Lecture 4. Surrogate Models. LIME and SHAP

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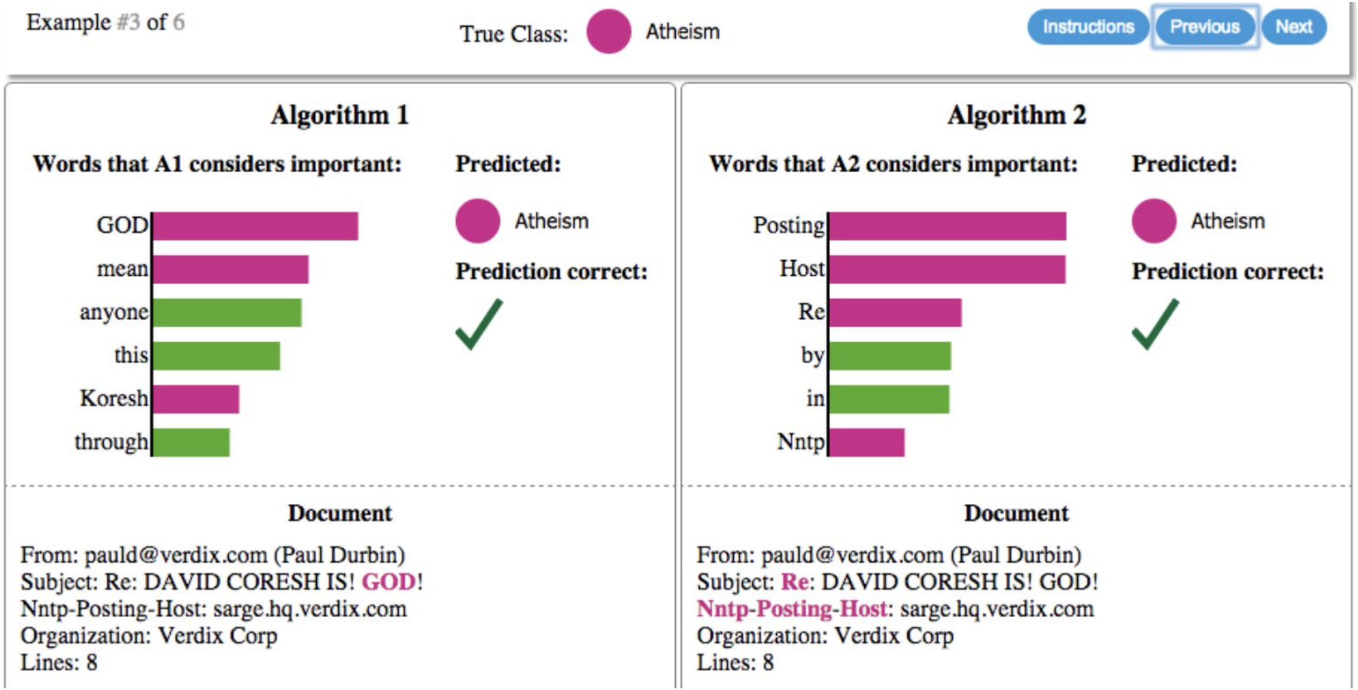
Part 1. LIME

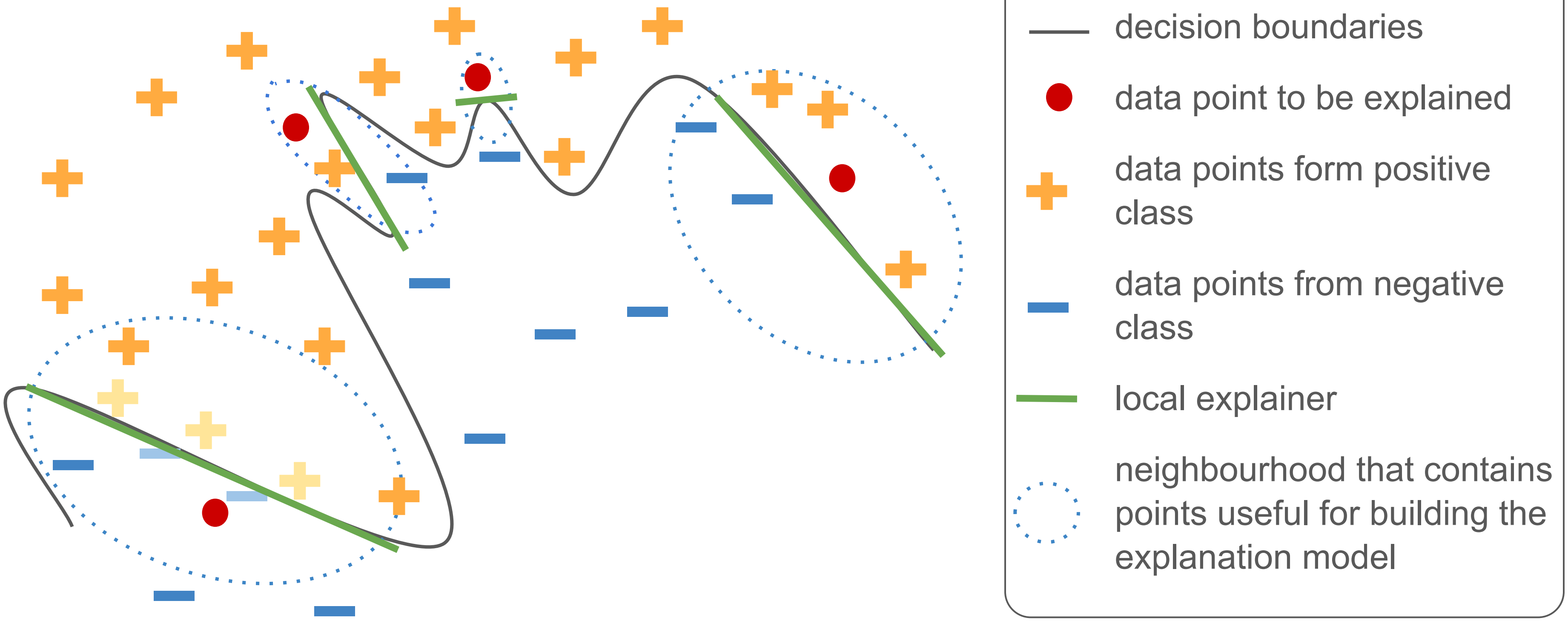
Why do we need more than just accuracy?



Explaining individual predictions of competing classifiers trying to determine if a document is about "Christianity" or "Atheism" on the "20 newsgroup" dataset. **Algorithm 1**: SVM trained on its manually clean version, accuracy: train 69.0%, test 88.6% **Algorithm 2**: SVM trained on the original dataset, accuracy: train 57.3%, test 94.0%

Credit: https://arxiv.org/pdf/1602.04938.pdf

Regression-based explanation



This kind of explanation is called **local** since we explain single instances (points) one by one

Local explanation by surrogate models

Let (X, y) be a dataset from $\mathbb{R}^{n \times d}$, i.e., an instance is described in d-dimensional space and f: $\mathbb{R}^d \rightarrow \mathbb{R}$ be a learned black box model, and x in $\mathbb{R}^d$ be an instance that should be explained

Main steps:

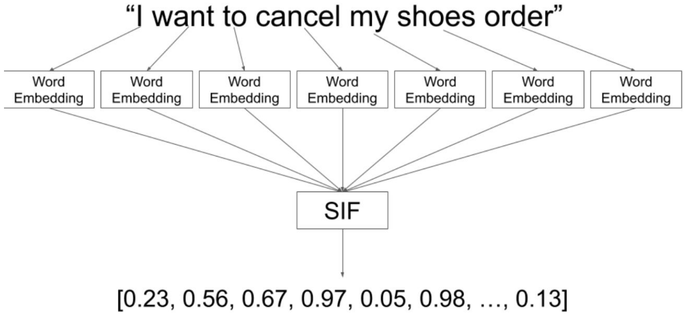
1. **By** introducing local **perturbations** to x generate an new data instances X_{new} in the neighbourhood of x
2. Feed them to the model to **get the target values** $y_{\text{new}} = f(X_{\text{new}})$
3. **Build an explainable model** g on $(X_{\text{new}}, y_{\text{new}})$ and (x, y_x)
4. Use this model g to **explain** $f(x)$

Interpretable space for white box models

Can we use the same space or we need something more?

White model g on images

White model g on word embeddings



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Feature importance is meaningless in these cases

We need a space that is **not too large**, such that the features allow for **a clear interpretation**

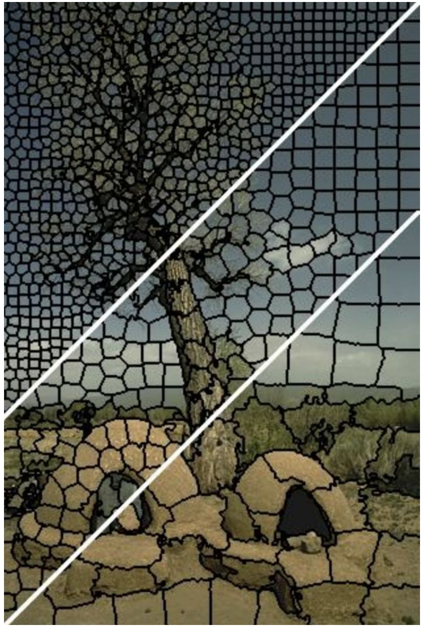
0 Step. Defining an interpretable space for g

Thus, given a black box model f: $\mathbb{R}^d \rightarrow \mathbb{R}$ trained on a dataset (X, y), we use a special transformation to interpretable space $\{0,1\}^{d'}$ and define a white box model g: $\mathbb{R}^{d'} \rightarrow \mathbb{R}$ (or $\{0,1\}^{d'} \rightarrow \mathbb{R}$)

Interpretable space is **specific for each type** of data

0 Step. Defining an interpretable space for g

- Numerical values in tabular data
  - applying a standard scaling: (value - mean) / std
- Categorical values in tabular data
  - one-hot encoding
- Image
  - segmentation (a kind of clustering)
- Texts
  - from the embeddings back to 0-1 vectors



An example of segmentation from https://ivrlwww.epfl.ch/supplementary_material/RK_SLICSuperpixels/index.html

Step 1. Introducing perturbations in tabular data

Let $x = (x_1, \ldots, x_d)$ be an instance described by d features

- for a **continuous** *i*-th attribute
  - *perturbation*: x'_i * std_i + mean_i, where $x'_i \sim N(0,1)$ is a random variable, mean_i and std_i are mean and standard deviation of the *i*-th attribute
  - *interpretable representation*: x'_i
- for a **categorical** *i*-th attribute taking *K* possible values
  - *perturbation*: $x_i \sim \mathrm{Cat}(K, \boldsymbol{\alpha})$, i.e., generalized Bernoulli distribution, where $\boldsymbol{\alpha}$ is a vector of probabilities of each of K values
  - *interpretable representation*: one-hot encoded feature

Step 1. Introducing perturbations in images

Let x be an instance described by d pixels

- *preprocessing*:
  1. applying a segmentation algorithm[1]
  2. consider the obtained K segments as clusters
- *perturbation*: randomly choose clusters with p = ⅓
- *interpretable space*: $\{0,1\}^K$, with 1 and 1 meaning that the *k*-th cluster has be selected or not for a given perturbation

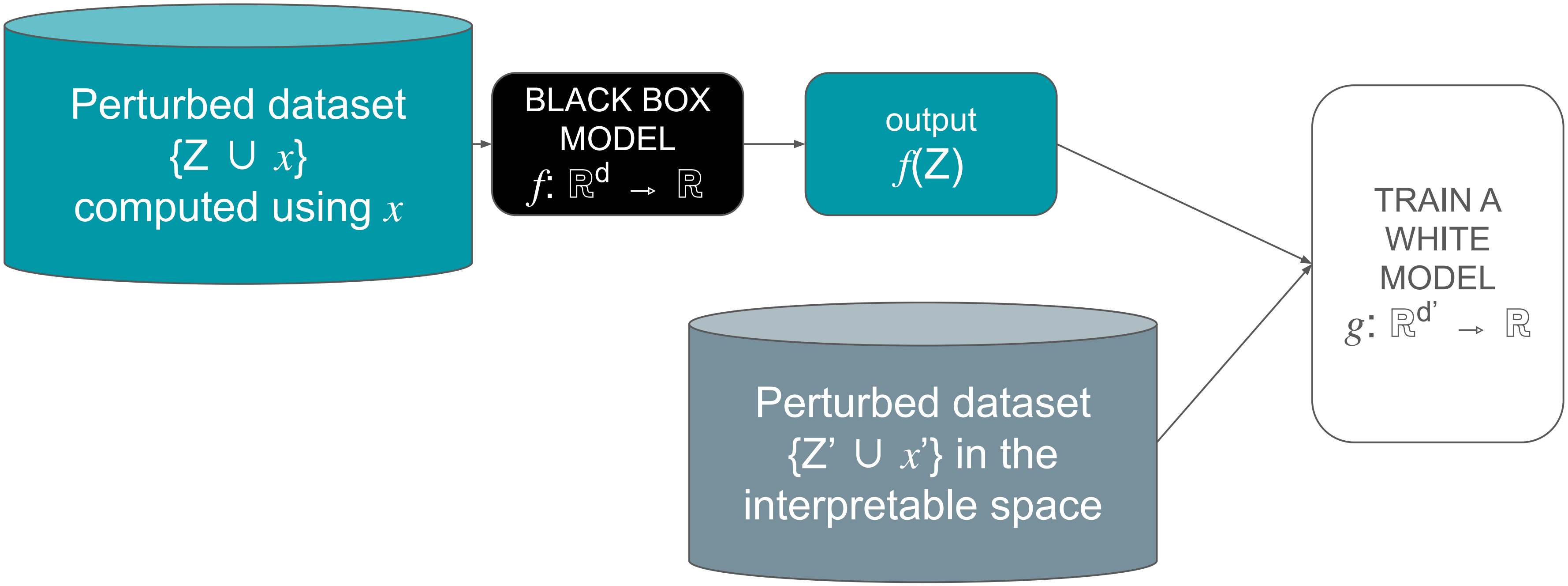
[1] Vedaldi, Andrea, and Stefano Soatto. "Quick shift and kernel methods for mode seeking." *European conference on computer vision*. Springer, Berlin, Heidelberg, 2008.

Step 1. Introducing perturbations in texts

Let $x \in \{1\}^d$ be a vector representing the words appearing in the text instance

- *perturbation*:
  1. select randomly a natural number between $k \in [1, d]$
  2. remove from x k randomly selected words
- *interpretable representation*: a $\{0,1\}^d$ - vector, where 0-values are those that have been removed during perturbation

2. Feed to the black box model

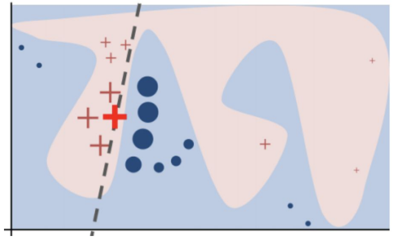


3. Fit an explainable model

The objective is given by $\mathcal{Z}(f, g, \pi_x(z)) = \sum_{z,z'} \boldsymbol{\pi_x(z)}[f(z) - g(z')]^2 + \boldsymbol{\Omega(g)}$

Not all the instances are of the same importance

Let x be the instance to be explained, and z be an perturbed one, then the weight of z is given by $\pi_x(z) = exp(-D(x,z)^2/\sigma^2)$, by default $\sigma = 0.75\sqrt{n}$ and D is the distance (e.g., cosine for texts, L2 for images, etc)



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Why do we do weighting: we put more importance to the instances that are close to the x

We need to use a reasonable number of features

We penalise too complex models using $\Omega(g)$, e.g., the height of the tree, the number of non-zero coefficients

Putting all together...

LIME provides an explanation by linear local surrogate model

The explanation is obtained as follows:

$$\xi(x) = \arg\min_{g \in G} \mathcal{L}(f, g, \pi_x) + \Omega(g)$$

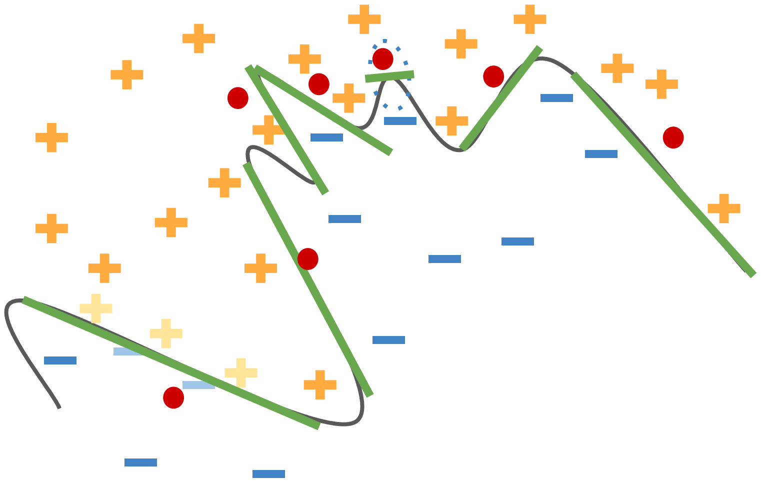
Specificities:

- interpretable representation
- importance of perturbed instances (weighted loss)
- regularization of the complexity of the model

How to trust our model?

With LIME we obtain explanation for a single prediction. Can we explain the whole model?

Yes! By selecting the most diverse instances



This kind of explanation is called **local** since we explain single instances (points) one by one

SP-LIME

Let $\mathscr{W}$ be an explanation matrix of size $|X| \times d'$, i.e., all instances are represented in the interpretable space

	a_1	a_2	a_3	a_4	a_5	a_6
$g(x'_1)$	$\lvert w_{11} \rvert$	$\lvert w_{12} \rvert$				
$g(x'_2)$		$\lvert w_{22} \rvert$	$\lvert w_{23} \rvert$	$w_{24}\rvert$		
$g(x'_3)$		$\lvert w_{32} \rvert$	$\lvert w_{33} \rvert$	$w_{34}\rvert$		
$g(x'_4)$					$\lvert w_{45} \rvert$	$\lvert w_{46} \rvert$

Submodular pick

Interpretable features	a_1	a_2	a_3	a_4	a_5	a_6
$g(x_1)$	$\|w_{11}\|$	$\|w_{12}\|$				
$g(x_2)$		$\|w_{22}\|$	$\|w_{23}\|$	$\|w_{24}\|$		
$g(x_3)$		$\|w_{32}\|$	$\|w_{33}\|$	$\|w_{34}\|$		
$g(x_4)$					$\|w_{45}\|$	$\|w_{46}\|$

Feature importance	I_1	I_2	I_3	I_4	I_5	I_6
$I_j = \sqrt{\sum_{i=1}^{n} \|w_{ij}\|}$	$\|w_{11}\|$	$\|w_{12}\|$ $\|w_{22}\|$ $\|w_{32}\|$	$\|w_{23}\|$ $\|w_{33}\|$	$\|w_{24}\|$ $\|w_{34}\|$	$\|w_{45}\|$	$\|w_{46}\|$

Submodular pick to get

1. Feature importance: which features are the most important for explanation

$$I_j = \sqrt{\sum_{i=1}^{n} |w_{ij}|}$$

2. Maximize the coverage for set of instances V

$$c(V, \mathcal{W}, I) = \sum_{j=1}^{d'} \mathbb{1}_{[\exists i \in V : w_{ij} > 0]} I_j$$

3. Select gradually features that maximize the coverage

$$V \leftarrow V \cup \arg\max_i i(V \cup \{i\}, \mathcal{W}, I)$$

Additional materials

Ribeiro, Marco Tulio, Sameer Singh, and Carlos Guestrin. "Why should i trust you?" Explaining the predictions of any classifier." *Proceedings of the 22nd ACM SIGKDD international conference on knowledge discovery and data mining*. 2016

Sebastian Gruber, Christoph Molnar, “LIME and sampling”, Limitations of Interpretable Machine Learning Methods, student seminar

Christoph Molnar Interpretable, “Local Surrogate (LIME)”, Machine Learning, A Guide for Making Black Box Models Explainable,

EXAMPLES (from the LIME package):

- Tabular data
- Texts (2-class and multiclass)
- Images
- Submodular pick

Part 2. SHAP

LIME. Quick recap

$$\xi(x) = \arg\min_{g \in G} \underbrace{\mathcal{L}(f, \underbrace{\boxed{g}}_{\text{linear model}}, \underbrace{\boxed{\pi_x}}_{\text{kernal}})}_{\text{weighted MSE errors}} + \underbrace{\boxed{\Omega(g)}}_{\text{penalty term}}$$

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

$$\pi_x(z) = \exp\left(\frac{-D(x,z)^2}{\sigma^2}\right)$$

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

$x = \boldsymbol{h}_x(x')$ converts a binary vector x' of interpretable inputs into the original input space

In LIME ϕ_i are chosen heuristically. Can we do better?

Yes, using Shapley values with nice theoretical properties.

Additive feature attribution model

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

- **feature attribution**: the quantity of interest of the model for each feature
- **additive**: summing the interest of single features results in the actual interest of the model

PROPERTIES:

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

Missingness A feature $x_i' = 0$ has not attributed impact, i.e., $x_i' = 0 \Longrightarrow \phi_i = 0$

Consistency Let $f_x(z') = f(h_x(z'))$ and $z' \setminus i$ denote setting $z_i' = 0$. For any two models f and f', if

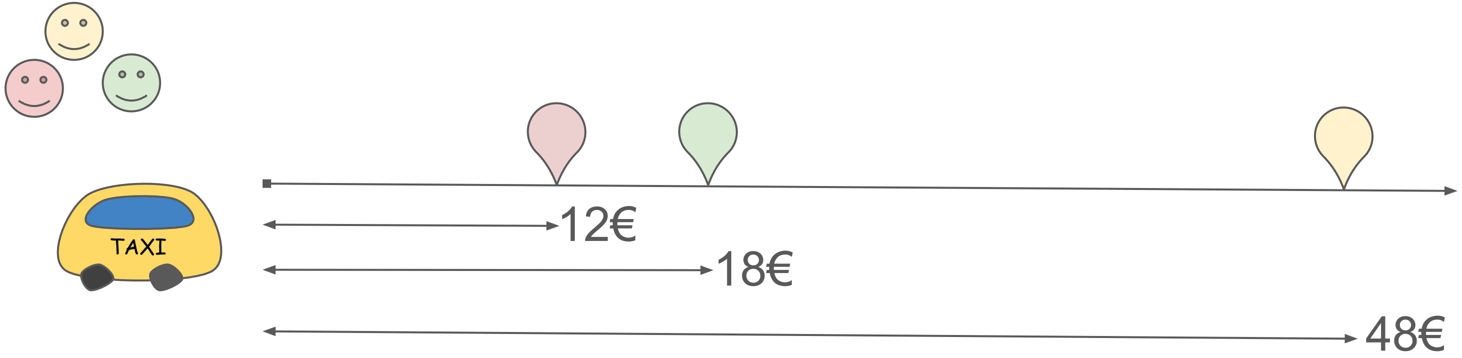
$f_x'(z') - f_x'(z' \setminus i) \geq f_x(z') - f_x(z' \setminus i)$ for all inputs $z_i' \in \{0,1\}^M$ then $\phi_i(f', x) \geq \phi_i(f, x)$.

Coalition game. Example

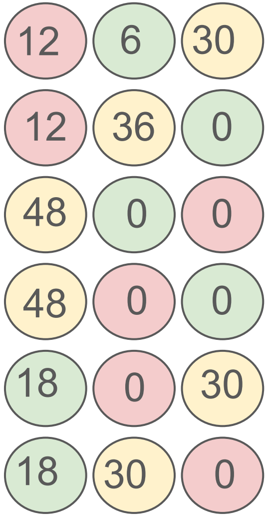
Three players take a taxi

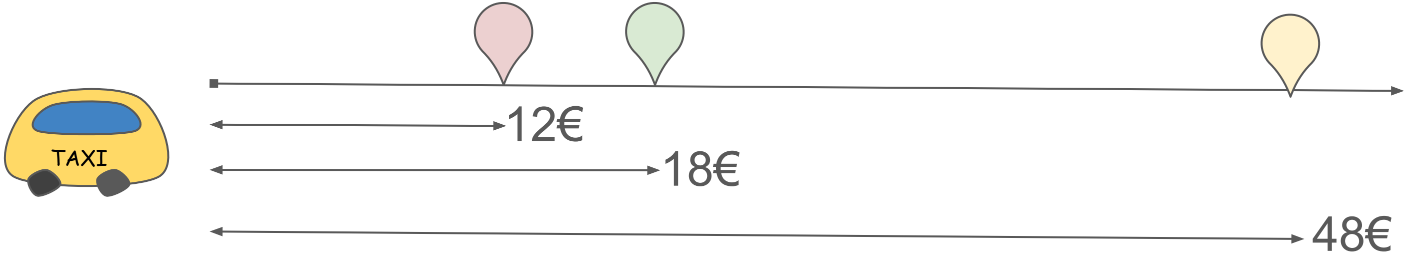
The value function v is the taxi driver's income. The players can make coalition to save some money

What is the **fair** price that each should pay if they take the taxi together?



Payoffs in the coalition



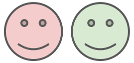


What is a fair contribution for each player?

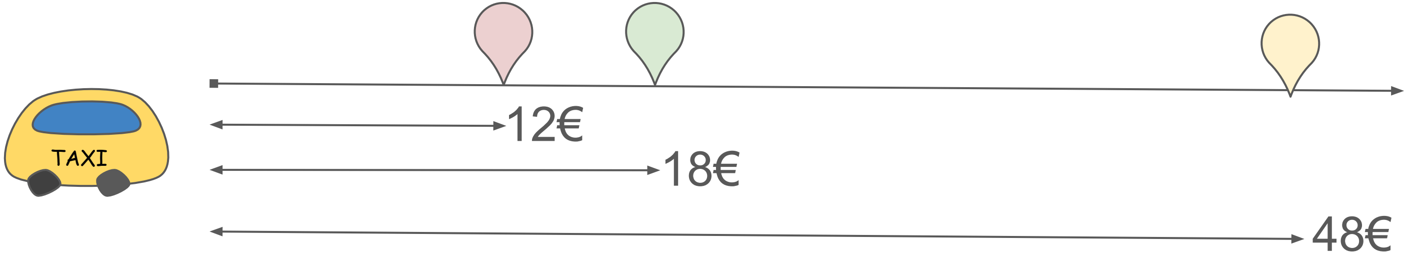
average values over the permutations

ϕ $\boxed{4} + \boxed{7} + \boxed{37} = 48$

Value function

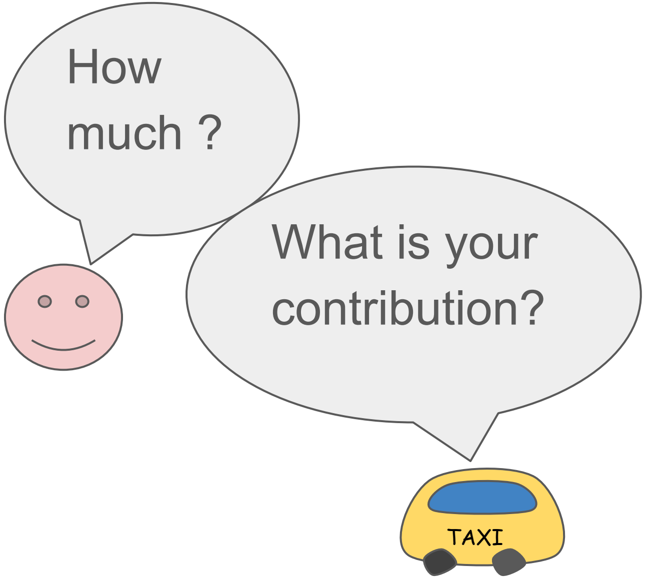
coalition*	v
	0
	12€
	18€
	48€
	18€
	48€
	48€
	48€

* these are the sets, there is not order between the instances



How the players may pay for the ride?

Individual contribution (alternative computing)

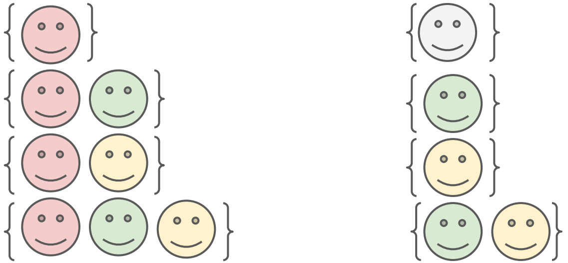


Coalitions with r: $S \cup \{r\}$

Coalitions without r: S

Difference in value functions

$v(S \cup \{r\}) - v(S)$

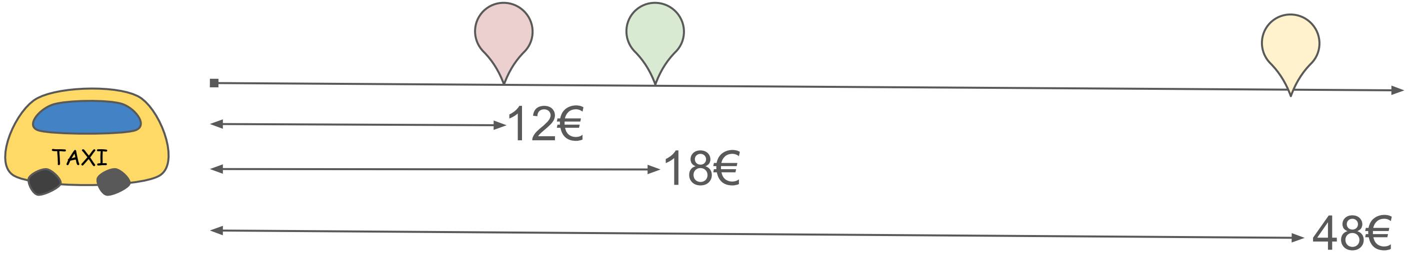


12€ - 0 = 12€

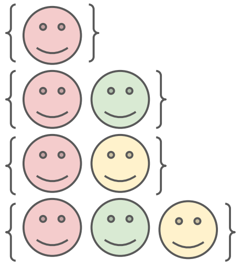
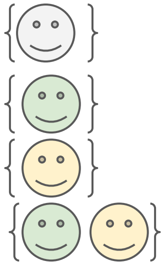
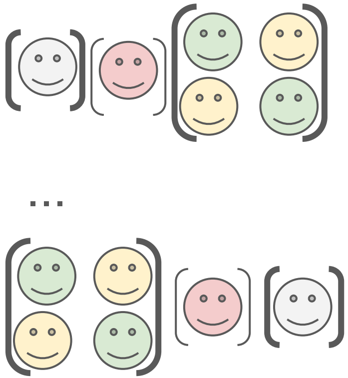
18€ - 18€ = 0

48€ - 48€ = 0

48€ - 48€ = 0



Individual contribution (alternative computing)

Coalitions with r: $S \cup \{r\}$	Coalitions without r: S	Difference in value functions $v(S \cup \{r\}) - v(S)$	How many permutation? $\lvert S\rvert!(\lvert F\rvert-\lvert S\rvert-1)!$	Weights $\frac{\lvert S\rvert!(\lvert F\rvert-\lvert S\rvert-1)!}{\lvert F\rvert!}$
		12€ - 0 = 12€ 18€ - 18€ = 0 48€ - 48€ = 0 48€ - 48€ = 0		2 / 3! = 1/3

The number of permutation for a coalition $S \cup \{r\}$: $\lvert S\rvert!(\lvert F\rvert - \lvert S\rvert-1)!$, where F is the set of the players, the total number of permutations is $\lvert F\rvert!$

More on permutations

Suppose we have 5 elements, i.e., F = {1, 2, 3, 4, 5}. We study a variable **1.** Let's find a number of permutations for the coalition **S = {2, 3}.** The rest is {4,5}

Thus, we search the permutation of the following form (2,3) (1) (4,5). It's obvious, that we have only 4 such kind of permutations, namely,

2, 3, 1, 4, 5
2, 3, 1, 5, 4
3, 2, 1, 4, 5
3, 2, 1, 5, 4

|S| = 2, |F| = 5, |F|-|S|-1 = 2 for $\frac{|S|!(|F|-|S|-1)!}{|F|!}$

Shapley regression values

Let F be a set of features, f_S is a linear model trained on a feature set S, and x_S represents if the input where the feature values from S are retained

Then Shapley regression values are given as follows:

$$\phi_i = \sum_{S \subseteq F \setminus \{i\}} \frac{|S|!(|F|-|S|-1)!}{|F|!} [f_{S \cup \{i\}}(x_{S \cup \{i\}}) - f_S(x_S)]$$

Example of the interpretable space

$f(x_1, x_2, x_3, x_4, x_5)$ is a function obtained by a black box model

Let $S = \{x_2, x_3\}$, then $z' = \{0, 1, 1, 0, 0\}$.

The input of the function f, i.e., $z_S = h_x(z')$ is $(\cdot, x_2, x_3, \cdot, \cdot)$

Simplified computing of Shapley values

Let S be a set of non-zero indices of z', i.e., $h_x(z') = z_S$, where z_S has missing values for features not in S, and

In SHAP as $f(z_S) = f(h_x(z'))$ one uses the conditional expectation, i.e.,

$$f(h_x(z')) = \underbrace{E[f(z)|z_S]}_{\text{expectation}} = E_{z_{\overline{S}}|z_S}[f(z)] \approx \underbrace{E_{z_{\overline{S}}}[f(z)]}_{\text{assuming feature independence*}} \approx \underbrace{f([z_S, E[z_{\overline{S}}]])}_{\text{assuming model linearity}}$$

expectation

assuming **feature independence***

assuming **model linearity**

*Instead of considering the conditional distribution and making the assumption on independence we may consider the interventional distribution $E[f(z)|do(Z_S=z_S)]$ and obtain the same results, see for details Janzing, D., Minorics, L., & Blöbaum, Feature relevance quantification in explainable AI: A causal problem. In *International Conference on Artificial Intelligence and Statistics* (pp. 2907-2916). PMLR.

Additive feature attribution model

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

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Additive feature attribution method

Additive feature attribution (AFA) methods have an explanation model that is a linear function of binary variables:

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

Theorem. Only one possible AFA explanation model g that satisfies properties of local accuracy, missingness, and consistency:

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

where $|z'|$ is the number of non-zeros entries in z', and $z' \subseteq x'$ represents all z' vectors where the non-zeros entries are a subset of the non-zeros entries in x'

Kernel SHAP (LIME + Shapley values)

$$\xi(x) = \arg\min_{g \in G} \mathcal{L}(f, g, \pi_x) + \cancel{\Omega(g)}$$

0

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

$$\mathcal{L}(f, g, \pi_x) = \sum_{z' \in Z} \pi_x(z')[f(h_x^{-1}(z')) - g(z')]^2$$

$$\pi_x(z) = \exp\left(\frac{-D(x,z)^2}{\sigma^2}\right)$$

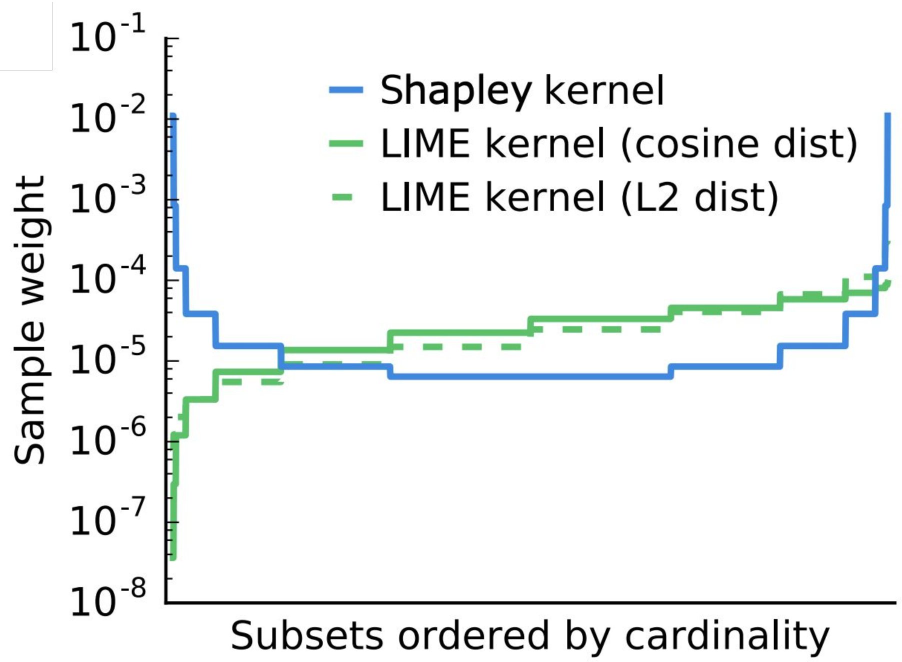
$$\boxed{\pi_x(z') = \frac{(M-1)}{(M\ choose\ |z'|)|z'|(M-|z'|)}}$$

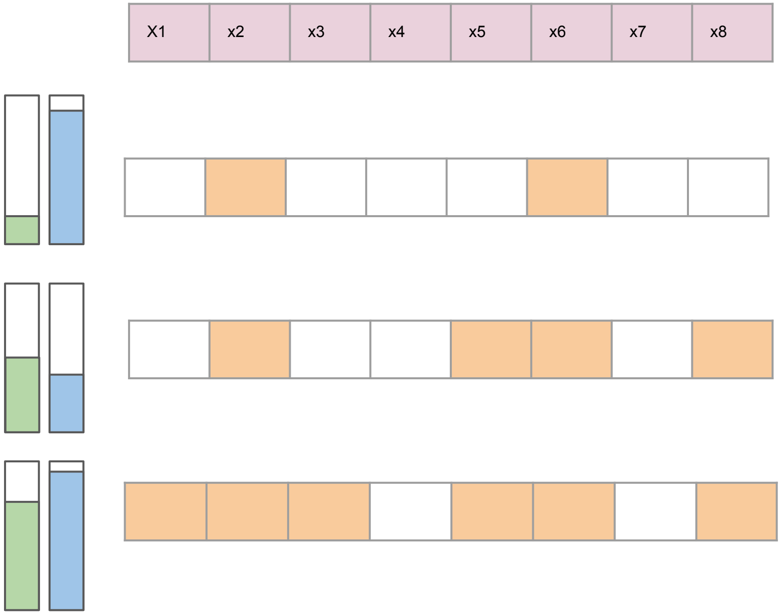
Proof for the kernel

Remark: $\pi_x(z') = \infty$ when $|z'| \in \{0,M\}$, which enforces $\phi_0 = f_x(\varnothing)$ and $f(x) = \sum_{0,\dots,M} \phi_i$, but they are eliminated in practice

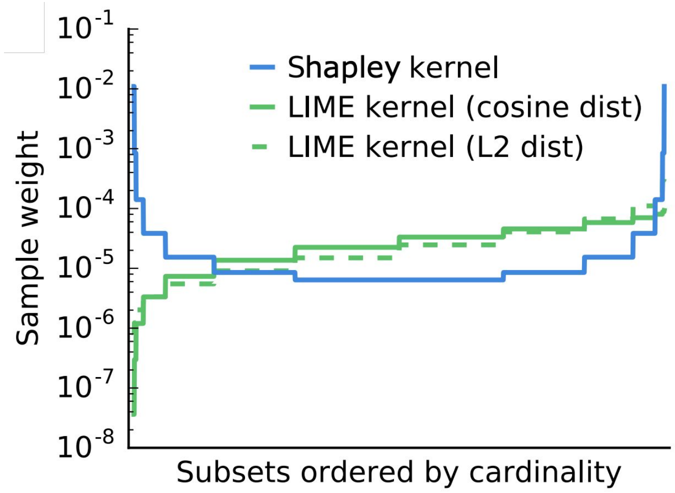
Kernels

SHAP values to measure feature importance





Kernel. The intuition behind



Let x = {3,4,2,4,5,3}. We need to compute explain the response of the model by SHAP and LIME. for Consider

For LIME z' = {0,0,0,1,1,0} in means that we introduce perturbation in 4 features, thus a new instance z will not be very similar to the original one

For SHAP it means that, we fix only x_4 and x_5 and averaged over other variables, thus me learn about the features' isolated main effect on the prediction. If on the opposite, z' = {1,1,1,0,0,1} learn about this features' total effect (main effect plus feature interactions).

If a coalition consists of half the features, we learn little about an individual features contribution

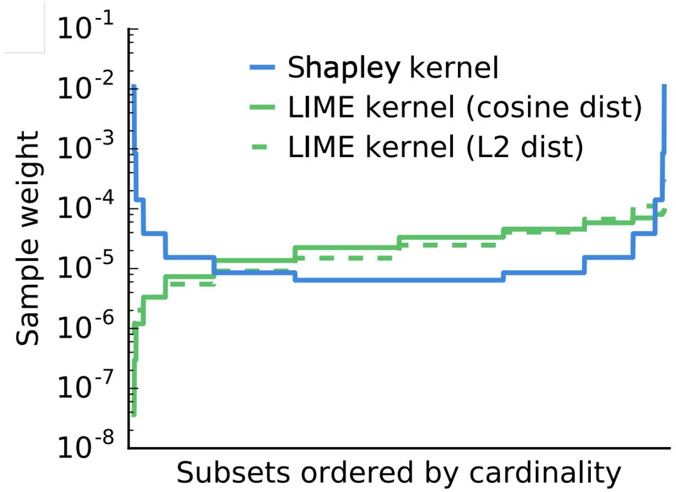
Complexity of the sampling

For an instance given in an M-dimensional space, the importance of the i-th feature is given by

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

Thus, we need to generate $O(2^{|M|})$ perturbation.

However, we may use a fixed number of perturbations which are simpled w.r.t. the kernel weight



SHapley Additive exPlanation Values. Summary

- additive
- good properties
- show how f relies on features
- Kernel SHAP model agnostic, potentially of high complexity

Model specific algorithms:

- TreeSHAP
- LinearSHAP
- GradientSHAP
- DeepSHAP