# 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 $X \to Y$ 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 $\epsilon$ 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

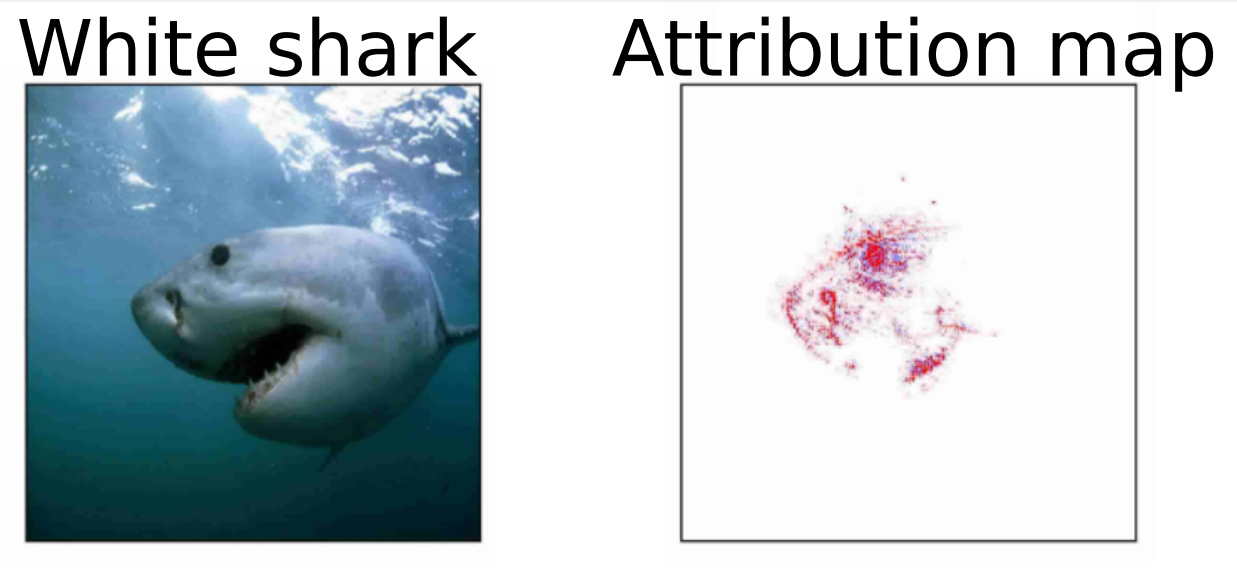
- What would $f$ predict if we vary one or more features?
  - Partial dependence plots (PDP)
  - Individual conditional expectation (ICE)

- What is the most likely input $x$ for a given prediction $y = f(x)$?
  - Input optimization

# Attribution maps

# Attribution maps

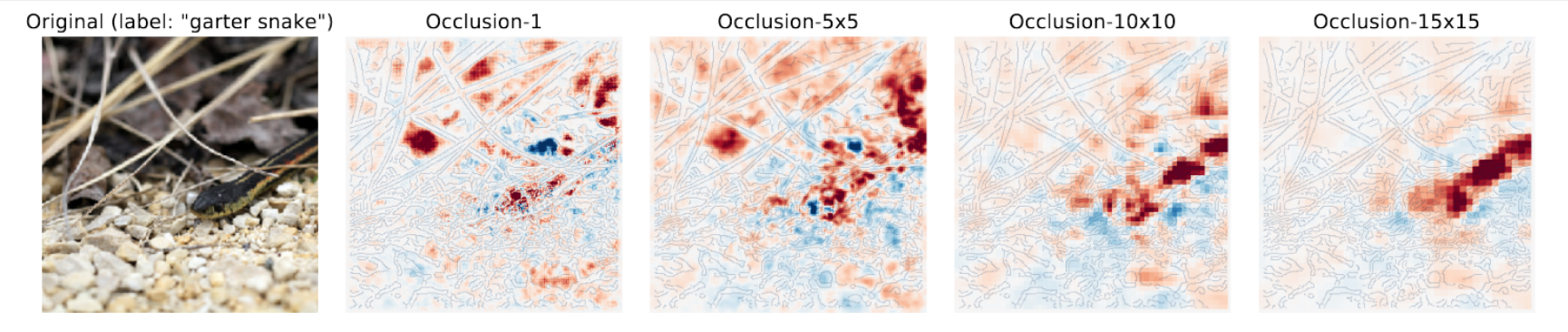
- Attribution maps are very popular with images, where the attribution of each pixel can be easily visualized
- Each input feature is assigned an attribution score (feature attribution)




[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

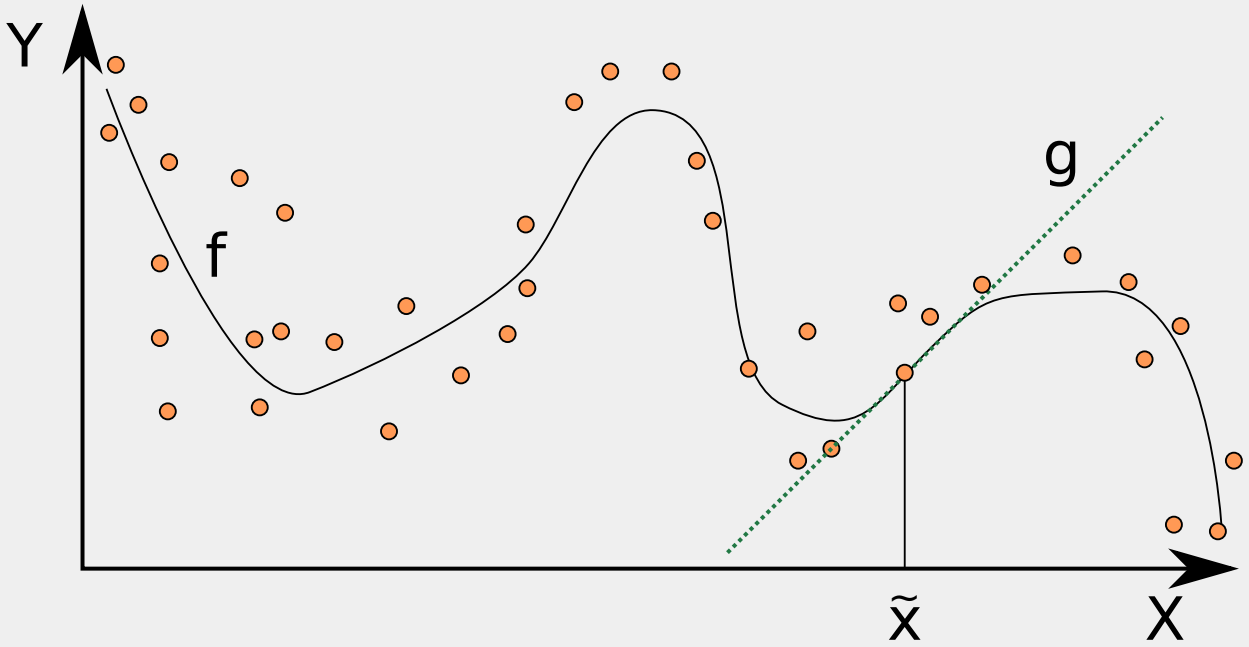


# Occlusion II

- 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 × 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]

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

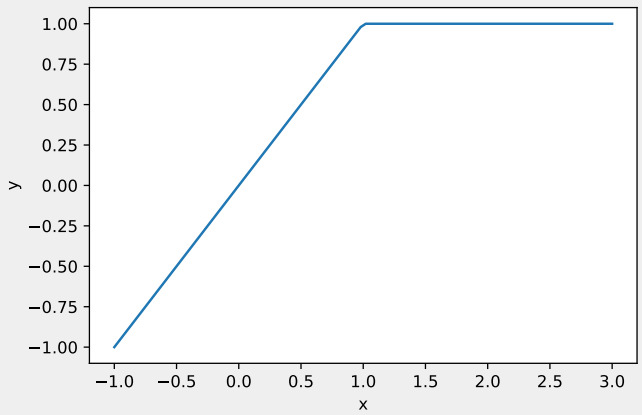
- IG satisfies several convincing axioms that other methods violate

## 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

## 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

## 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

## 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] exploits 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

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

  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-$\epsilon$)

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

  - $a_i$ 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

- $\sigma^2$ 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 $j$th 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 $b_i$

Original Image

Interpretable Components

# 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 $\theta_j$ 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 $j$th 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 $j$th contribution to those features
- We have to test for all subsets $S \subseteq F \backslash \{j\}$

# 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

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

- 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 $S \subseteq F \backslash \{j\}$
- 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.

$$1, 2, 3$$
$$1, 3, 2$$
$$2, 1, 3$$
$$2, 3, 1$$
$$3, 1, 2$$
$$3, 2, 1$$

# 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

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

- 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

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

  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 $\pi_i$, compute the set of features $S_{ij}$ from $\pi_i$, i.e. all features until feature $j$ occurs in $\pi_i$
  - 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 $\phi_j$ and the binary values $b_i^{(j)}$

# Shapley values - Kernel SHAP II

- The weights $\phi_j$ are the Shapley values
- Notice that LIME with loss function

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

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 $\phi = (\phi_1, \ldots, \phi_p)$ for

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

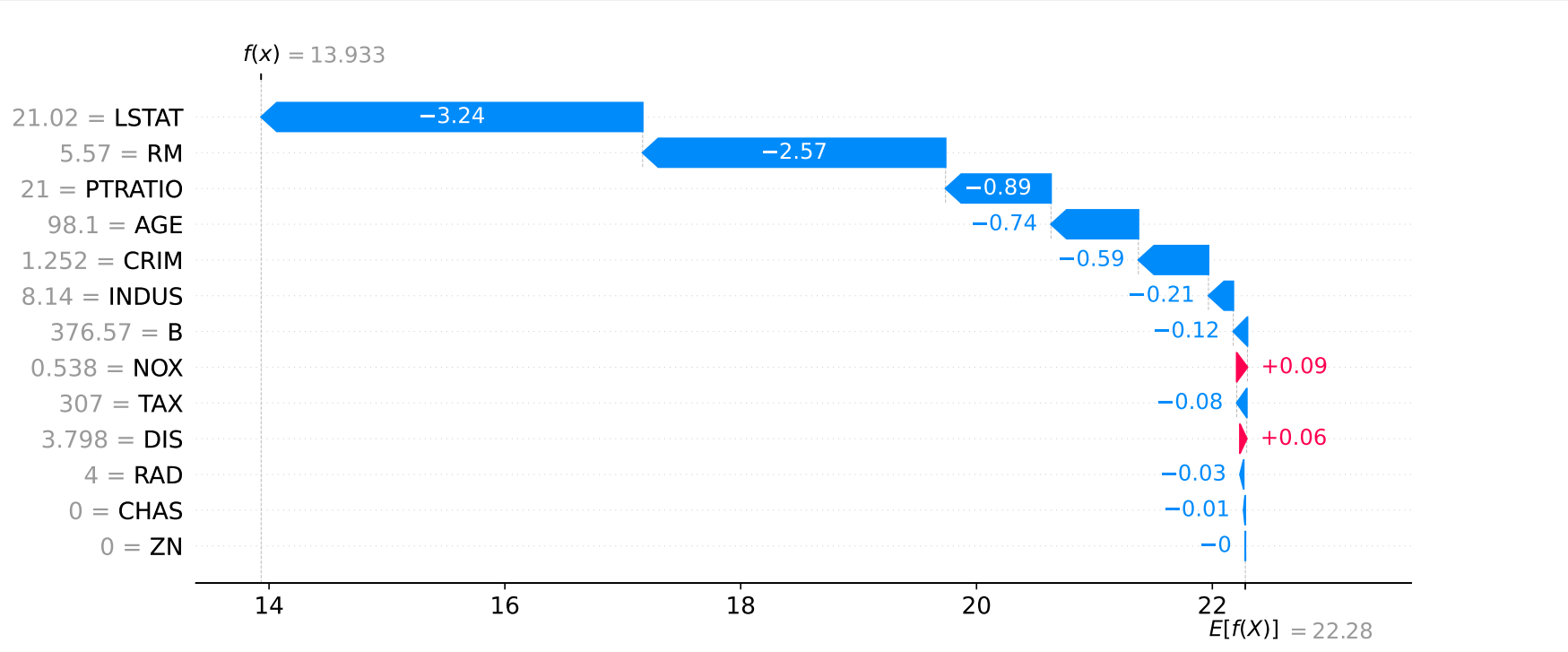
where $k_i = |b_i|$ is the number of ones in the binary representation of the $i$th sample

- 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 $\theta$ correspond to the Shapley values $\phi$ 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]:

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

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

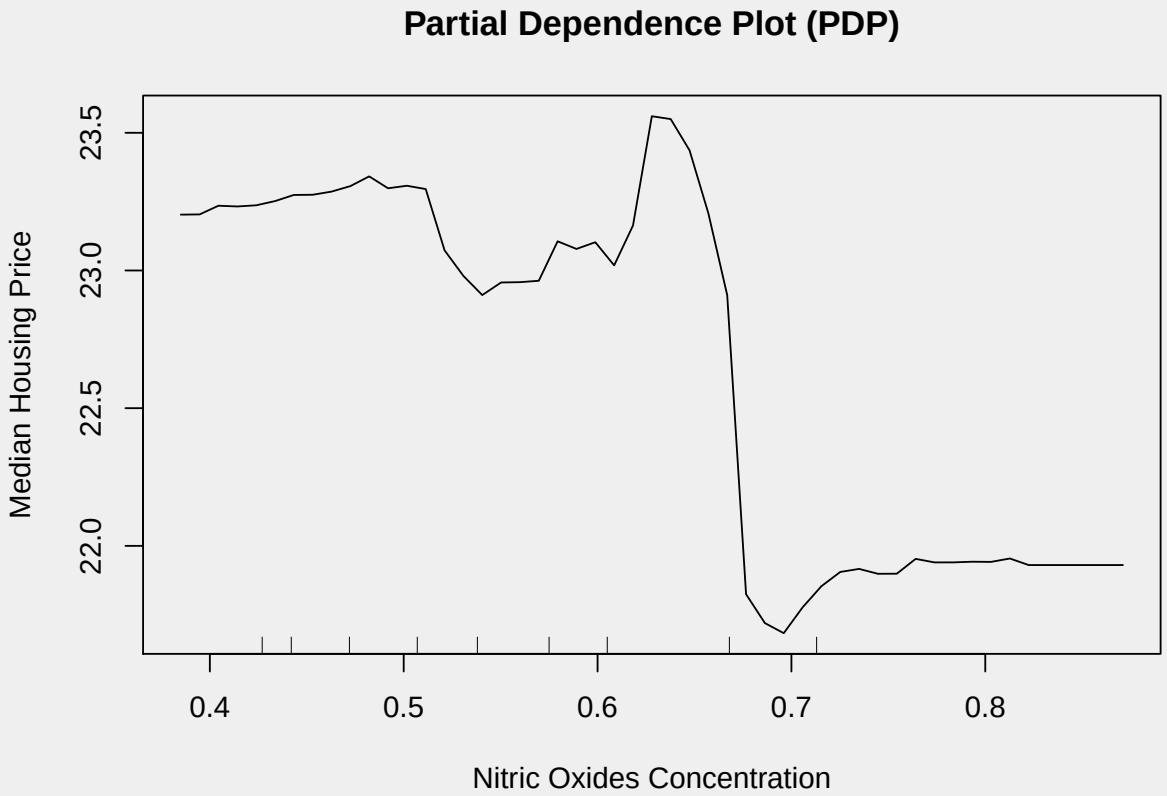
- In practice we use the training data $(x_i, y_i)_{i=1}^n$ to estimate the $\mathrm{PDP}$, i.e.

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

# Partial Dependence Plot - Example

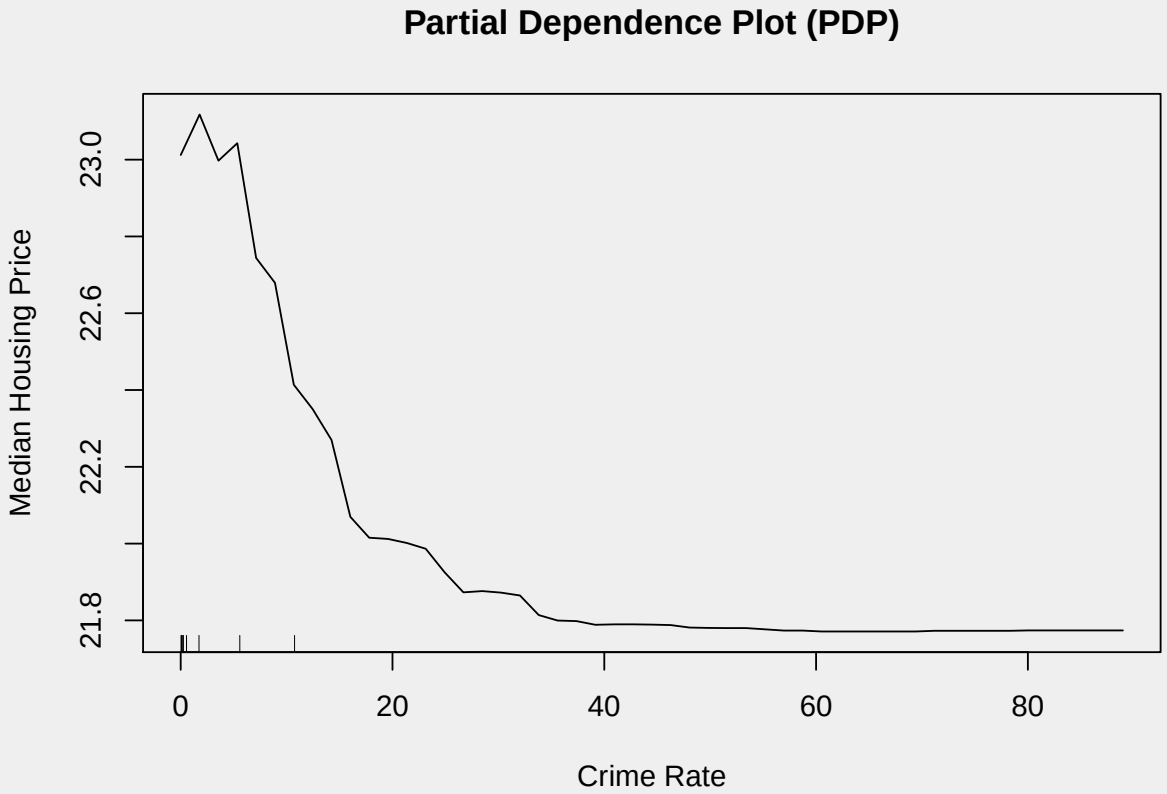
- Boston housing data: Housing data for 506 census tracts of Boston from the 1970 census
- X: capita crime rate, proportion of non-retail business acres per town, nitric oxides concentration, average number of rooms per dwelling, proportion of owner-occupied units built prior to 1940, ...
- Y: median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