CXPlain: Causal Explanations for Model Interpretation under Uncertainty

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Introduction

- Explanation methods for machine learning models are important, but complex models are difficult to interpret
- Wide variety of machine learning models make it challenging to develop a fast, accurate, unified and optimized approach to importance attribution for any machine learning models
- State-of-the-art explanation methods typically have significant uncertainty, difficult to judge if the explanation results are accurate

Drawbacks of Existing Methods

Computational cost and Applicability

Table 1: Comparison of CXPlain to several representative methods for feature importance estimation.

	CXPlain	SG [8] / IG [10]	DeepSHAP [1, 6]	LIME [16]	SHAP [6]
Accuracy	high	moderate	high	high	high
Model-agnostic	✓	×	×	✓	✓
Uncertainty estimates	✓	×	×	×	×
Computation time	fast	fast	fast	slow	slow

Drawbacks of Existing Methods

Uncertainty in explanation

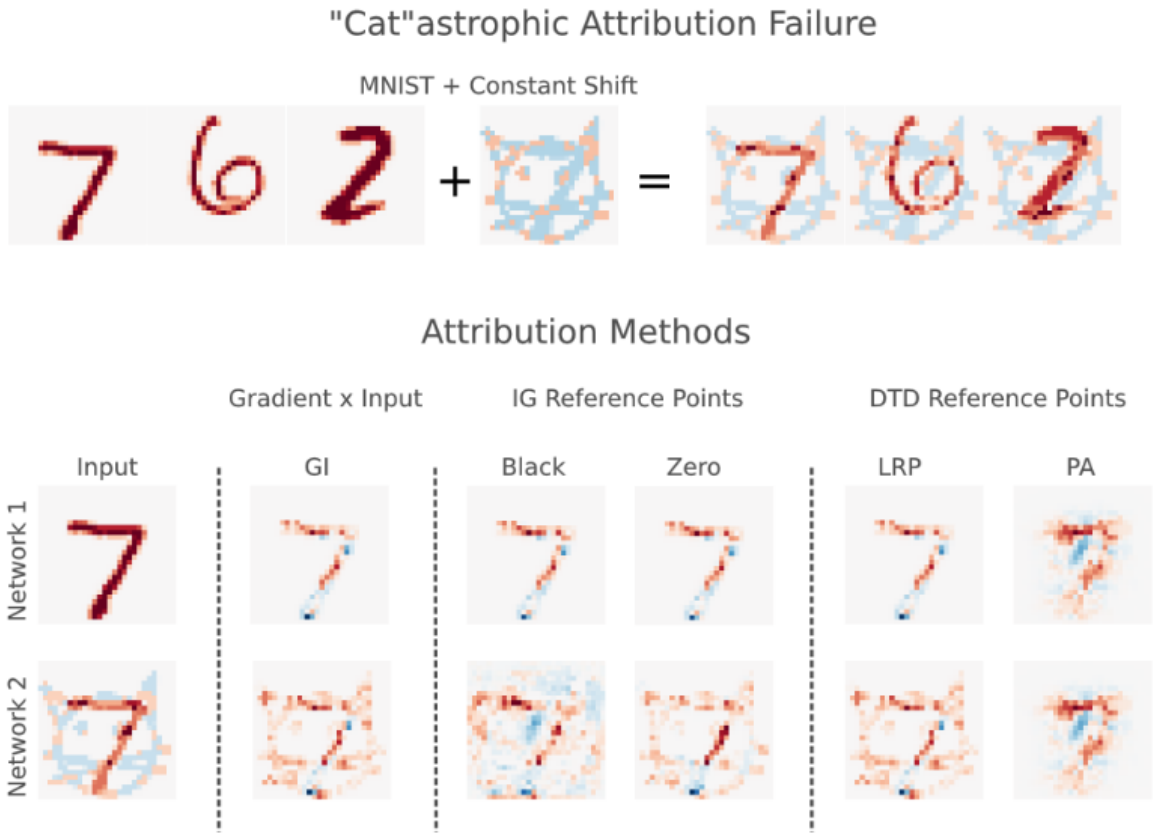

Figure 6: Evaluation of attribution method sensitivity using MNIST. Gradient x Input, IG with both a black and zero reference point and DTD with a LRP reference point, do not satisfy input invariance and produce different attribution for each network. DTD with a PA reference point is not sensitive to the transformation of the input.

1

[1] Pieter-Jan Kindermans, Sara Hooker, Julius Adebayo, Maximilian Alber, Kristof T Schütt, Sven Dähne, Dumitru Erhan, and Been Kim. The (un) reliability of saliency methods. arXiv preprint arXiv:1711.00867, 2017.

Drawbacks of Existing Methods

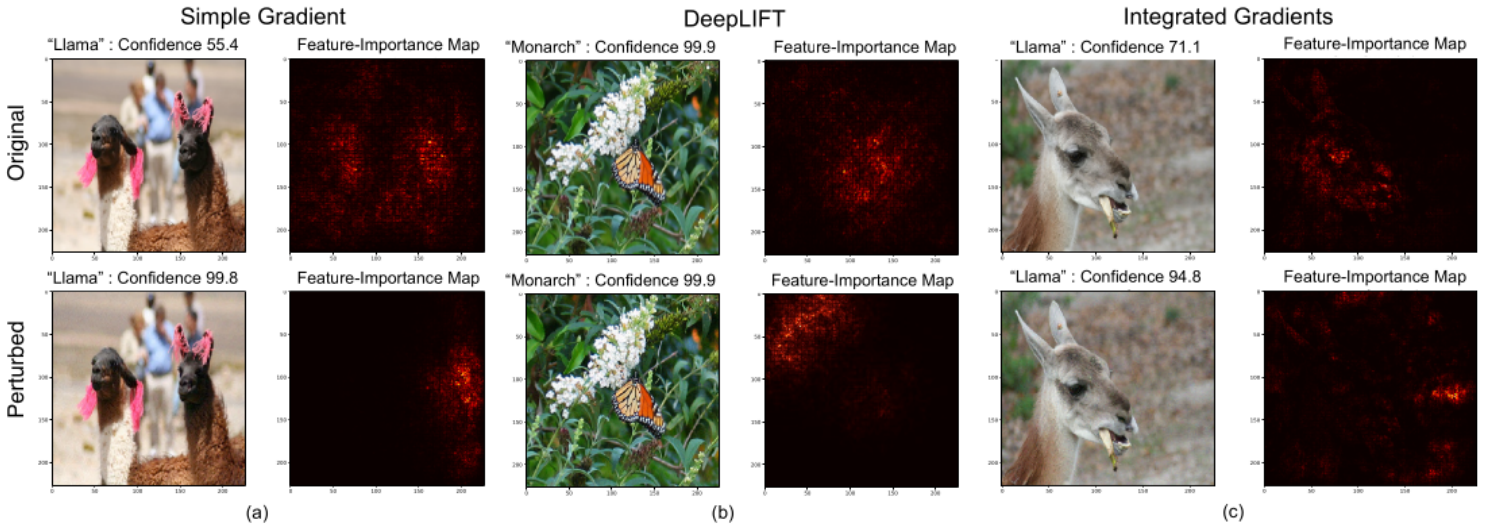

Figure 1: **Adversarial attack against feature-importance maps.** We generate feature-importance scores, also called saliency maps, using three popular interpretation methods: (a) simple gradients, (b) DeepLIFT, and (c) integrated gradients. The **top row** shows the the original images and their saliency maps and the **bottom row** shows the perturbed images (using the center attack with $\epsilon = 8$, as described in Section 2) and corresponding saliency maps. In all three images, the predicted label does not change from the perturbation; however, the saliency maps of the perturbed images shifts dramatically to features that would not be considered salient by human perception.

2

[2] Amirata Ghorbani, Abubakar Abid, and James Zou. Interpretation of neural networks is fragile. AAAI Conference on Artificial Intelligence, 2019.

CXPlain

- Causal Explanation Model
- Estimate feature importance for **any** machine learning model
- Significantly **more accurate** and **faster** in evaluation than existing model-agnostic methods
- Provide uncertainty estimates for feature importance by bootstrap resampling
- Uncertainty estimates are strongly correlated with the accuracy of the explanation model

Idea: train a seperate explanation model to produce the importance scores for each input features.

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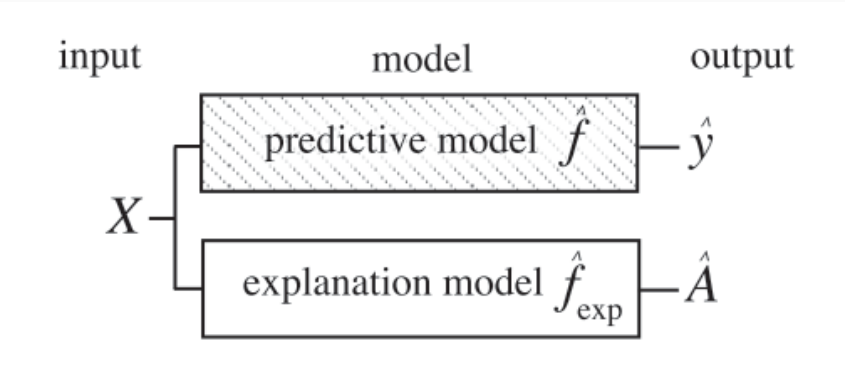
Problem Setup

Predictive model

- Suppose we have a predictive model $\hat{f} : X \rightarrow \hat{y} \in \mathbb{R}^k$, where X consists of p input features $\{x_i\}_{i=1}^{p}$
- The predictive model is scored by an objective function $\mathcal{L}$
- No other restrictions on $\hat{f}$, no need for knowledge on how $\hat{f}$ produces its output

Explanation model

- Goal: train an explanation model $\hat{f}_{exp} : X \rightarrow \hat{A} \in \mathbb{R}^p$, where each element $\hat{a}_i$ corresponds to the importance score of input feature x_i.



Causal Objective

Given input features X, we compute the outputs of the predictive model $\hat{f}$ with and without the ith input feature x_i:

$$\hat{y}_{X \setminus \{i\}} = \hat{f}(X \setminus \{i\}), \quad \hat{y}_X = \hat{f}(X) \tag{1}$$

Then we compute the errors of the predictive model $\hat{f}$ with and without x_i using the loss function $\mathcal{L}$ of $\hat{f}$:

$$\varepsilon_{X \setminus \{i\}} = \mathcal{L}(y, \hat{y}_{X \setminus \{i\}}), \quad \varepsilon_X = \mathcal{L}(y, \hat{y}_X) \tag{2}$$

The **causality** of input feature x_i to model output y is defined as the **marginal decrease** in the predictive error:

$$\Delta\varepsilon_{X,i} = \varepsilon_{X \setminus \{i\}} - \varepsilon_X \tag{3}$$

Causal Objective

We get the **importance scores** by normalizing the causalities:

$$\omega_i(X) = \frac{\Delta\varepsilon_{X,i}}{\sum_{j=1}^{p} \Delta\varepsilon_{X,j}} \tag{4}$$

Finally, we define the **causal objective** as the Kullback-Leibler divergence between the target importance distribution Ω and the one computed by the explanation model:

$$\mathcal{L}_{\text{causal}} = \frac{1}{N} \sum_{l=1}^{N} \text{KL}(\Omega_{X_l}, \hat{A}_{X_l}), \tag{5}$$

where $\Omega(i) = \omega_i(X)$, and $\hat{A}(i) = \hat{a}_i$ are the output of $\hat{f}_{exp}$.

Remarks

Mask input features

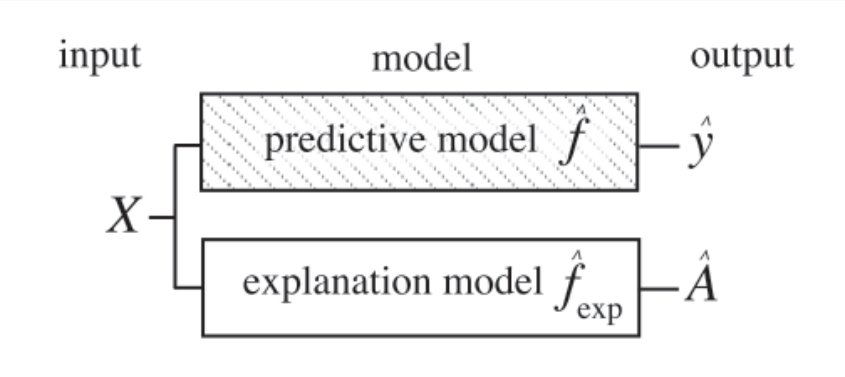
- Replace x_i with zeros when the zero value has no special meaning
- Replace x_i with mean value across the entire dataset
- Advanced schemes considering the distribution of the features can be more principled alternatives

Precompute importance scores

- To precompute the importance score for one training sample X with p features, $p + 1$ evaluations of the predictive model are required
- For high-dimensional images, we can group non-overlapping regions of adjacent pixels into feature groups

Remarks

CXPlain models



$$\hat{f}_{\text{exp}} : X = (x_1, x_2, \ldots, x_p) \rightarrow (\omega_1(X), \omega_2(X), \ldots, \omega_p(X)) \qquad (6)$$

- Any supervised machine learning model that can be trained with a custom objective can be used as explanation models
- In this work, the authors use DNNs, specifically MLPs and U-nets

Uncertainty Quantification

The uncertainty associated in feature importance estimate $\hat{a}$ can be quantified via bootstrap ensemble methods.

- Randomly draw N training samples X with repeats from the original training set (of size N), and train an explanation model on the selected set.
- Repeat the process M times to obtain a bootstrap ensemble of M explanation models.
- Use the median of the outputs as the assigned output, and use the $\frac{\alpha}{2}$ and $1-\frac{\alpha}{2}$ quantiles to form the confidence intervals $\mathrm{CI}_\gamma = [c_{\frac{\alpha}{2}}, c_{1-\frac{\alpha}{2}}]$ at confidence level $\gamma = 1-\alpha$.
- The width of CI_γ can be used to quantify the uncertainty of $\hat{a}$.

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Questions to answer

- How does the feature importance estimation performance of CXPlain compare to that of the state-of-the-art methods? (Accuracy)
- How does the computational performance of CXPlain compare to existing model-agnostic and model-specific methods for feature importance estimation? (Computational cost)
- Are uncertainty estimates of CXPlain models qualitatively and quantitatively correlated with their ability to accurately determine feature importance? (Quality of uncertainty quantification)

Tasks

Binary classification tasks:

- 8 vs. 3 MNIST benchmark (model accuracy: 99.85%)
- Gorilla vs. Zebra ImageNet benchmark (model accuracy: 96.73%)
- The test set contains 100 unseen images

Metrics

Accuracy of important features

- To quantify the accuracy of important features predicted, we measure the change in the classification models' confidence after masking the top 10 and 30% of the most importanct pixels for MNIST and ImageNet test images respectively:

$$\Delta\text{log-odds} = \text{log-odds}(p_{\text{original}}) - \text{log-odds}(p_{\text{masked}}) \tag{7}$$

- $\text{log-odds}(p) = \log\left(\frac{p}{1-p}\right)$
- Higher Δlog-odds means higher accuracy in important feature estimation
- Mann-Whitney-Wilcoxon (MWW) tests are used to calculate p-values for comparison between distributions.

Metrics

Uncertainty Quantification

- We want to test whether the uncertainty estimates u_i of input feature x_i are correlated with the errors in feature importance estimation on test set. That is to say, whether a small uncertainty provided by the ensemble models leads to a high accuracy in the estimation of importance scores.
- The authors state that typically the per-feature ground-truth values of importance scores are not available, so the Rank Error

$$\text{RE}_i = |\text{rank}_{\Delta\text{log-odds}}(i) - \text{rank}_{\hat{f}_{exp}}(i)|$$

defined as the difference in the rank of feature x_i implied by Δlog-odds and the rank implied by $\hat{f}_{exp}$ is used as the error in importance estimation.

Metrics

Uncertainty Quantification

- Pearson correlation coefficient $\rho_{X,Y} = \frac{\text{cov}(X,Y)}{\sigma_X \sigma_Y}$ is used to measure the correlation between RE_i and u_i
- The coefficient ρ is computed on the top 2.5% of pixels by Δlog-odds across the test set of $N = 100$ images.
- Fisher z-transform is applied to the correlation scores to correct the skew in the distribution of sample correlation.

Results

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