be the class of linear models
- $\mathcal{L}$ is the main loss function we want to minimize
- $\Omega(g)$ is a penalty on the complexity of g, which for instance gives preference to models with fewer parameters
- $\pi_{\tilde{x}}(x)$ is a weight function that measures the proximity of x to $\tilde{x}$, whereby a local approximation of f is enforced

LIME - Basic idea

- Let $x_1, \ldots, x_n$ be a set of n training points
- For regression problems, the $\mathcal{L}$ function can be

$$\mathcal{L}(f, g, \pi_{\tilde{x}}) = \sum_i (f(x_i) - g(x_i))^2 \, \pi_{\tilde{x}}(x_i)$$

- The weight function can be given by an exponential kernel

$$\pi_{\tilde{x}}(x_i) = \exp\left\{ -\frac{d(\tilde{x}, x_i)^2}{\sigma^2} \right\}$$

  where d is a distance function

- σ^2 controls how local the approximation should be

LIME - In practice I

- The data used for training f might not be appropriate for estimating g
- We require samples $(x_i)_i$ close to $\tilde{x}$, where LIME uses the following scheme:
  - Draw a binary vector b_i of length p at random
  - Compute $x_i = h_{\tilde{x}}(b_i)$
- The function $h_{\tilde{x}}$ creates a sample x_i from b_i by masking parts of the reference $\tilde{x}$ (occlusion)

LIME - In practice II

- For instance, $h_{\tilde{x}}$ could mask features by replacing them with feature means $\bar{x}^{(j)}$, i.e. the jth feature of $x_i = h_{\tilde{x}}(b_i)$ is given by

$$x_i^{(j)} = \begin{cases} \tilde{x}^{(j)} & \text{if } b_i^{(j)} = 1 \\ \bar{x}^{(j)} & \text{if } b_i^{(j)} = 0 \end{cases}$$

LIME - In practice III

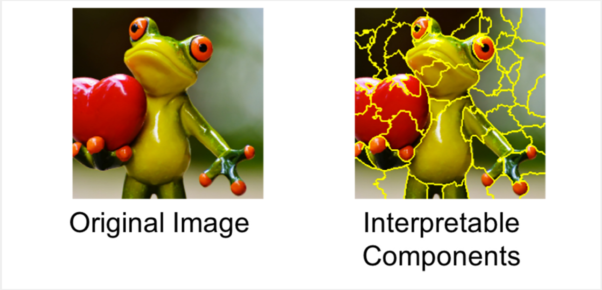
- Example topic models:
  - A data point x is a word count vector, where each entry $x^{(j)}$ denotes the number of occurrences of word j in a text document
  - $h_{\tilde{x}}(b_i)$ could mask features by replacing them with zeros, i.e.

$$h_{\tilde{x}}(b_i) = \begin{cases} \tilde{x}^{(j)} & \text{if } b_i^{(j)} = 1 \\ 0 & \text{if } b_i^{(j)} = 0 \end{cases}$$

  - Hence, samples x_i are created from the reference $\tilde{x}$ by replacing some of the counts with zeros

LIME - In practice IV

- Example image classification:
  - x is a an image, where each entry $x^{(j)}$ denotes a pixel or super-pixel
  - A sample $x_i = h_{\tilde{x}}(b_i)$ consists of the reference image $\tilde{x}$ where a some pixels or super-pixels have been masked, as defined by the binary vector b_i



LIME - In practice V

- The interpretable model g is typically defined on the binarized points b_i
- The loss for regression problems then becomes

$$\mathcal{L}(f, g, \pi_{\tilde{x}}) = \sum_i (f(x_i) - g(b_i))^2 \, \pi_{\tilde{x}}(x_i)$$

Shapley values

Shapley values - Motivation

- Assume a linear model

$$f(x) = \theta_1 x^{(1)} + \theta_2 x^{(2)} + \cdots + \theta_p x^{(p)}$$

- If features are standardized we can interpret the coefficient θ_j as the *global* importance of the *j*th feature

- Given a specific input x, the contribution of feature j to the prediction $f(x)$ is given by

$$\begin{aligned} \phi_j(f, x) &= \theta_j x^{(j)} - \mathbb{E}\left[\theta_j X^{(j)}\right] \\ &= \theta_j \left(x^{(j)} - \mathbb{E}\left[X^{(j)}\right]\right) \end{aligned}$$

assuming features are independent

Shapley values - Motivation I

- For non-linear models we need a more advanced definition
- Let F denote the set of p features and $S \subseteq F$ a subset
- Furthermore, let $f(x^{(S)})$ be the prediction of a machine learning model where only a subset of features S is used
- Let $S = F \backslash \{j\}$, then the contribution of the jth feature can be measured as

$$f(x^{(S \cup \{j\})}) - f(x^{(S)})$$

  - $f(x^{(S \cup \{j\})})$ is the prediction with feature j
  - $f(x^{(S)})$ the prediction without feature j

Shapley values - Motivation II

- In practice, features are rarely independent, i.e. feature j might only be informative in combination with other features
- In this case we have to attribute some of feature jth contribution to those features
- We have to test for all subsets $S \subseteq F \setminus \{j\}$

Shapley values - Example I

- Let the feature set F consist of $p = 3$ elements, i.e. $F = \{1, 2, 3\}$

- Assume we observe the following predictions

$$
\begin{aligned}
&f(x^{(\{1\})}) = 100, \quad f(x^{(\{1,2\})}) = 500, \\
&f(x^{(\{2\})}) = 100, \quad f(x^{(\{1,3\})}) = 300, \quad f(x^{(\{1,2,3\})}) = 1100 \\
&f(x^{(\{3\})}) = 100, \quad f(x^{(\{2,3\})}) = 300,
\end{aligned}
$$

- Clearly, features are not contributing independently to the predictions

- For independent features we would expect

$$f(x^{(\{1,2\})}) = f(x^{(\{1\})}) + f(x^{(\{2\})})$$

Shapley values - Example II

- How much should we attribute to each feature?
- We fix a particular feature j and evaluate its contribution to all subsets $S \subseteq F \setminus \{j\}$
- To simplify notation, let

$$\xi_j(S) = f(x^{(S \cup \{j\})}) - f(x^{(S)})$$

- For $j = 3$ and $S = \{1, 2\}$ we have

$$\xi_j(S) = 1100 - 500 = 600$$

- For $j = 2$ and $S = \{3\}$ we have

$$\xi_j(S) = 300 - 100 = 200$$

Shapley values - Example III

- $\xi_j(S)$ denotes the contribution of feature j to the prediction based on features S
- The Shapley value for feature j is the average over all contributions
- We evaluate all $p!$ permutations of p features, i.e.

$$\begin{gathered} 1, 2, 3 \\ 1, 3, 2 \\ 2, 1, 3 \\ 2, 3, 1 \\ 3, 1, 2 \\ 3, 2, 1 \end{gathered}$$

Shapley values - Example IV

- A permutation is interpreted as a sequence of features entering the set of features S
- For instance, for $2, 1, 3$ we first have feature 2 entering S and afterwards feature 1. Feature 3 is the last to join S
- We then evaluate the contribution of each feature, i.e. for $2, 1, 3$ we evaluate $\xi_2(\{\})$, $\xi_1(\{2\})$, and $\xi_3(\{1, 2\})$

Shapley values - Example V

	$j=1$		$j=2$		$j=3$	
1,2,3	$\xi_1(\{\})$	$=100$	$\xi_2(\{1\})$	$=400$	$\xi_3(\{1,2\})$	$=600$
1,3,2	$\xi_1(\{\})$	$=100$	$\xi_2(\{1,3\})$	$=800$	$\xi_3(\{1\})$	$=200$
2,1,3	$\xi_1(\{2\})$	$=400$	$\xi_2(\{\})$	$=100$	$\xi_3(\{1,2\})$	$=600$
2,3,1	$\xi_1(\{2,3\})$	$=800$	$\xi_2(\{\})$	$=100$	$\xi_3(\{2\})$	$=200$
3,1,2	$\xi_1(\{3\})$	$=200$	$\xi_2(\{1,3\})$	$=800$	$\xi_3(\{\})$	$=100$
3,2,1	$\xi_1(\{2,3\})$	$=800$	$\xi_2(\{3\})$	$=200$	$\xi_3(\{\})$	$=100$

- The rows are the permutations, the columns represent features to enter the set S
- The Shapley value $\phi_j(f,x)$ for feature j is the average over all $p! = |F|!$ rows in column j
- Hence, permutations are assumed to be uniformly distributed

Shapley values - Example VI

- How often do we observe a particular entry $\xi_j(S)$ in column j?
- We can permute all features before j enters and all features after j enters
- Hence, an entry $\xi_j(S)$ occurs

$$|S|!(|F| - |S| - 1)!$$

times in column j

Shapley values - Definition I

Shapley value [Shapley, 1951]

The shapley value for the *j*th feature is defined as

$$\phi_j(f,x) = \sum_{S \subseteq F \setminus \{j\}} \frac{|S|!(|F|-|S|-1)!}{|F|!} \xi_j(S)$$
$$= \sum_{S \subseteq F \setminus \{j\}} \frac{|S|!(|F|-|S|-1)!}{|F|!} \left(f(x^{(S \cup \{j\})}) - f(x^{(S)})\right)$$

- The sum is over 2^{p-1} permutations
- For large feature sets the Shapley value is computationally very expensive or even impossible to compute

Shapley values - Linear models I

- Assume f is a linear model of the from

$$f(x) = \theta_1 x^{(1)} + \theta_2 x^{(2)} + \cdots + \theta_p x^{(p)}$$

- Given independent features, the Shapley values for this model reduce to

$$\phi_j(f, x) = \theta_j \left(x^{(j)} - \mathbb{E}\left[X^{(j)} \right] \right)$$

  [Štrumbelj and Kononenko, 2014]

- This is what we expected from our previous discussion

Shapley values - Properties I

- *Efficiency:*
$$\sum_j \phi_j(f,x) = f(x) - \mathbb{E}_X f(X)$$

- *Symmetry:* If two features j and k contribute equally to all subsets, then
$$\phi_j(f,x) = \phi_k(f,x)$$
for all x

- *Dummy:* If feature j does not influence the prediction $f(x^{(S)})$ for all S, then
$$\phi_j(f,x) = 0$$

Shapley values - Properties II

- *Additivity:* If $f(x) = \sum_m f_m(x)$ then

$$\phi_j(f, x) = \sum_m \phi_j(f_m, x)$$

  i.e. f could be a random forest or any other bagging method

Shapley values - In practice I

- How do we remove features from the prediction of our machine learning model f?
- The optimal but impractical way would be to train a model f_S for each subset S
- Instead, we often use

$$f(x^{(S)}) = \mathbb{E}\left[f(X)\,|\,X^{(S)} = x^{(S)}\right]$$

  where all elements of X that are not given by $\{X^{(S)} = x^{(S)}\}$ are considered random

- The expectation can be estimated from our training data, which however requires many evaluations of the model f

Shapley values - In practice II

- Assuming that our model f is linear, we obtain

$$f(x^{(S)}) = \mathbb{E}\left[f(X) \mid X^{(S)} = x^{(S)}\right] = f\left(\mathbb{E}[X \mid X^{(S)} = x^{(S)}]\right)$$

- Furthermore, assuming independent features we obtain

$$f(x^{(S)}) = f(\bar{x}^{(S)})$$

where

$$\bar{x}^{(S)} = \begin{cases} x^{(j)} & \text{if } j \in S \\ \mathbb{E}\, X^{(j)} & \text{if } j \notin S \end{cases}$$

i.e. all features not in S have been replaced by their expectation

Shapley values - Monte Carlo I

- Summing over 2^{p-1} contributions is often too expensive
- We may utilize Monte Carlo approximations (law of large numbers) to estimate the Shapley value [Štrumbelj and Kononenko, 2014]
  - Draw k permutation $\pi_i = (r_1, \ldots, r_p)$ with $r_m \in \{1, \ldots, p\}$ from a uniform distribution
  - For each permutation π_i, compute the set of features S_{ij} from π_i, i.e. all features until feature j occurs in π_i
  - The Monte Carlo approximation of the Shapley value is given by

$$\phi_j(f, x) \approx \frac{1}{k} \sum_{i=1}^{k} \left(f(x^{(S_{ij} \cup \{j\})}) - f(x^{(S_{ij})}) \right)$$

Shapley values - Kernel SHAP I

- SHapley Additive exPlanations (SHAP) [Lundberg and Lee, 2017]
- Kernel SHAP reformulates the computation of Shapley values as a linear regression problem using the LIME framework
- The interpretable model g is assumed to be a linear regression model

$$g(b_i) = \phi_0 + \sum_{j=1}^{p} \phi_j b_i^{(j)}$$

i.e. the contributions of the linear model depend on the weights ϕ_j and the binary values $b_i^{(j)}$

Shapley values - Kernel SHAP II

- The weights ϕ_j are the Shapley values
- Notice that LIME with loss function

$$\mathcal{L}(f, g, \pi_{\tilde{x}}) = \sum_i \left(f(x_i) - g(b_i)\right)^2 \pi_{\tilde{x}}(x_i)$$

and $\Omega(g) = 0$ corresponds to weighted ordinary least squares

$$\begin{aligned}\hat{\theta} &= \arg\min_{\theta} \left\| W^{1/2}(y - X\theta) \right\|_2^2 \\ &= (X^\top W X)^{-1} X^\top W y\end{aligned}$$

where $X \in \{0, 1\}^{2^p \times p}$ denotes a matrix containing all possible binary vectors b_i of length p as rows, $W = (w_{ii})$ is a weight

Shapley values - Kernel SHAP III

matrix with $w_{ii} = \pi_{\tilde{x}}(x_i)$ and $y = (y_i)$ is the vector of targets $y_i = f(x_i)$

- The coefficients $\hat{\theta}$ are the Shapley values $\phi = (\phi_1, \dots, \phi_p)$ for

$$\pi_{\tilde{x}}(x_i) = \frac{p-1}{\binom{p}{k_i} k_i (p-k_i)}$$

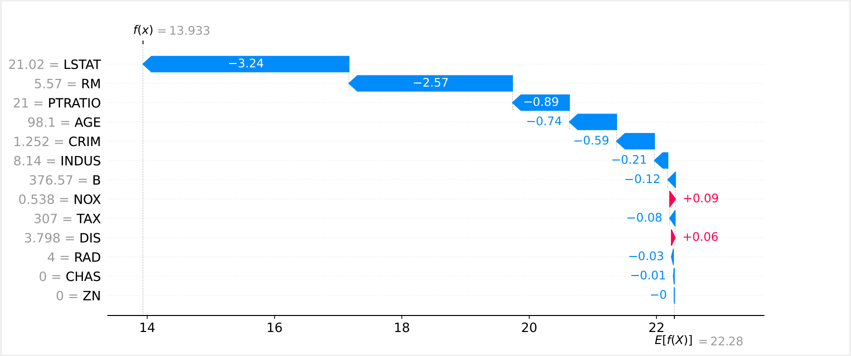
where $k_i = |b_i|$ is the number of ones in the binary representation of the ith sample

- Notice that $|b_i|$ measures the similarity between x_i and x, therefore this particular choice of $\pi_{\tilde{x}}$ is indeed a weight based on a distance measured

Shapley values - Kernel SHAP IV

- Recall that the *i*th sample x_i is generated from x by randomly generating a binary representation b_i and afterwards masking all features j in $\tilde{x}$ where $b_i^{(j)} = 0$
- The linear regression coefficients θ correspond to the Shapley values ϕ only when we consider all possible binary vectors b_i
- In practice, Kernel SHAP uses a sampled subset of binary vectors
- An improved method has been proposed [Kwon and Zou, 2022]

Shapley values - Example



Partial Dependence Plot

Partial Dependence Plot

- Let f be a black-box model such as a neural network
- What is the effect of individual predictors $X^{(j)}$ on the response variable Y as captured by our model f?

Partial Dependence Plot

- Partial dependence plots (PDP) [Friedman, 2001]:

$$\mathrm{PDP}_j(x) = \int f(x, x^{(-j)}) \mathrm{pr}(x^{(-j)}) dx^{(-j)}$$

  where $x^{(-j)} = (x^{(1)}, \ldots, x^{(j-1)}, x^{(j+1)}, \ldots x^{(p)})$

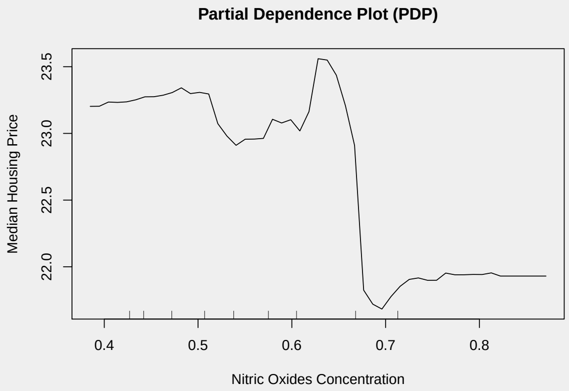
- In practice we use the training data $(x_i, y_i)_{i=1}^n$ to estimate the PDP, i.e.

$$\widehat{\mathrm{PDP}}_j(x) = \frac{1}{n} \sum_{i=1}^{n} f(x, x_i^{(-j)})$$

Partial Dependence Plot - Example

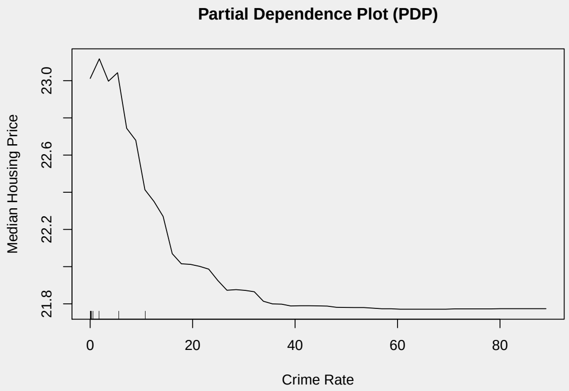
- Boston housing data: Housing data for 506 census tracts of Boston from the 1970 census
- X: capita crime rate, proportion of non-retail business acres per town, nitric oxides concentration, average number of rooms per dwelling, proportion of owner-occupied units built prior to 1940, ...
- Y: median value of owner-occupied homes in USD 1000's

Partial Dependence Plot - Example



- Housing prices drop when *nitric oxides concentration* reaches $\sim$ 0.68

Partial Dependence Plot - Example



- Housing prices drop quickly with crime rate

Partial Dependence Plot - ICE

- The individual conditional expectation (ICE) is an extension of the PDP
- It plots each component of the PDP sum individually, i.e.

$$\widehat{\mathrm{ICE}}_{ij}(x) = f(x, x_i^{(-j)})$$

- Hence, we have

$$\widehat{\mathrm{PDP}}_j(x) = \frac{1}{n} \sum_{i=1}^{n} \widehat{\mathrm{ICE}}_{ij}(x)$$

Input Optimization

Input optimization I

- Assume that f is a classifier for images
- We want to find inputs x not contained in the training set that correspond to predictions of a given classification
- This analysis might help to understand if f is sensitive to the correct features
- For a given output y we solve the optimization problem

$$\hat{x} = \arg\min_{x} \mathcal{L}(f(x), y)$$

- The loss function $\mathcal{L}$ typically corresponds to the loss function used for training f

Input optimization II

- As for training f we may use gradient descent to compute $\hat{x}$
- The result $\hat{x}$ depends strongly on the initial value for solving the optimization problem
- Using multiple initial conditions allows to generate multiple inputs $(x_i)_i$ corresponding to the same prediction y

SOFTWARE

- SHAP:
  `https://shap.readthedocs.io`
- iNNvestigate (Keras/Tensorflow):
  `https://github.com/albermax/innvestigate`
- Captum (PyTorch):
  `https://github.com/pytorch/captum`

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