

Explainability of Neural Networks (XAI)

CPSC680: Trustworthy Deep Learning

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Readings

- Readings are updated on the website (syllabus page)
- **Lecture 5 readings:**
 - [LIME](#) (local interpretation)
 - [SHAP](#) (attribution)

Content

- Methods using Surrogate Models
- Counterfactual Explanations

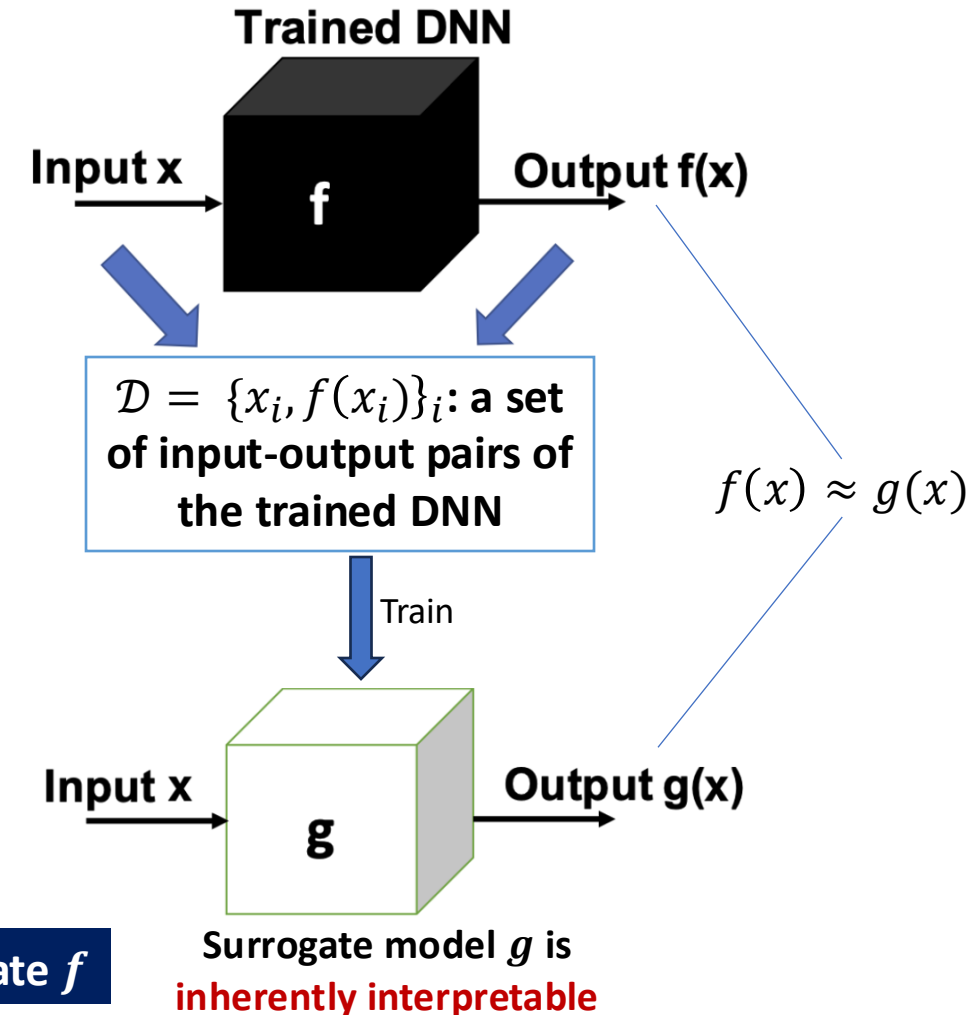
Content

- Methods using Surrogate Models
- Counterfactual Explanations

Local Explanations with Surrogate Models

- **Explanation with Surrogate Model**

- **Post-hoc, model-agnostic** explanation
- Learn **an inherently interpretable model** (e.g. decision trees, linear models) that **(locally) approximates** the behaviors of the original model.
- We can analyze the **local** behaviors of f around x_0 using g .



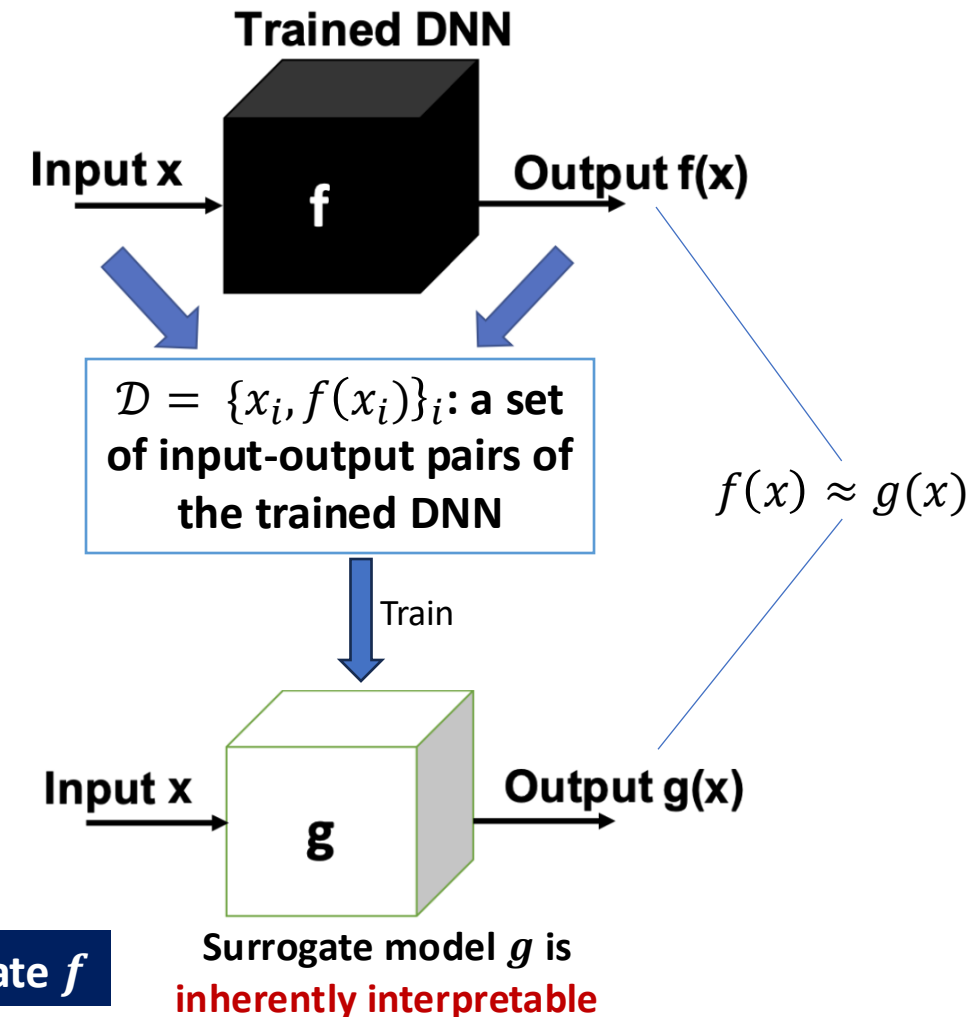
Use $\mathcal{D} = \{x_i, f(x_i)\}_i$ as traing data for g to approximate f

Local Explanations with Surrogate Models

- **Explanation with Surrogate Model**

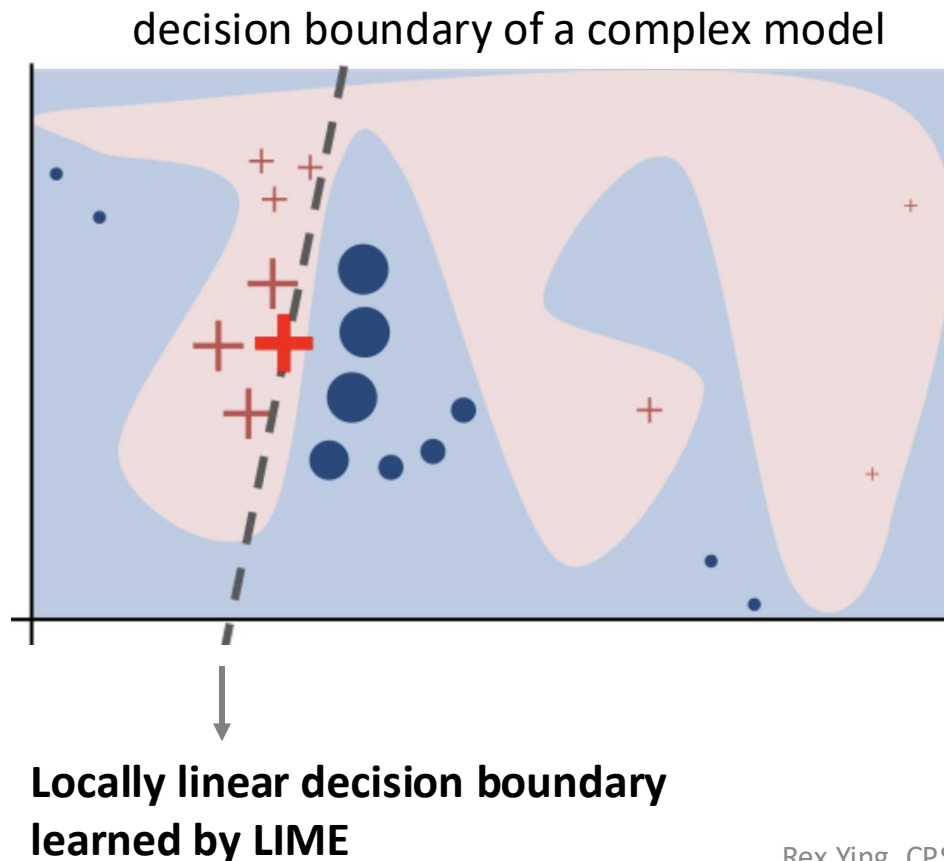
- Given input instance x_0 and model f .
- Steps:
 1. Sample points around x_0
 2. Use model to predict labels for each example $(x_i, f(x_i))$
 3. Weight examples according to the distance to the input instance x_0
 4. Learn a linear model on weighted samples
 5. Use simple linear model to explain

Use $\mathcal{D} = \{x_i, f(x_i)\}_i$ as training data for g to approximate f



Intuition of LIME

- **Local Interpretable Model-Agnostic Explanations (LIME)**



- the **pink** and **blue** background: complex decision function f of the black-box model
- **+** : instance to be explained
- **•** **+** : instances with different predicted labels by f
- **Size of •** **+** : the **proximity** to the instance to be explained
(larger size \Leftrightarrow closer to the explained instance)

LIME samples instances around the given instance **+**, and weighs them by the **proximity** to the instance **+**.

Goal of LIME: learn a local surrogate model around the given instance **+**

LIME for Tabular Data

- **LIME**

- Given input instance x_0 and model f .

- Steps:

- ➔ 1. **Sample points around x_0**
 2. Use model to predict labels for each example $(x_i, f(x_i))$
 3. Weight examples according to the distance to the input instance x_0
 4. Learn a linear model on weighted samples
 5. Use simple linear model to explain

Sampling Mechanism

- **For continuous features:** Adding a Gaussian noise $x_i \sim \mathcal{N}(x_0, \sigma I)$
- **For categorical features:** perturb by sampling according to the training distribution

LIME for Tabular Data

- **LIME**

- Given input instance x_0 and model f .

- Steps:

1. Sample points around x_0
2. Use model to predict labels for each example $(x_i, f(x_i))$

➡ **3. Weight examples according to the distance to the input instance x_0**

4. Learn a linear model on weighted samples
5. Use simple linear model to explain

Weighting Function

$\pi_{x_0}(z)$: **similarity kernel** for the recovered representation z around the original input x_0

$$\pi_{x_0}(x_i) = e^{-\frac{D(x_0, x_i)^2}{\sigma^2}}$$

- **D is the distance function** (e.g., L_2 distance)
- σ is a hyper-parameter for the kernel

LIME targets at **local approximation** \Rightarrow samples z with relatively **larger $\pi_{x_0}(z)$** (i.e., smaller distance **$D(x_0, x_i)$**) should have larger weights during the training of the surrogate model

LIME for Tabular Data

- **LIME**

- Given input instance x_0 and model f .

- Steps:

1. Sample points around x_0
2. Use model to predict labels for each example $(x_i, f(x_i))$
3. Weight examples according to the distance to the input instance x_0
- ➡ **4. Learn a linear model g on weighted samples**
5. Use simple linear model to explain

Training Objective

The training objective of LIME to search a surrogate model around input x :

$$g^* = \operatorname{argmin}_{g \in \mathcal{G}} \mathcal{L}(f, g, \pi_{x_0}) + \Omega(g)$$

- \mathcal{G} is the class of interpretable models (linear model or decision tree)
- $\mathcal{L}(f, g, \pi_{x_0})$ is the loss function that penalizes the differences between f and g
- $\Omega(g)$ controls the complexity of the model g

LIME for Tabular Data: Objective and Loss

Training objective of LIME to search a surrogate model around input x_0 :

$$g^* = \operatorname{argmin}_g \mathcal{L}(f, g, \pi_{x_0}) + \boxed{\Omega(g)} \rightarrow \text{Control complexity of the interpretable model}$$

where

$$\mathcal{L}(f, g, \pi_{x_0}) = \sum_{x_i \in \mathcal{D}} \boxed{\pi_{x_0}(x_i)} \boxed{(f(x_i) - g(x_i))^2}$$

$$\pi_{x_0}(x_i) = e^{-\frac{D(x_0, x_i)^2}{\sigma^2}}$$

Sample x_i closer to x_0 contributes more to the loss

optimize g to locally approximate the behavior of f

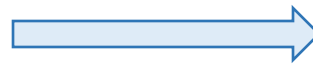
- $\Omega(g)$: a measure of **complexity** of the surrogate model g
 - $\Omega(g)$: the depth of tree for a decision tree; the number of weights for a linear model
 - A simple local surrogate is preferred! (Occam's Razor)
 - Lasso is a possible choice

LIME for Images: Data Representation (1)

- Given an original input $x \in \mathbb{R}^d$, let $x' \in \{0, 1\}^M$ denote a binary vector as its **interpretable representation**
 - M is the number of features in the interpretable representation
 - For **images**, x' can be a binary vector indicating the “presence” or “absence” of a **patch of similar pixels**
 - For **text**, x' can be a binary vector indicating the “presence” or “absence” of a **word**
 - Example:**



1 denotes “presence” of the pixel
0 denotes “absence” of the pixel



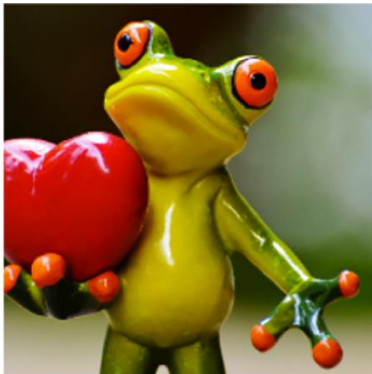
0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0
0	0	0	1	1	1	0	0	0
0	0	1	1	1	1	0	0	0
0	0	1	1	1	1	0	0	0
0	0	1	1	1	1	0	0	0
0	0	1	1	1	0	0	0	0
0	0	0	0	0	0	0	0	0

x : Original image

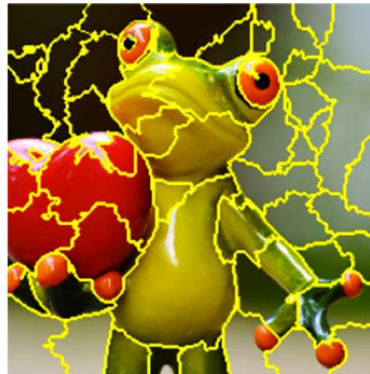
x' : Interpretable representation

Choice of Interpretable Representation

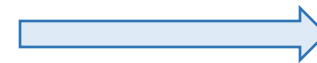
- Given an original input $x \in \mathbb{R}^d$, let $x' \in \{0, 1\}^M$ denote a binary vector as its **interpretable representation**
 - In the context of images, a segmentation method can be used to decompose the image into interpretable components (see `skimage.segmentation`)



Original Image



Interpretable
Components

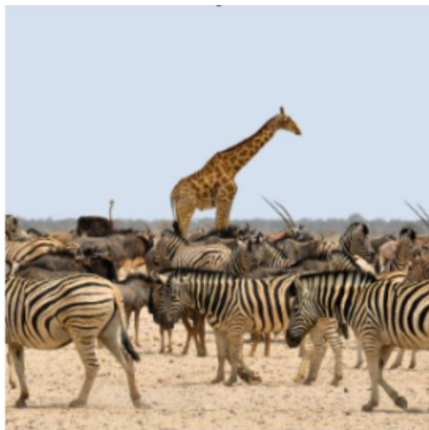


0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0
0	0	0	1	1	1	0	0	0
0	0	1	1	1	1	0	0	0
0	0	1	1	1	1	0	0	0
0	0	1	1	1	1	0	0	0
0	0	1	1	1	0	0	0	0
0	0	0	0	0	0	0	0	0

Mask corresponding to a
super-pixel (segment)

Details of LIME: Data Representation (2)

- Based on an **interpretable representation** $x' \in \{0, 1\}^M$, a **perturbed sample** $z' \in \{0, 1\}^M$ contains a **fraction of the nonzero elements of x'**
- $z \in \mathbb{R}^d$: **recovered explanation** in the original domain
- Example:

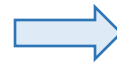


$x \in \mathbb{R}^d$
Original image



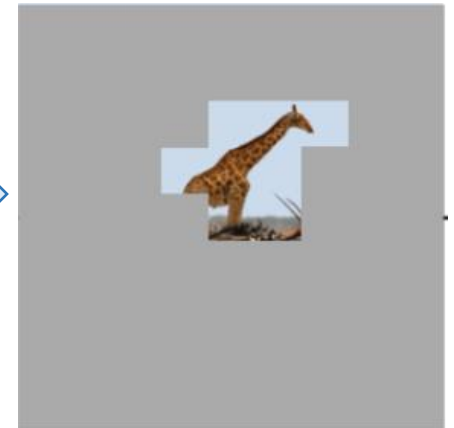
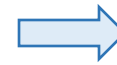
0	0	0	0	0	0	0	0	0	0
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0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0

$x' \in \{0, 1\}^M$
Interpretable representation



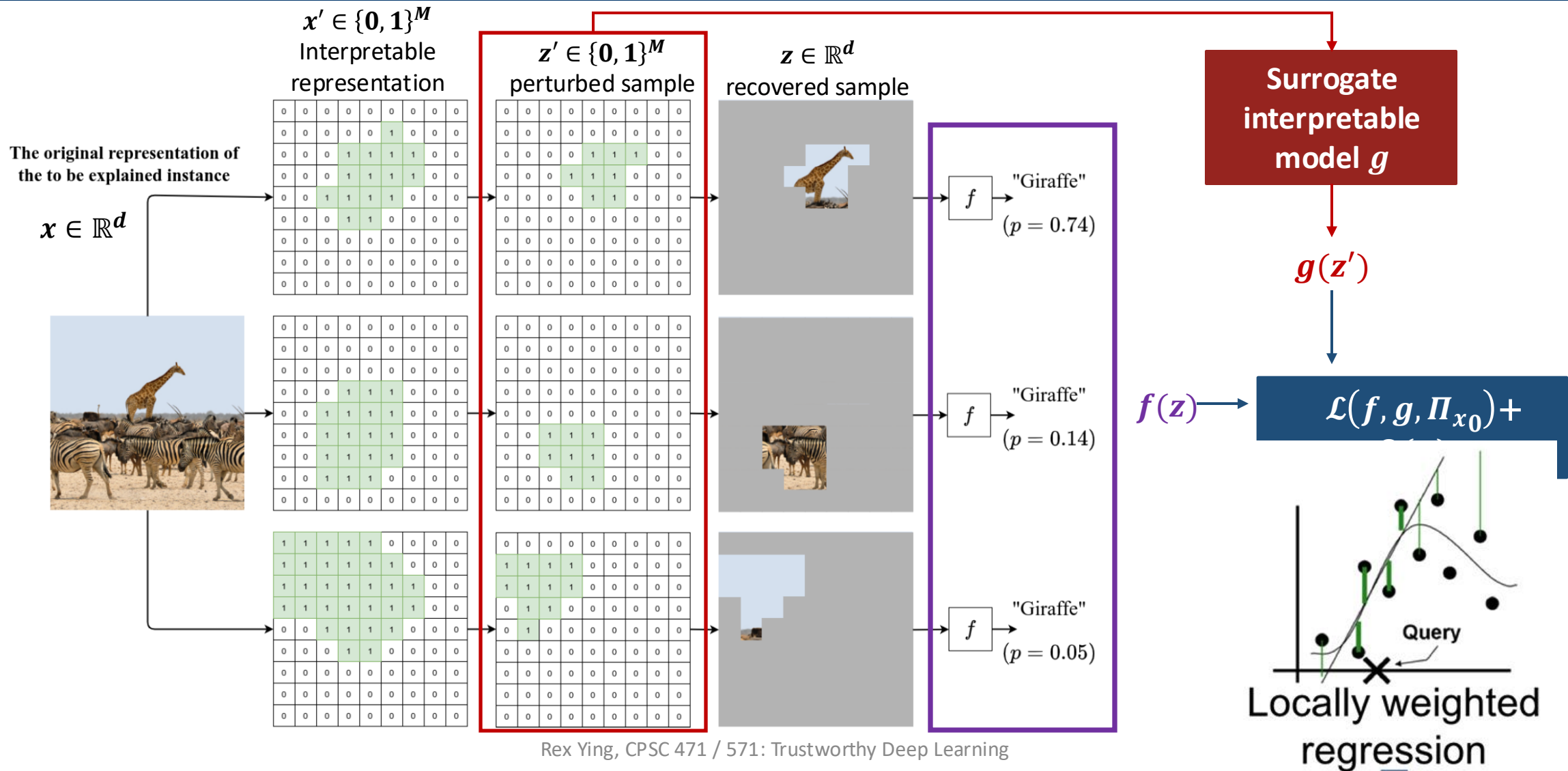
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0	0	0	0	0	0	0	0	0	0
0	0	0	0	1	1	1	0	0	0
0	0	0	1	1	1	0	0	0	0
0	0	0	0	1	1	0	0	0	0
0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0

$z' \in \{0, 1\}^M$
perturbed sample



$z \in \mathbb{R}^d$
explanation

LIME for Images - Architecture



Evaluation: Important Feature Selection (1)

- **Dataset:** sentiment analysis datasets (BOOKs and DVDs)[1]
- **Features: bag of words (BOW)**

		she	loves	pizza	is	delicious	a	good	person	people	are	the	best	BOW: number of times each word occurs in a sentence
Input sentence	She loves pizza, pizza is delicious	1	1	2	1	1	0	0	0	0	0	0	0	

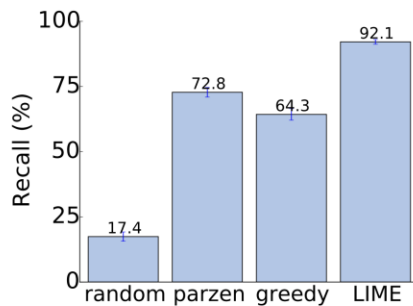
- Measure **faithfulness of explanations** for classifiers that are intrinsically interpretable
 - Train a **sparse logistic regression** or **decision tree** to select 10 most important features as the ground truth
- Generate explanations for each prediction in the test set and compute **the fraction of truly important features** recovered by the explanations

Evaluation: Important Feature Selection (2)

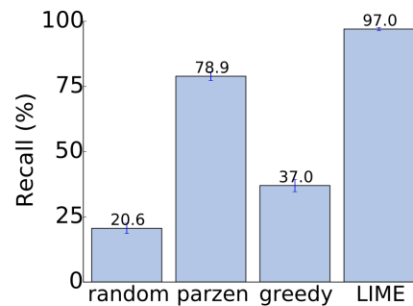
- **Baselines:**

- **Random:** randomly pick 10 features
- **Parzen:** pick 10 features with the highest absolute gradients
- **Greedy:** greedily remove 10 features that contribute the most to the predicted class and take these 10 features as an explanation

- **Recall:** $\frac{TP}{TP+FN}$ (true positive rate; TP: True Positive, FN: False Negative)

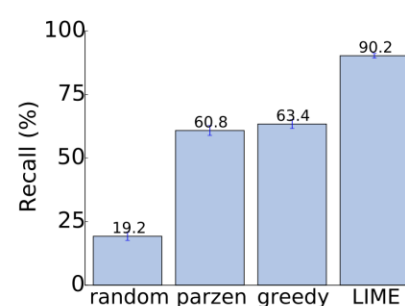


(a) Sparse LR

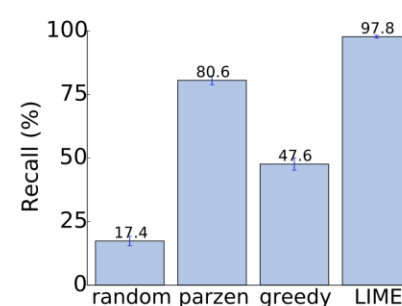


(b) Decision Tree

BOOKs dataset



(a) Sparse LR



(b) Decision Tree

DVDs dataset

LIME provides faithful explanations with > 90% recall for both logistic regression and decision trees!

Shapley Additive Explanation

- **SHAP**: a **local additive feature attribution** methods based on **Shapley values** for each input feature
- Given a black-box model f and an input $x \in \mathbb{R}^d$ to be explained
 - $z \in \{0,1\}^M$: interpretable representation of x recall the representation used in LIME
 - $h_x: \{0,1\}^M \rightarrow \mathbb{R}^d$ recovering function that maps to original domain \mathbb{R}^d

- **Surrogate model:**

$$g(z) = \overset{\text{null output}}{\boxed{\phi_0}} + \sum_{i=1}^M \overset{\text{Shapley value of the } i\text{-th feature}}{\boxed{\phi_i}} z_i$$

- $z_i \in \{0,1\}$: the i -th element of z_i , indicating the **presence/absence of the i -th feature**
- $g(z)$ locally approximates $f(x)$ when $x = h_x(z)$

map to the original domain

Shapley Values in Cooperative Game Theory

- The concept of Shapley values is originally from **cooperative game theory**
- **Cooperative games** model scenarios where agents can benefit by cooperating together and a binding agreement.
 - Probably not the part of game theory you've heard of

Cooperative game

- Players can benefit by cooperating
- Binding agreements are possible
- Answer the question: **How to divide the surplus when joining the grand coalition?**

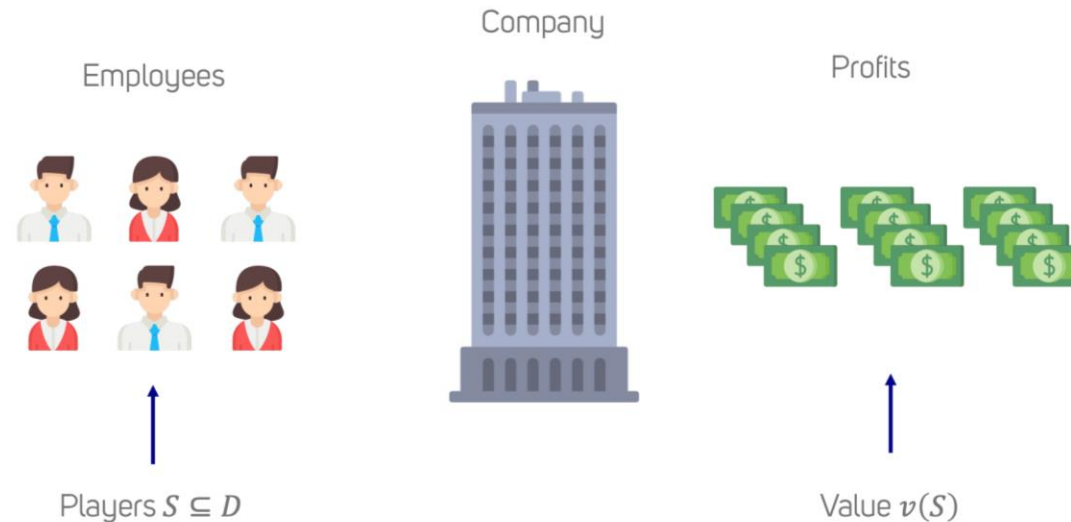
Non-cooperative game

- Players are independent
- No cooperation, focus on individual actions
- Answer the question: **What is the “good” strategy for each player to maximize their *individual* return?**

Nash equilibrium, zero-sum game

Shapley Values in Cooperative Game Theory

- **Example of a cooperative game:**



- **Question:** How to measure each player's contribution? How to divide a surplus (profit) to shareholders so that everyone is satisfied?
- **Lloyd Shapley's idea:** members should receive payments **proportional to their average marginal contributions \Rightarrow Shapley Values**

Shapley Values in Cooperative Game Theory

- Consider the following example where there are three players and got 19\$
- The marginal contribution of player A

- to coalition $S = \emptyset$ is $7 - 0 = 7\$$ $/ (3 * 1)$
- to coalition $S = \{B\}$ is $7 - 4 = 3\$$ $/ (3 * 2)$
- to coalition $S = \{C\}$ is $15 - 6 = 9\$$ $/ (3 * 2)$
- to coalition $S = \{B, C\}$ is $19 - 9 = 10\$$ $/ (3 * 1)$

- The player A should get

$$\frac{1}{3} \left(\frac{1}{\binom{2}{0}} 7 + \frac{1}{\binom{2}{1}} 3 + \frac{1}{\binom{2}{1}} 9 + \frac{1}{\binom{2}{2}} 10 \right) = 7.667$$

Marginal contribution

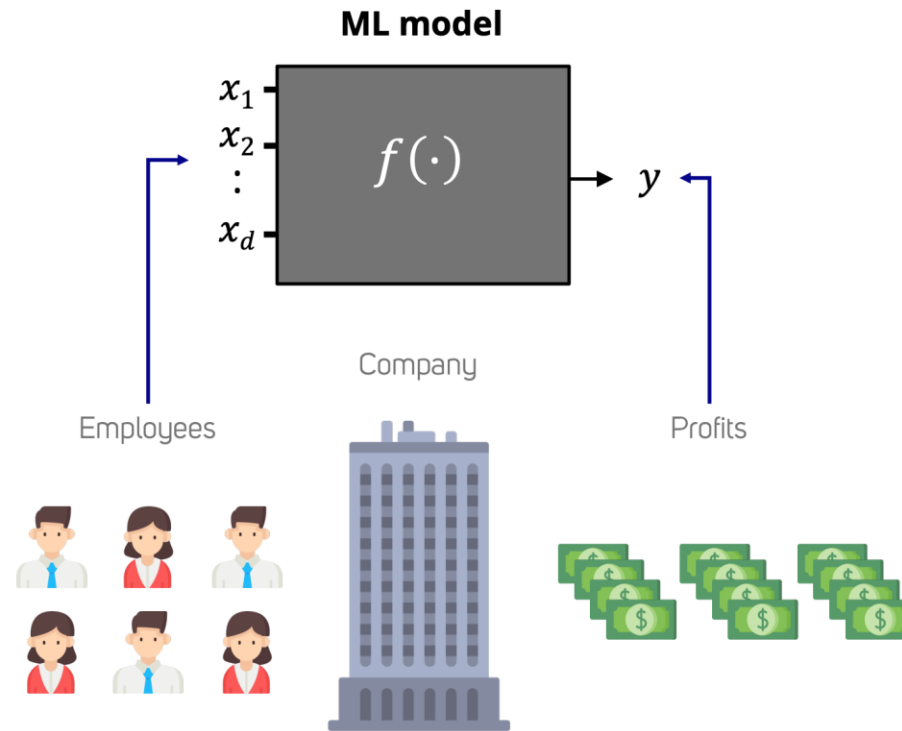
Every coalition with the same size is equally likely to appear

All sizes are equally likely to appear.



Shapley Values in Cooperative Game Theory

- In context of a deep learning system:



features \Leftrightarrow players prediction \Leftrightarrow profit

Calculating Shapley Values

- f : black-box model; $x \in \mathbb{R}^d$: input to be explained; \mathbf{h}_x : reverse map to \mathbb{R}^d
- **Shapley value** for the i -th input feature:

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

Setting $z'_i = 0$ (removing the i -th feature)

All possible binary representations of subset features of x , $|Z| = 2^M$

Very small $|z'|$ (close to 0) or very large $|z'|$ (close to M) result in larger weights. Why?

- $z' \subseteq x'$ represents all z' vectors where the non-zero entries are a **subset** of the non-zero entries in x'
- $|z'|$: the number of non-zero entries in z'
- M : number of features in the **interpretable representation**

Example of SHAP

Example: calculating the **Shapley value of feature 4**:

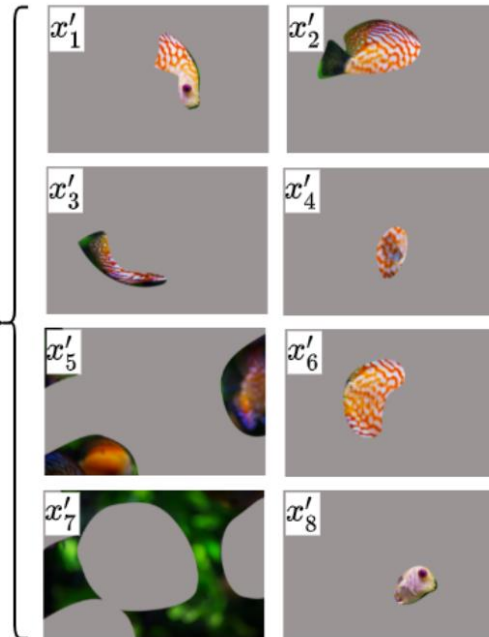
x'	x_1	x_2	x_3	x_4
$z' \subseteq x'$	x_1	x_2	x_3	x_4
$z' \setminus 4$	x_1	x_2	x_3	x_4



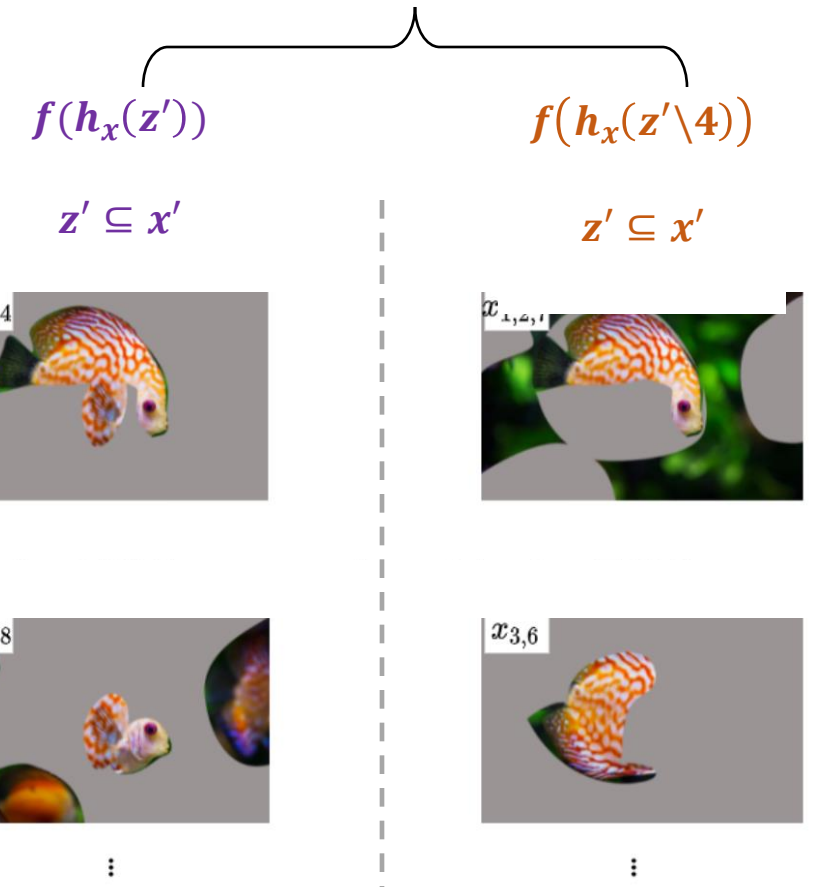
"Discus Fish"

Feature
extractor

x' : interpretable representation
(8 features in total)



Compute $f(h_x(z')) - f(h_x(z' \setminus 4))$, and
weighted average over all possible subset z'



Properties of SHAP (1)

- **Linearity:** The importance score of a linear combination of two models is a linear combination of the importance score

$$\phi_i(f_1 + \alpha f_2) = \phi_i(f_1) + \alpha \phi_i(f_2)$$

- **Dummy:** If the model is not sensitive to a feature, its importance score should be zero

$$\forall z \quad \delta_i(z) := f(h_x(z)|z_i = 1) - f(h_x(z)|z_i = 0) = 0 \Rightarrow \phi_i = 0$$

- **Symmetry:** Symmetric features get similar importance scores

$$\forall z \quad \delta_i(z) = \delta_j(z) \Rightarrow \phi_i = \phi_j$$

- **Efficiency:** The sum of importance scores of all features recovers the prediction

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

The model output is fully distributed to all input features.

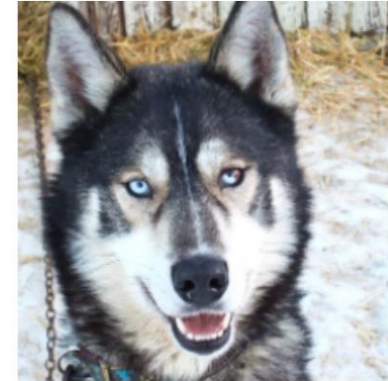
Properties of SHAP (2)

- **Theorem:** Shapley value is a *unique* solution concept that satisfies four axioms: *linearity*, *dummy*, *symmetry*, and *efficiency*.
- **Pros:** *This uniqueness* implies that the Shapley values is the “best” (only one) method to allocate importance scores to input features if we accept four properties (axioms)
- **Cons:** **Computationally expensive.**
 - E.g., to compute exactly the Shapley value with 50 features, we need to compute the summation over $2^{50} > 10^{15}$ perturbation $z' \in Z$.
 - We need to do Monte-Carlo sampling to approximate the Shapley values. In practice, 1000 – 10000 perturbations are sufficient.

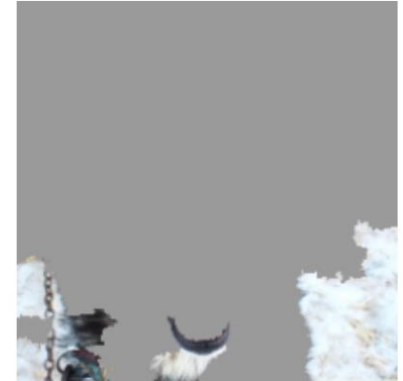
What are Pros and Cons of SHAP?

Questions!

- **Efficiency**
- **Stability**
- Modeling **Correlation**
- **Robustness**
 - How likely will the identified explanations tend to be adversarial examples
- **Granularity**
 - Can the method find fine-grained explanations for any instance



(a) Husky classified as wolf



(b) Explanation

The equivalence between LIME and SHAP

- **Theorem:** The Shapley values is a **special case** of the LIME framework

LIME	SHAP
<ul style="list-style-type: none"> • LIME solves the following optimization problem $w^* = \operatorname{argmin}_w \sum_{x \in \mathcal{D}} \pi_x(z) [f(x) - (w^\top x + b)]^2 + \Omega(w)$ <p>where \mathcal{D} is the set of perturbations around x_0</p>	<ul style="list-style-type: none"> • Importance score using Shapley value $\phi_i = \sum_{z' \subseteq x'} \frac{ z' ! (M - z' - 1)!}{M!} [f(\mathbf{h}_x(z')) - f(\mathbf{h}_x(z' \setminus i))]$ <p>x' is the interpretable representation of x</p>

If

- $\Omega(w) = 0$
- $\pi_x(z) = \frac{(M-1)}{\binom{M}{|z|} |z| (M-|z|)}$
- $\mathcal{D} = \{h_{x_0}(z') \mid z' \subseteq x'\}$

Then $w^* = \phi_i$

No control over the complexity of g

Weighting function: Small $|z'|$ (few 1's in z')
and large $|z'|$ (i.e. many 1's in z') get the largest weights

The perturbation set is the set of all possible
binary combinations of features in x , $|\mathcal{D}| = 2^M$

Rex Ying, CPSC 471 / 571: Trustworthy Deep Learning

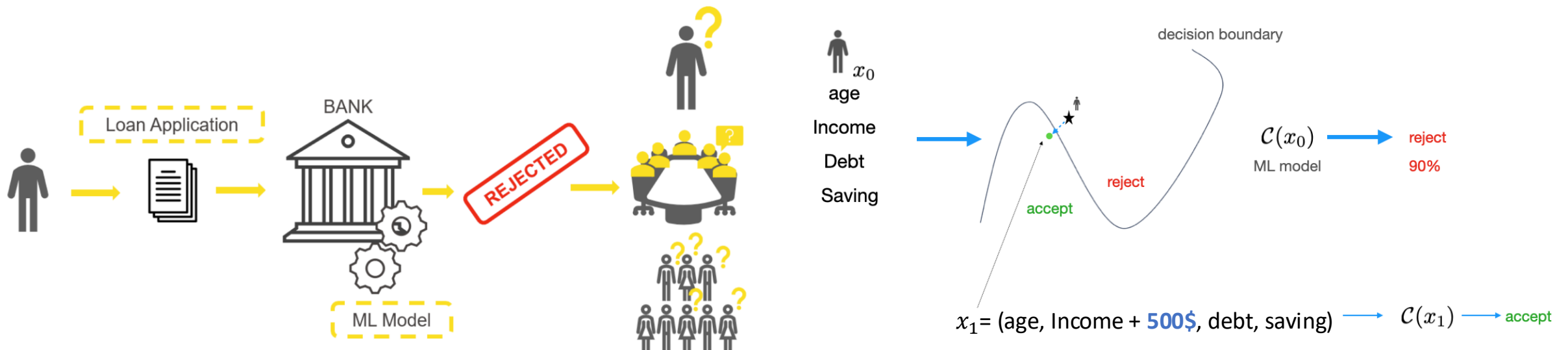
See proof in the [original paper](#)

Content

- Methods using Surrogate Models
- Counterfactual Explanation

Counterfactual Explanations

- Counterfactual explanation considers **"what-if" scenarios** of model predictions, addressing the question of **how slight adjustments** in the input can lead to different model predictions.
 - useful in consequential applications such as loan approvals, university admission, etc.



**You should increase your income by 500\$
in order to be accepted**

Counterfactual Explanations

- **Goal:** Find a counterfactual example
 - can change the model prediction to a desired outcome
 - a change in the input instance should be minimal in order to reduce the implementation cost for users (loan applicants, students, etc)

- **Formulation:**

The diagram illustrates the mathematical formulation of counterfactual explanations. It features the equation $x_{CF} = \operatorname{argmin}_{x' \in \mathcal{X}} d(x_0, x')$ with a constraint $s.t. f(x') = y^{\text{target}}$. Annotations include: a green arrow pointing from x_{CF} to the text 'Counterfactual Explanation'; a blue arrow pointing from $d(x_0, x')$ to the text 'distance function (implementation cost)'; an orange arrow pointing from $x' \in \mathcal{X}$ to the text 'Feasible action space'; and a red arrow pointing from the constraint equation to the text 'Constraint to get desired outcome'.

$$x_{CF} = \operatorname{argmin}_{x' \in \mathcal{X}} d(x_0, x')$$

Counterfactual Explanation

distance function (implementation cost)

Feasible action space

$s.t. f(x') = y^{\text{target}}$

Constraint to get desired outcome

Counterfactual Explanations

- **Formulation:**

$$x_{CF} = \underset{x' \in \mathcal{X}}{\operatorname{argmin}} d(x_0, x') \\ \text{s.t. } f(x') = y^{\text{target}}$$

The above problem has a non-linear constraint, which is difficult to solve

- **Reformulation:** Using Lagrange multipliers to convert to unconstrained optimization problem:

$$x_{CF} = \underset{x' \in \mathcal{X}}{\operatorname{argmin}} d(x_0, x') + \lambda \mathcal{L}(f(x'), y^{\text{target}})$$

where

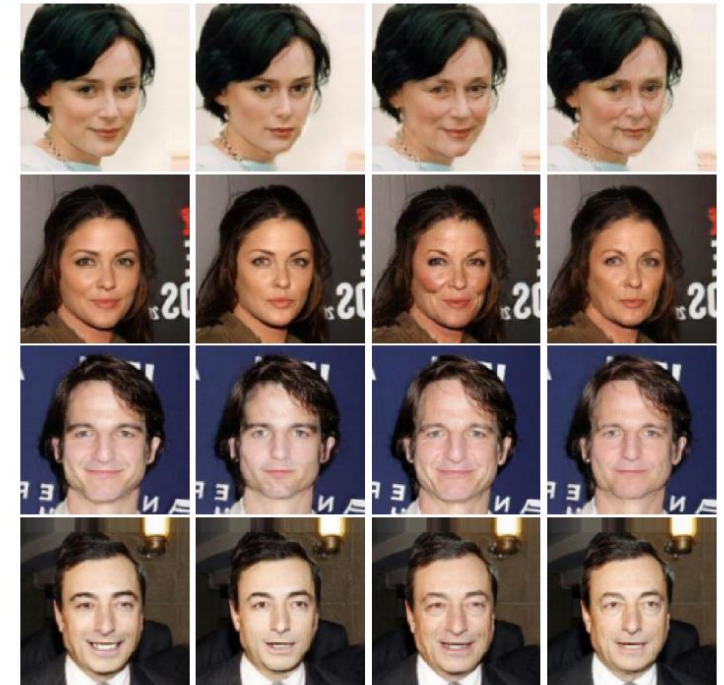
$$\mathcal{L}(f(x'), y^{\text{target}}) = (f(x') - y^{\text{target}})^2 \longrightarrow \text{Least Square Error}$$

This problem is differentiable and can be solved by Projected Gradient Descent Algorithm

Generative Approaches

- $x_{CF} = \operatorname{argmin}_{x' \in \mathcal{X}} d(x_0, x')$
s.t. $f(x') = y^{\text{target}}$
- x' can be obtained through **generative models**
 - Variational autoencoder
 - Diffusion model
- **Objective 1**: reconstruction (also distribution loss)
- **Objective 2**: target constraint (y^{target})

Young Young Old Old
Smiling Serious Smiling Serious



Summary

- **Surrogate models** learns a local approximation of the decision boundary at a given instance
 - The local approximation is done by a simple explainable model such as linear regression or decision tree
 - Explanation is at the granularity of “interpretable representation”
 - A kernel function is used
- **Shapley value** has a game theoretic interpretation of contribution in a coalition game
 - Can be used to weight the contribution of each perturbation
- **Counterfactual explanation** deals with the “what-if” question
 - The model finds a perturbation that causes the model to switch its prediction