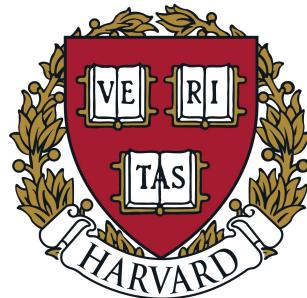
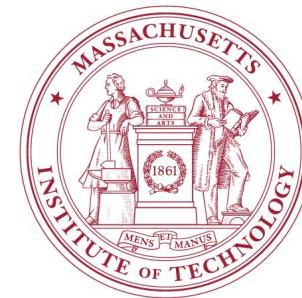


Explaining Machine Learning Predictions: State-of-the-art, Challenges, Opportunities

Hima Lakkaraju



Julius Adebayo



Sameer Singh





Hima Lakkaraju
Harvard University



Julius Adebayo
MIT



Sameer Singh
UC Irvine

Slides and Video: explainml-tutorial.github.io

Motivation



Machine Learning is EVERYWHERE!!

Friend Requests

- 3 mutual friends
- 2 mutual friends
- 2 mutual friends

People You May Know

- 2 mutual friends

See All

this week's bestselling models.

Canon PowerShot A495 10.0 MP Digital Camera with 3.3x Optical Zoom and 2.5- Inch LCD (Blue)	Canon PowerShot A3000IS 10 MP Digital Camera with 4x Optical Image Stabilized Zoom and 2.7- Inch LCD	Canon PowerShot ELPH 300 HS 12 MP CMOS Digital Camera with Full 1080p HD Video (Black)	Canon PowerShot S95 10 MP Digital Camera with 3.8x Wide Angle Optical Image Stabilized Zoom and 3.0-Inch inch LCD



Motivation

Model understanding is absolutely critical in several domains -- particularly those involving *high stakes decisions*!



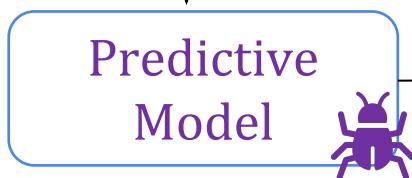
Motivation: Why Model Understanding?

Input



Model understanding facilitates debugging.

This model is
incorrect
make
on!! Let
model



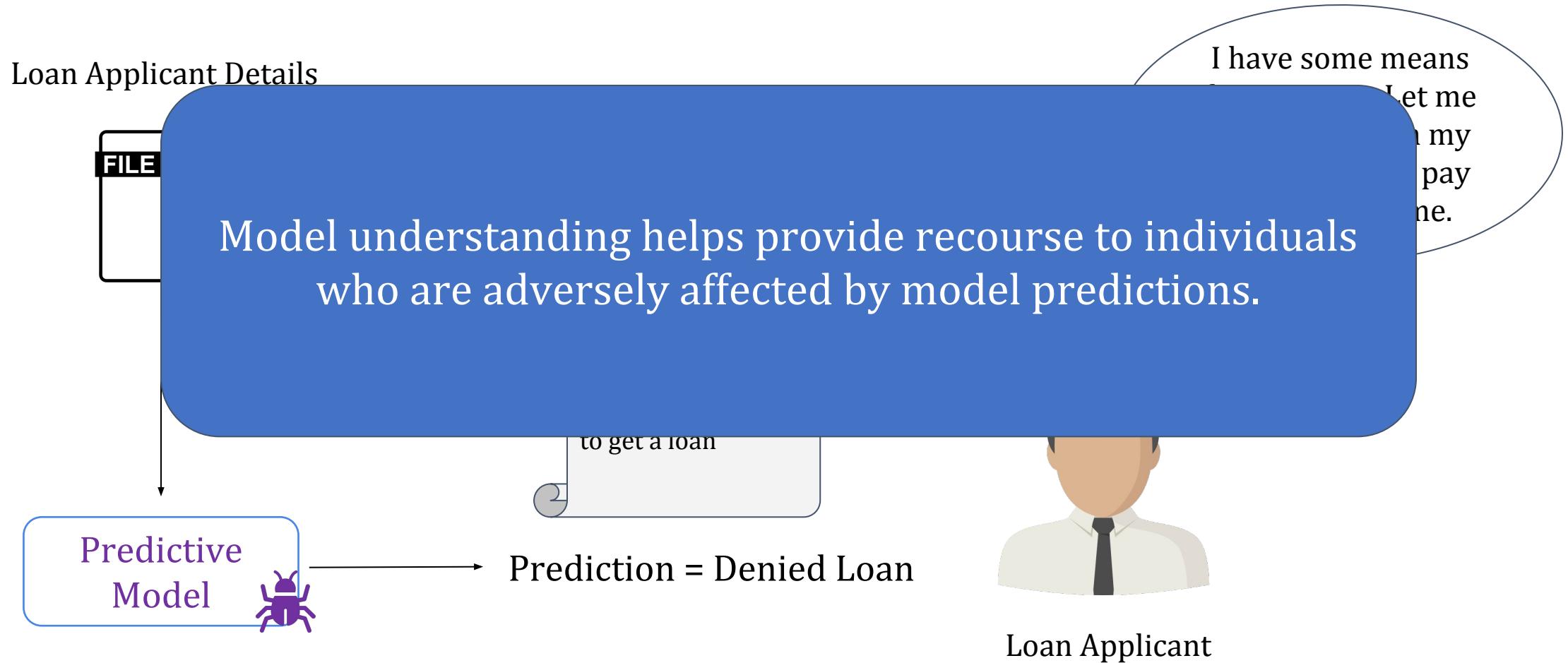
Prediction = Siberian Husky



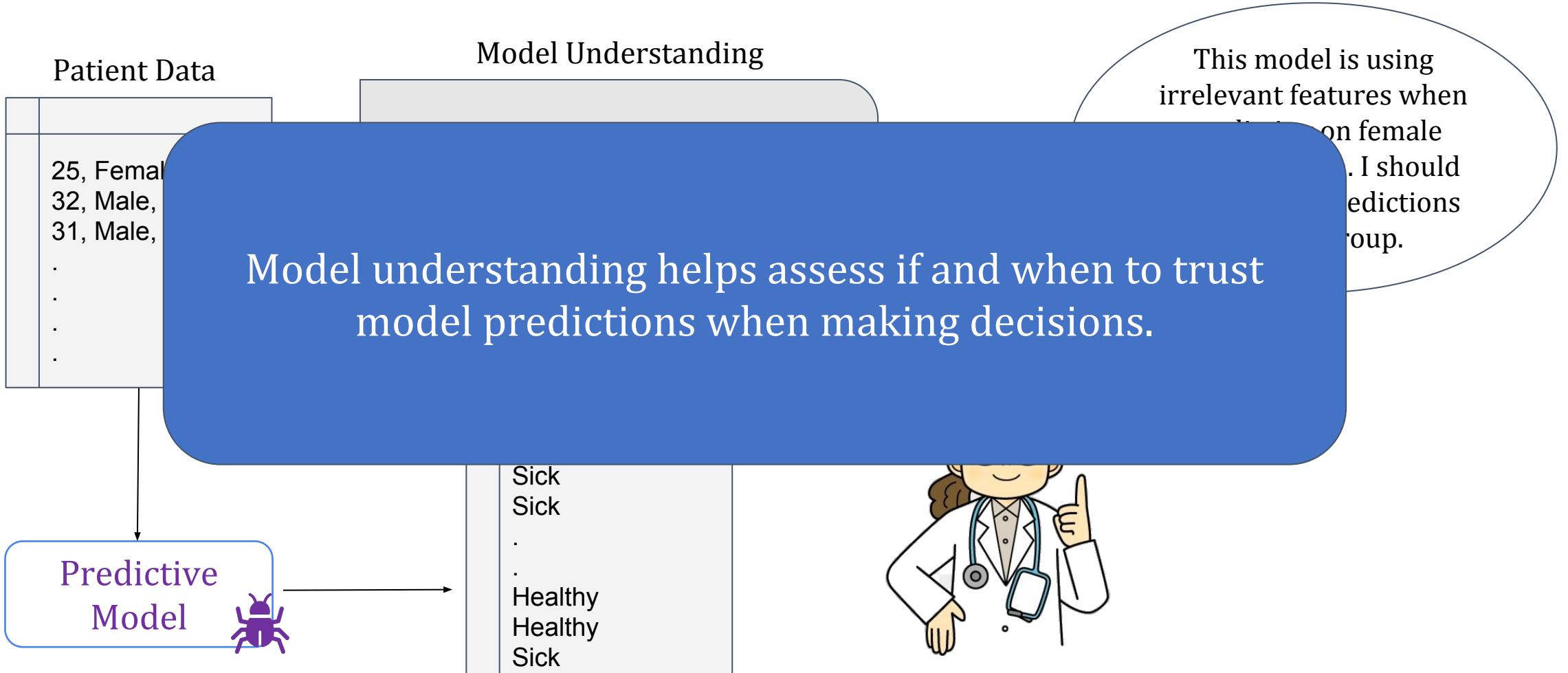
Motivation: Why Model Understanding?



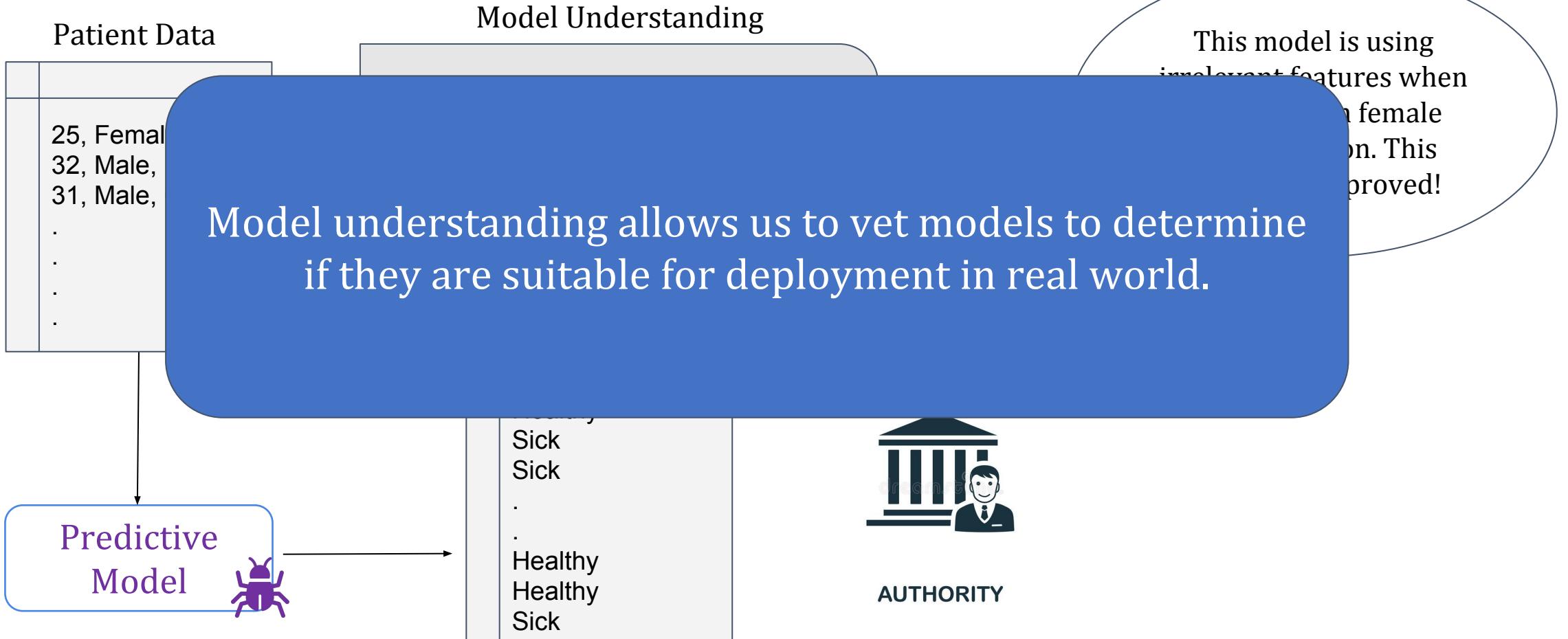
Motivation: Why Model Understanding?



Motivation: Why Model Understanding?



Motivation: Why Model Understanding?



Motivation: Why Model Understanding?

Utility

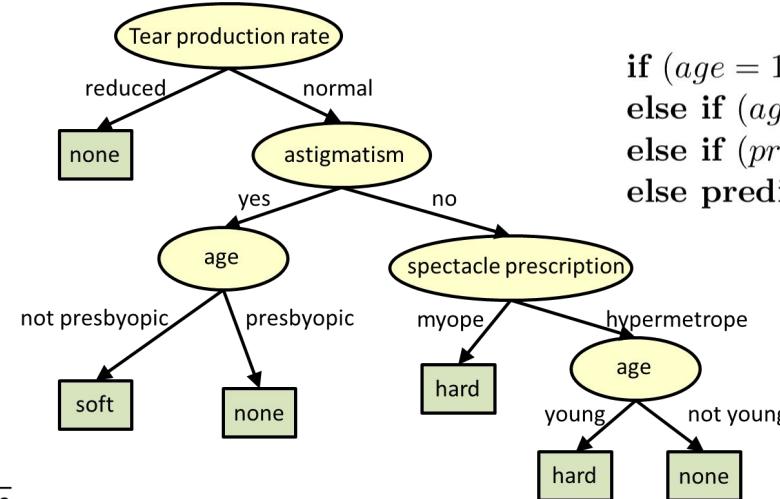
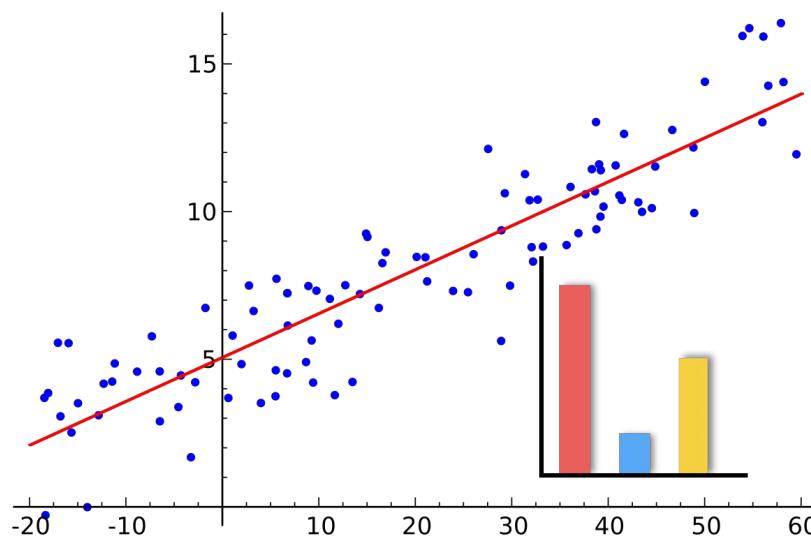
- Debugging
- Bias Detection
- Recourse
- If and when to trust model predictions
- Vet models to assess suitability for deployment

Stakeholders

- End users (e.g., loan applicants)
- Decision makers (e.g., doctors, judges)
- Regulatory agencies (e.g., FDA, European commission)
- Researchers and engineers

Achieving Model Understanding

Take 1: Build *inherently interpretable* predictive models

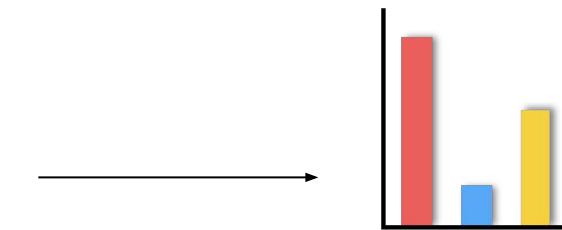
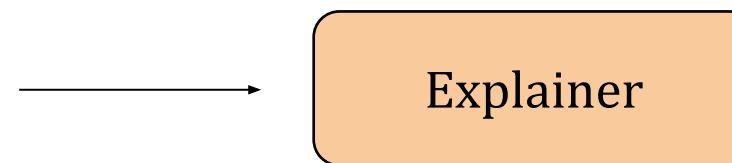
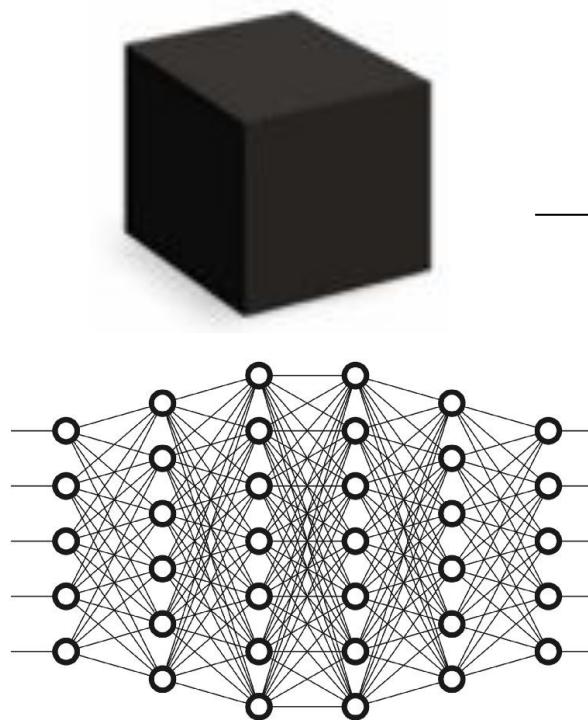


```

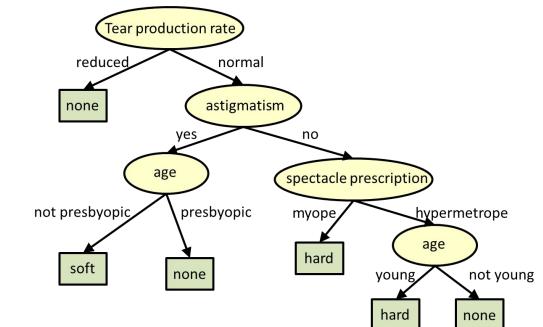
if (age = 18 – 20) and (sex = male) then predict yes
else if (age = 21 – 23) and (priors = 2 – 3) then predict yes
else if (priors > 3) then predict yes
else predict no
  
```

Achieving Model Understanding

Take 2: *Explain* pre-built models *in a post-hoc manner*

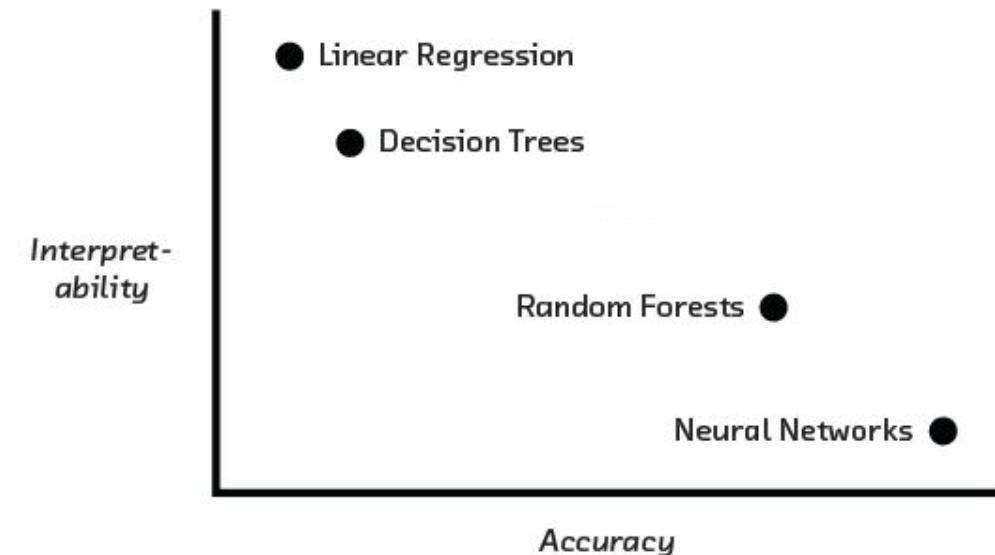
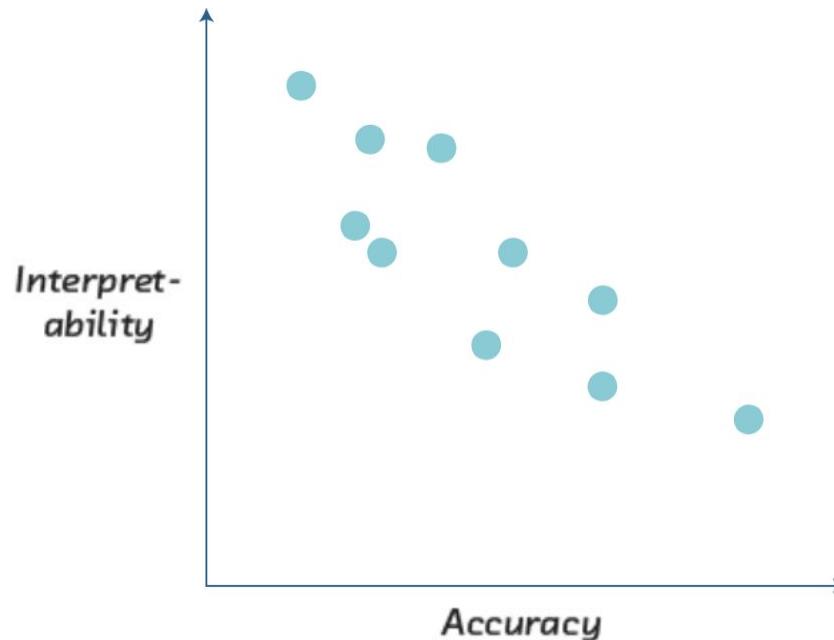


```
if (age = 18 – 20) and (sex = male) then predict yes
else if (age = 21 – 23) and (priors = 2 – 3) then predict yes
else if (priors > 3) then predict yes
else predict no
```



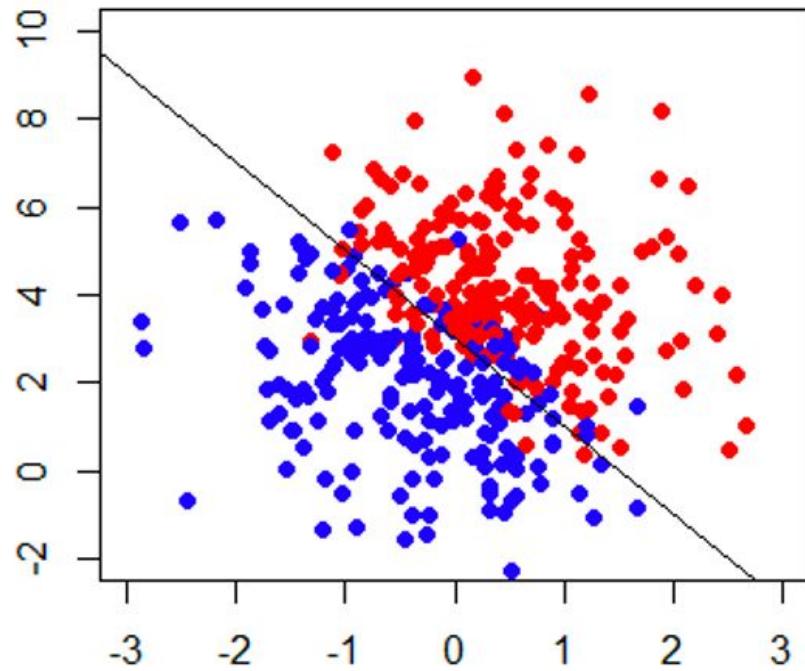
Inherently Interpretable Models vs. Post hoc Explanations

Example

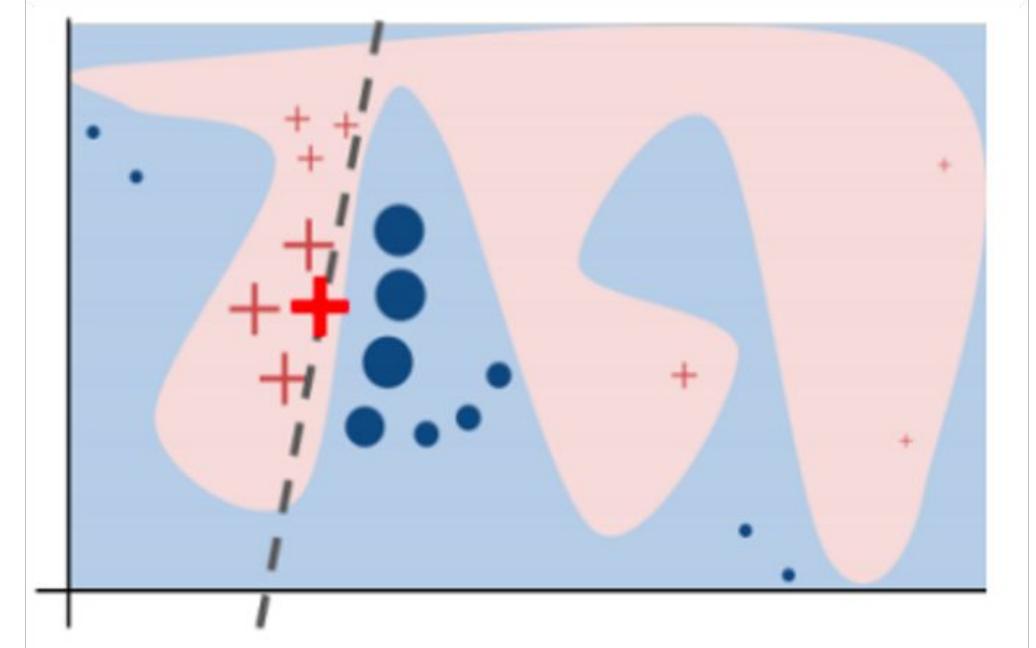


In *certain* settings, *accuracy-interpretability trade offs* may exist.

Inherently Interpretable Models vs. Post hoc Explanations



can build interpretable +
accurate models



complex models might
achieve higher accuracy

Inherently Interpretable Models vs. Post hoc Explanations

Sometimes, you don't have enough data to build your model from scratch.

And, all you have is a (proprietary) black box!



Inherently Interpretable Models vs. Post hoc Explanations

If you *can build* an interpretable model which is also adequately accurate for your setting, DO IT!

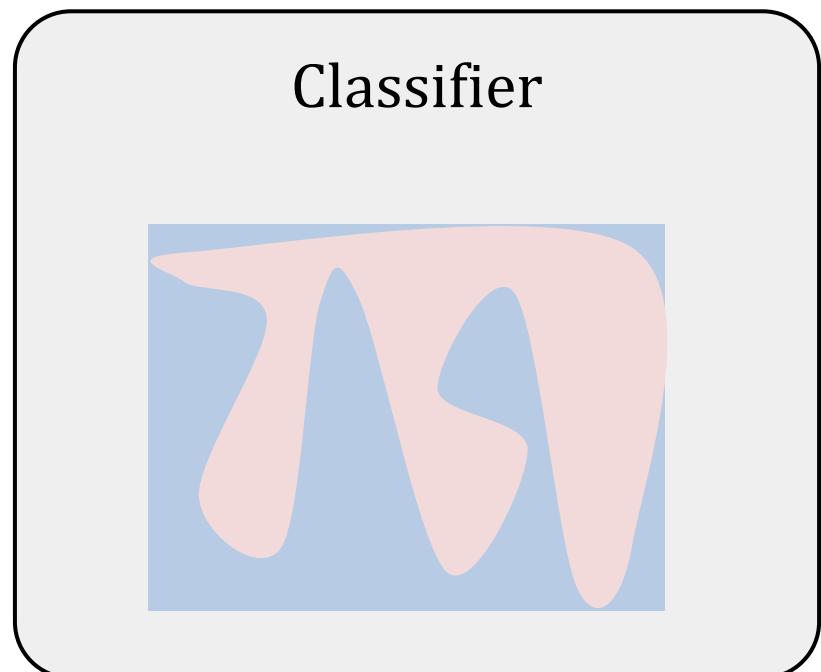
Otherwise, ***post hoc explanations*** come to the rescue!

This tutorial will focus on post hoc explanations!

What is an Explanation?

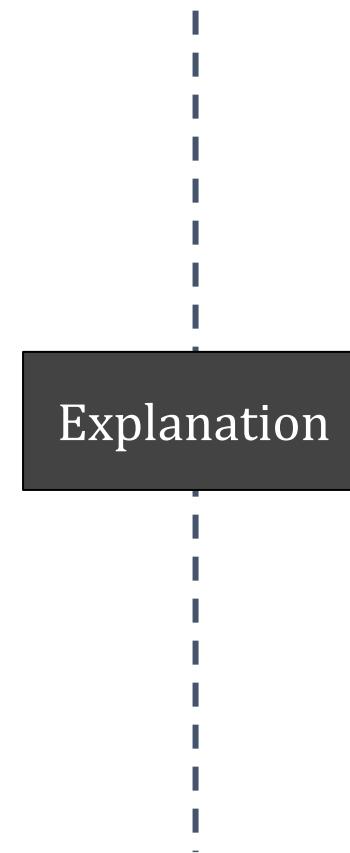
What is an Explanation?

Definition: Interpretable description of the model behavior



Classifier

Faithful



Explanation

Understandable

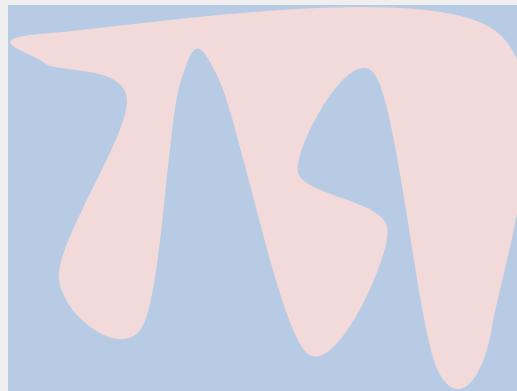


User

What is an Explanation?

Definition: Interpretable description of the model behavior

Classifier



Send all the model parameters θ ?

User

Send many example predictions?



Summarize with a program/rule/tree

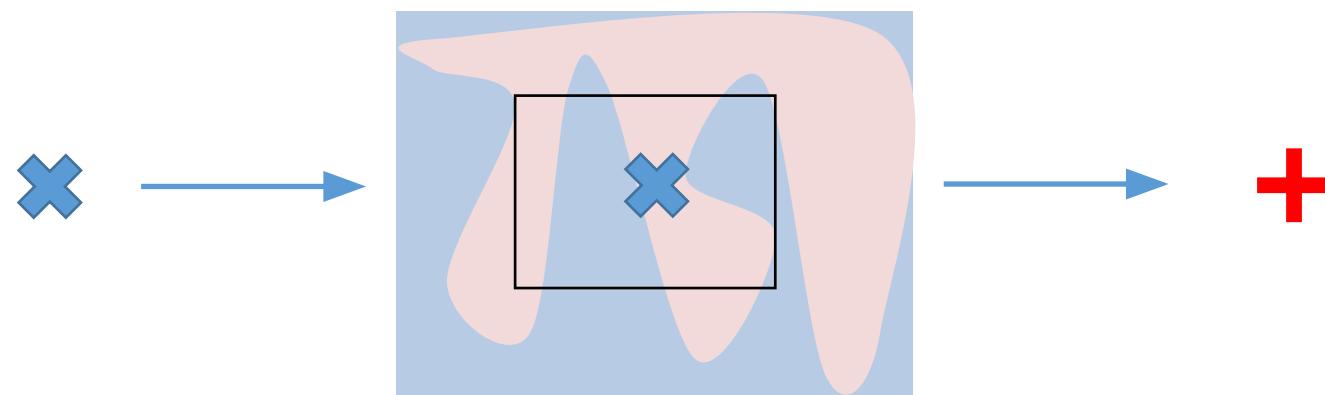
Select most important features/points

Describe how to *flip* the model prediction

...

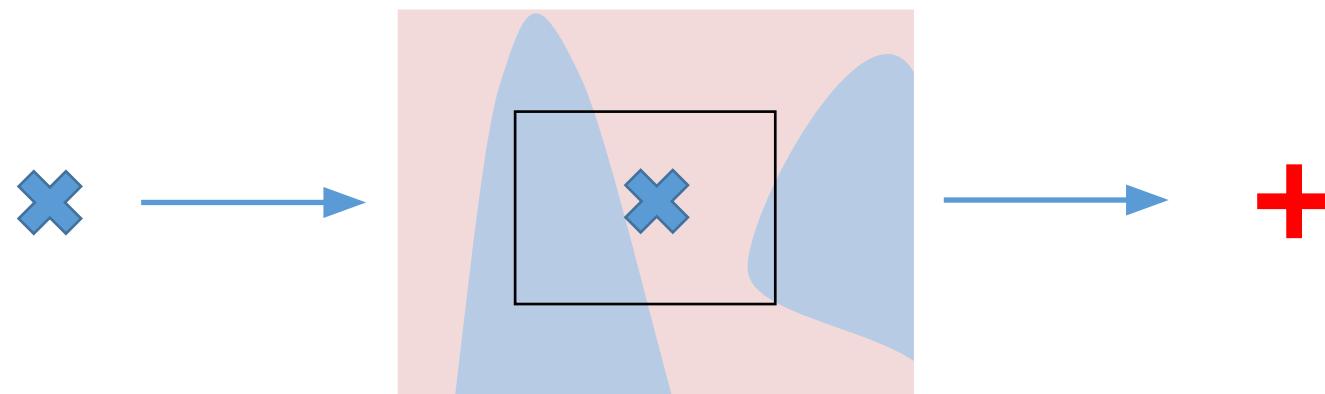
Local versus Global Explanations

Global explanation may be too complicated



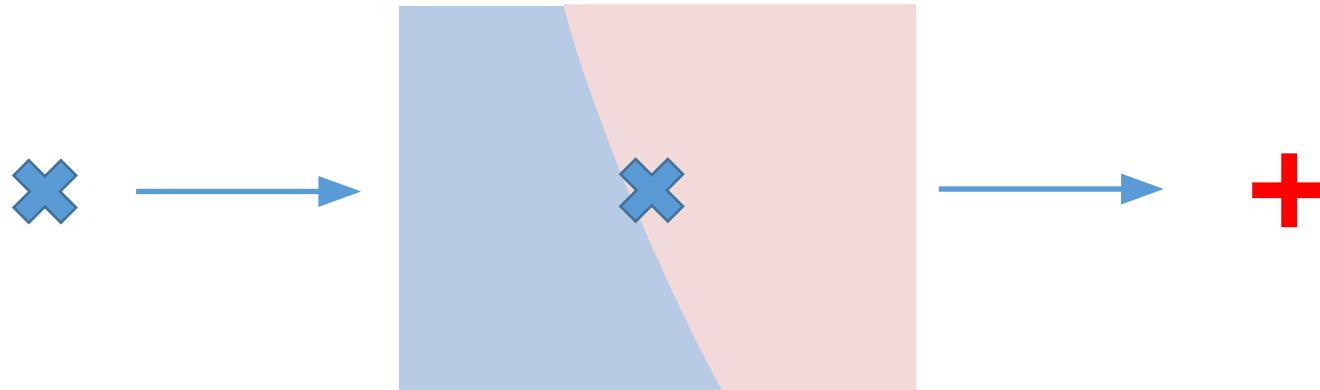
Local versus Global Explanations

Global explanation may be too complicated



Local versus Global Explanations

Global explanation may be too complicated

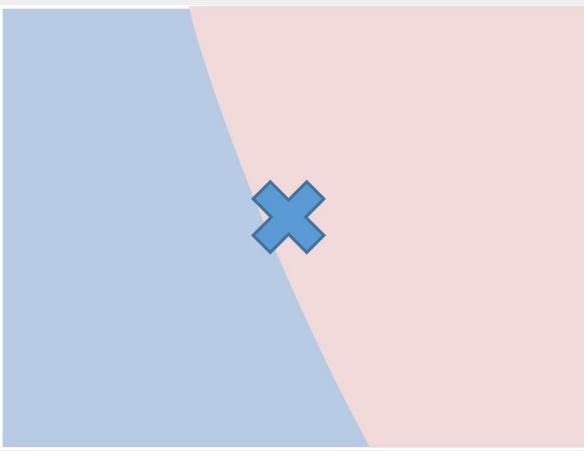


Definition: Interpretable description of the model behavior
in a target neighborhood.

Local Explanations

Definition: Interpretable description of the model behavior
in a target neighborhood.

Classifier



User



Send many example predictions?

Summarize with a program/rule/tree

Select most important features/points

Describe how to *flip* the model prediction

⋮

⋮

⋮

Local Explanations vs. Global Explanations

Explain individual predictions

Help unearth biases in the *local neighborhood* of a given instance

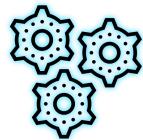
Help vet if individual predictions are being made for the right reasons

Explain complete behavior of the model

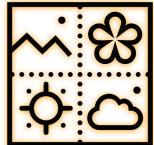
Help shed light on *big picture biases* affecting larger subgroups

Help vet if the model, at a high level, is suitable for deployment

Tutorial on Post hoc Explanations



Approaches for Post hoc Explainability



Explanations in **Different Modalities**



Evaluation of Explanations

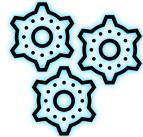


Limits of Post hoc Explainability

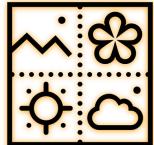


Future of Post hoc Explainability

Tutorial on Post hoc Explanations



Approaches for Post hoc Explainability



Explanations in Different Modalities



Evaluation of Explanations

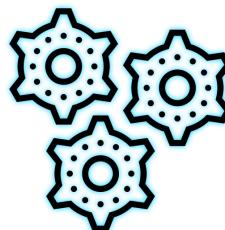


Limits of Post hoc Explainability

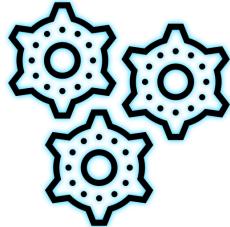


Future of Post hoc Explainability

Approaches for Post hoc Explainability



Approaches for Post hoc Explainability

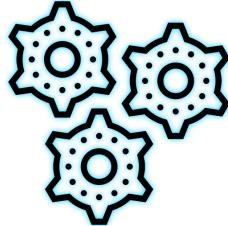


Local Explanations

- Feature Importances
- Rule Based
- Saliency Maps
- Prototypes/Example Based
- Counterfactuals

Global Explanations

- Collection of Local Explanations
- Representation Based
- Model Distillation
- Summaries of Counterfactuals



Approaches for Post hoc Explainability

Local Explanations

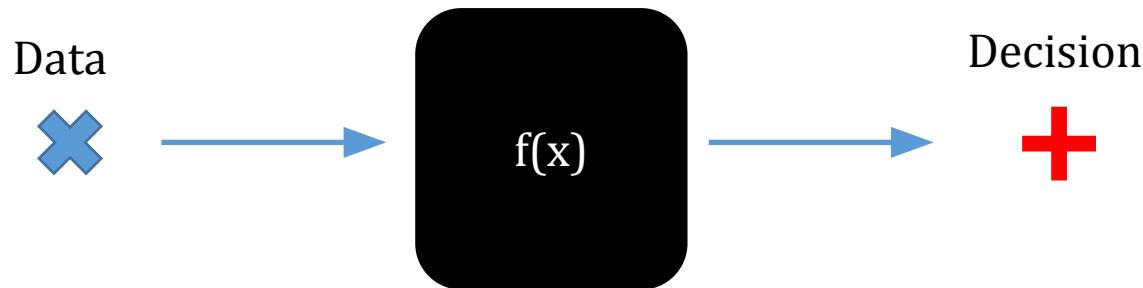
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Being Model-Agnostic...

No access to the internal structure...



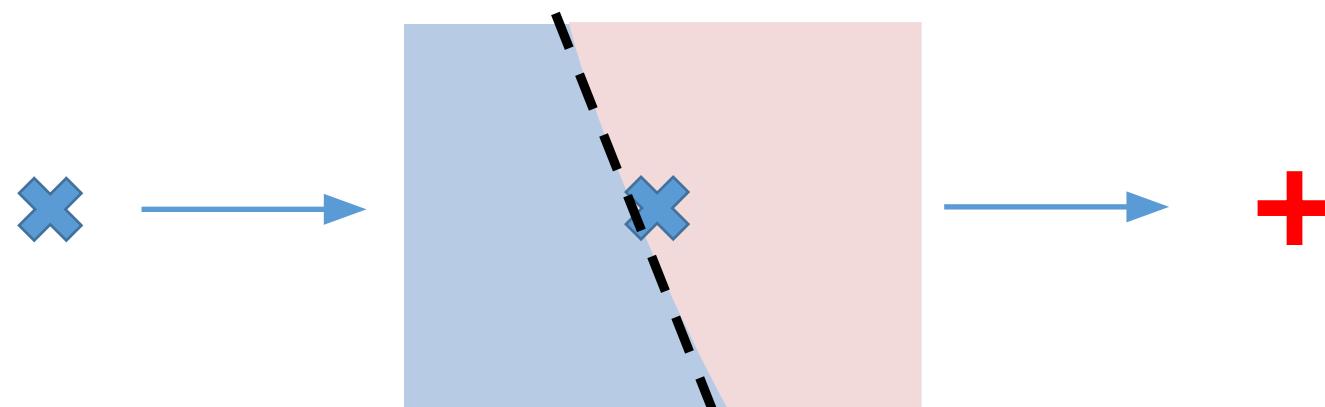
Not restricted to specific models

Practically easy: not tied to PyTorch, Tflow, etc.

Study models that you don't have access to!

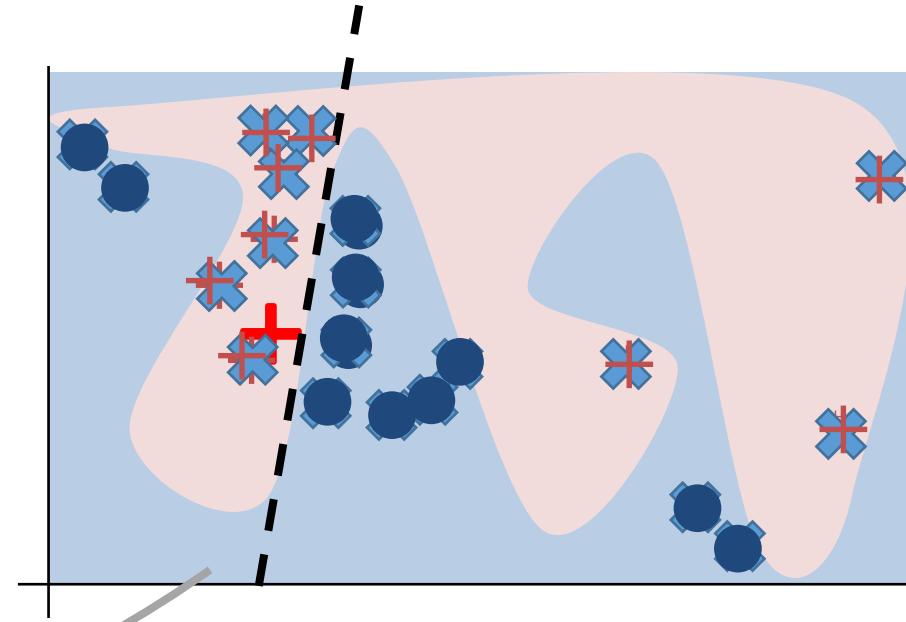
LIME: Sparse, Linear Explanations

Identify the important dimensions,
and present their relative importance



LIME: Sparse Linear Explanations

1. Sample points around x_i
2. Use model to predict labels for each sample
3. Weigh samples according to distance to x_i
4. Learn simple model on weighted samples
5. Use simple model to explain



LIME Example - Images



Original Image

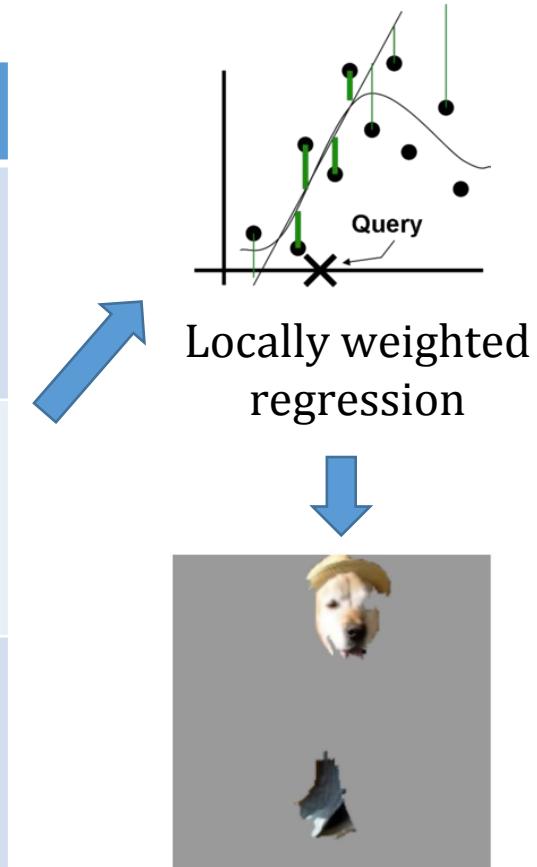
 $P(\text{labrador}) = 0.21$

LIME is quite customizable:

- How to perturb?
- Distance/similarity?
- How *local* you want it to be?
- How to express explanation

Perturbed Instances	$P(\text{Labrador})$
	0.92
	0.001
	0.34

Maybe to a fault?



Predict Wolf vs Husky

Only 1 mistake!



Predicted: **wolf**
True: **wolf**



Predicted: **husky**
True: **husky**



Predicted: **wolf**
True: **wolf**



Predicted: **wolf**
True: **husky**

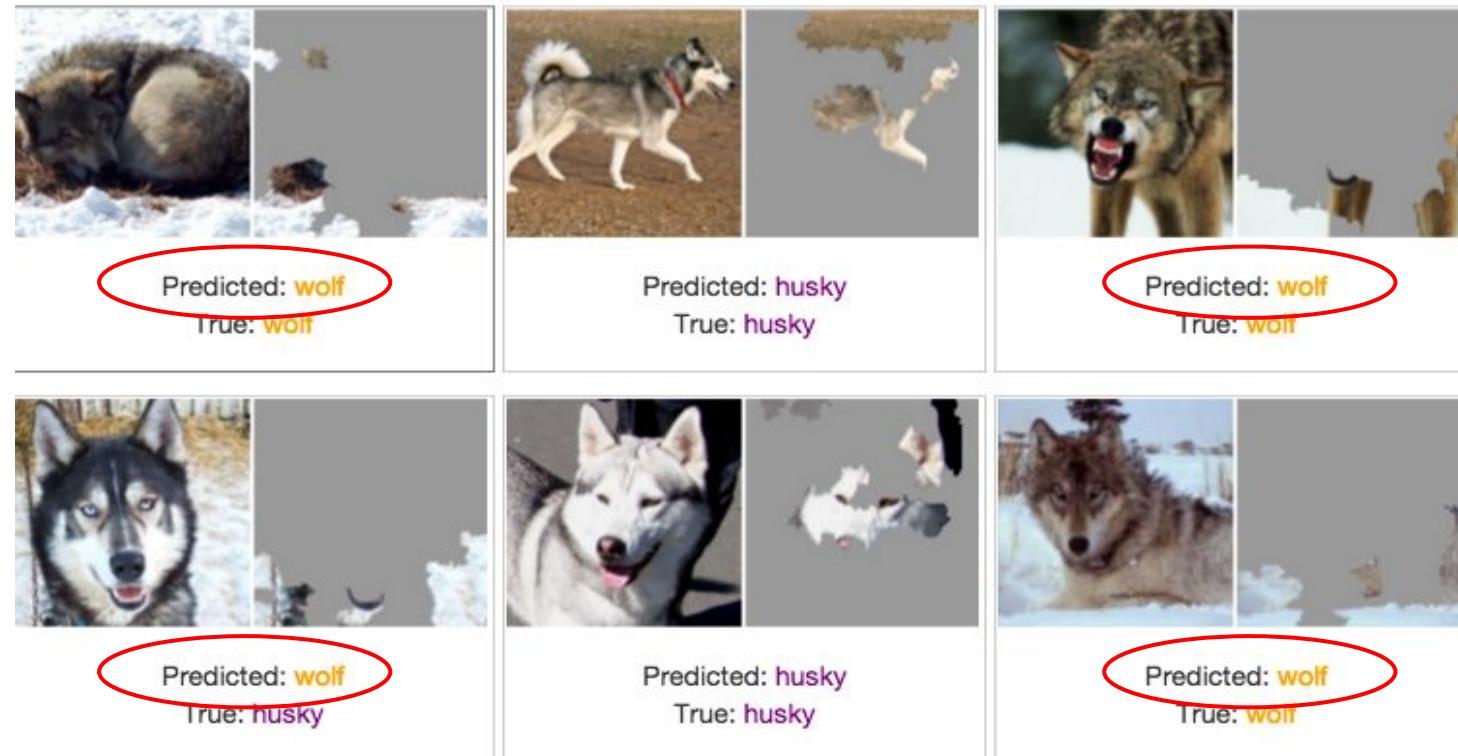


Predicted: **husky**
True: **husky**



Predicted: **wolf**
True: **wolf**

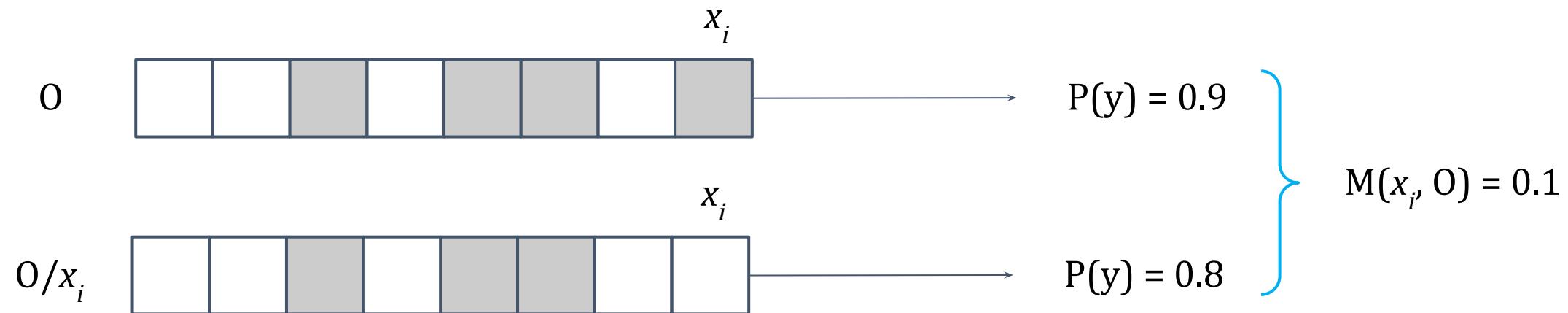
Predict Wolf vs Husky



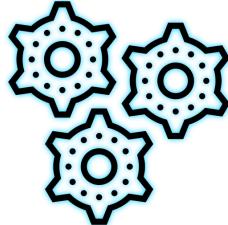
We've built a great snow detector...

SHAP: Shapley Values as Importance

Marginal contribution of each feature towards the prediction, averaged over all possible permutations.



Fairly attributes the prediction to all the features.



Approaches for Post hoc Explainability

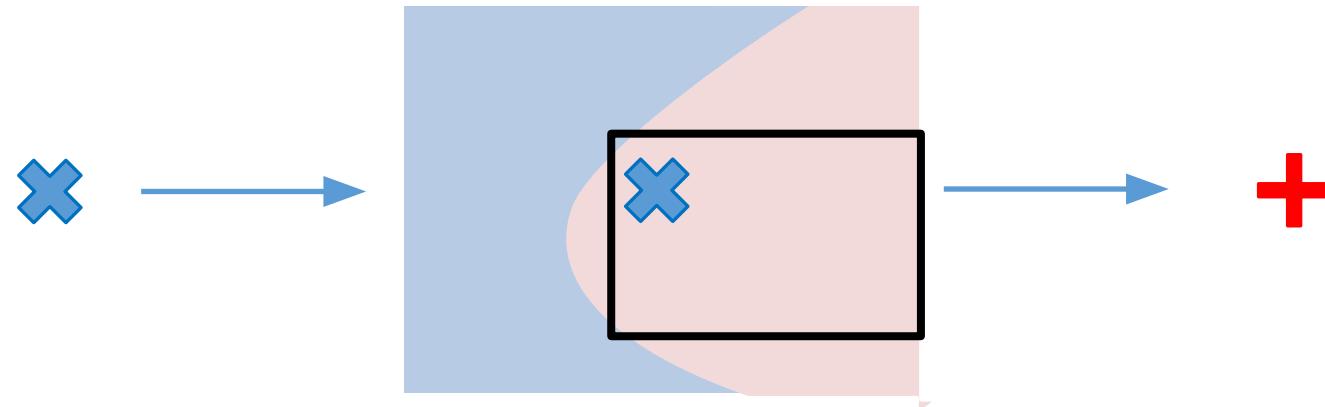
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Anchors: Sufficient Conditions

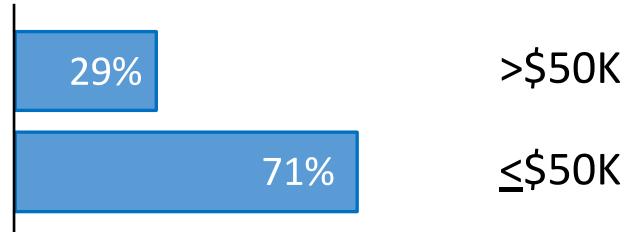


Identify the conditions under which the classifier has the same prediction

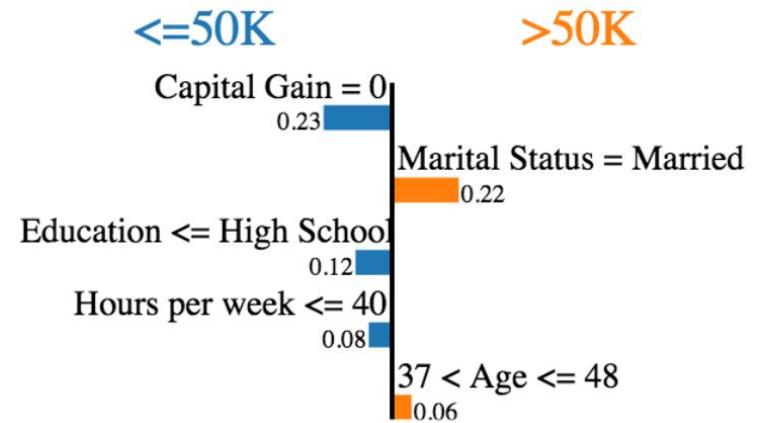
Salary Prediction

Feature	Value
Age	$37 < \text{Age} \leq 48$
Workclass	Private
Education	$\leq \text{High School}$
Marital Status	Married
Occupation	Craft-repair
Relationship	Husband
Race	Black
Sex	Male
Capital Gain	0
Capital Loss	0
Hours per week	≤ 40
Country	United States

Salary

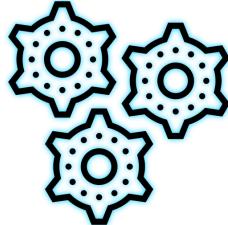


LIME



Anchors

**IF Education \leq High School
Then Predict Salary \leq 50K**



Approaches for Post hoc Explainability

Local Explanations

- Feature Importances
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- Counterfactuals

Global Explanations

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Saliency Map Overview

Input

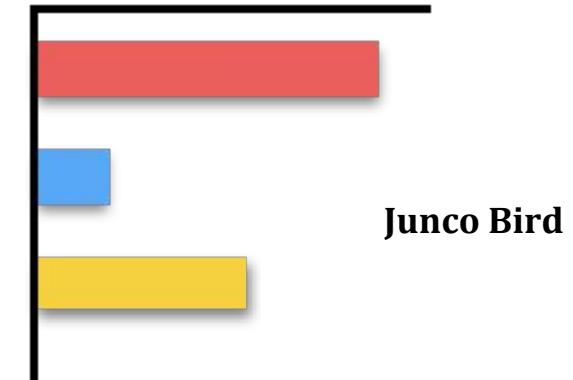


Model

$$F_{\theta}$$
A large red mathematical expression F_{θ} centered on a black background, representing the model's function.



Predictions



Saliency Map Overview

Input

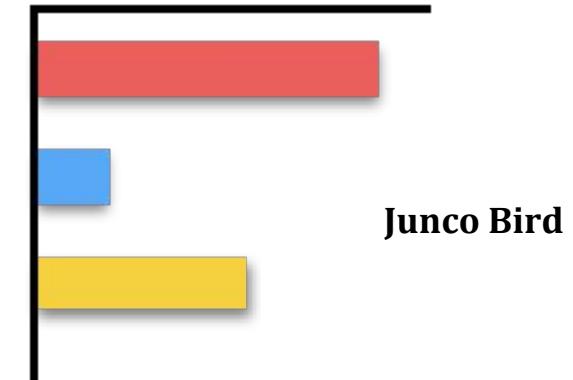


Model

$$F_{\theta}$$



Predictions



What parts of the input are most relevant for the model's prediction: '**Junco Bird**'?

Saliency Map Overview

Input

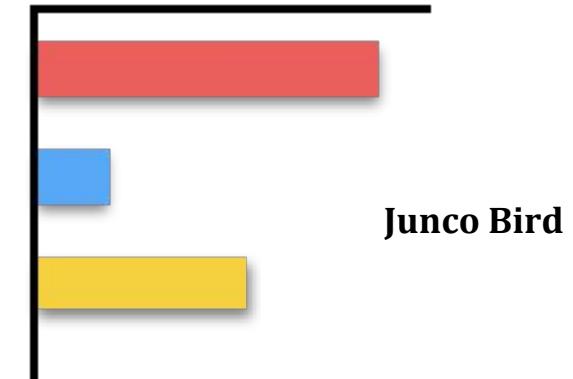


Model

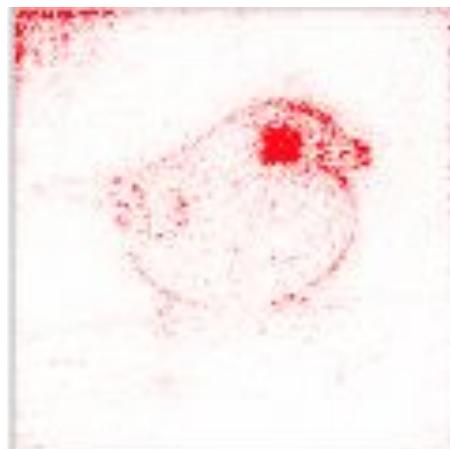
$$F_{\theta}$$



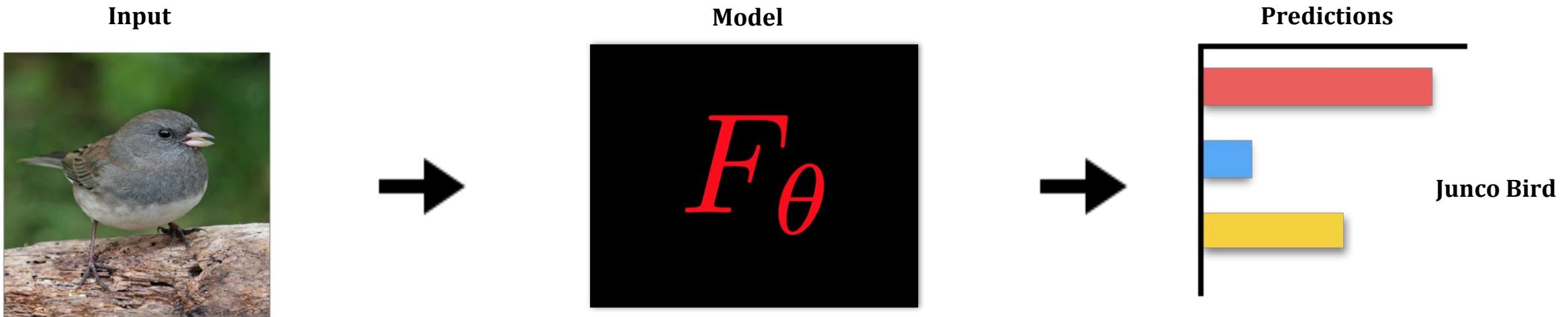
Predictions



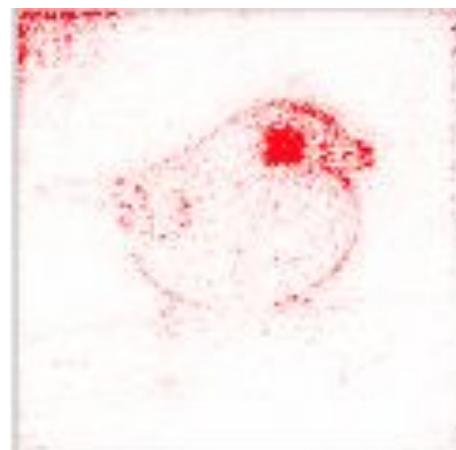
What parts of the input are most relevant for the model's prediction: '**Junco Bird**'?



Saliency Map Overview



What parts of the input are most relevant for the model's prediction: '**Junco Bird**'?



- Feature Attribution
- 'Saliency Map'
- Heatmap

A Linear Model Detour

$$y = w^\top x \quad x \in \mathbb{R}^d$$

$$y = w_1 x_1 + w_2 x_2 + \dots + w_d x_d$$

A Linear Model Detour: Sensitivity

$$y = w^\top x \quad x \in \mathbb{R}^d$$

$$y = w_1 x_1 + w_2 x_2 + \dots + w_d x_d$$

How much does a unit change in an input dimension induce in the output?

A Linear Model Detour: Sensitivity

$$y = w^\top x \quad x \in \mathbb{R}^d$$

$$y = w_1 x_1 + w_2 x_2 + \dots + w_d x_d$$

How much does a unit change in an input dimension induce in the output?

$$\nabla_x y = w$$



$$\text{Sensitivity} \equiv (w_1, w_2, \dots, w_d)$$

A Linear Model Detour: Attribution

$$y = w^\top x \quad x \in \mathbb{R}^d$$

$$y = w_1 x_1 + w_2 x_2 + \dots + w_d x_d$$

how can we apportion the output across all the input dimensions?

Another notion of relevance

$$y = w^\top x \quad x \in \mathbb{R}^d$$

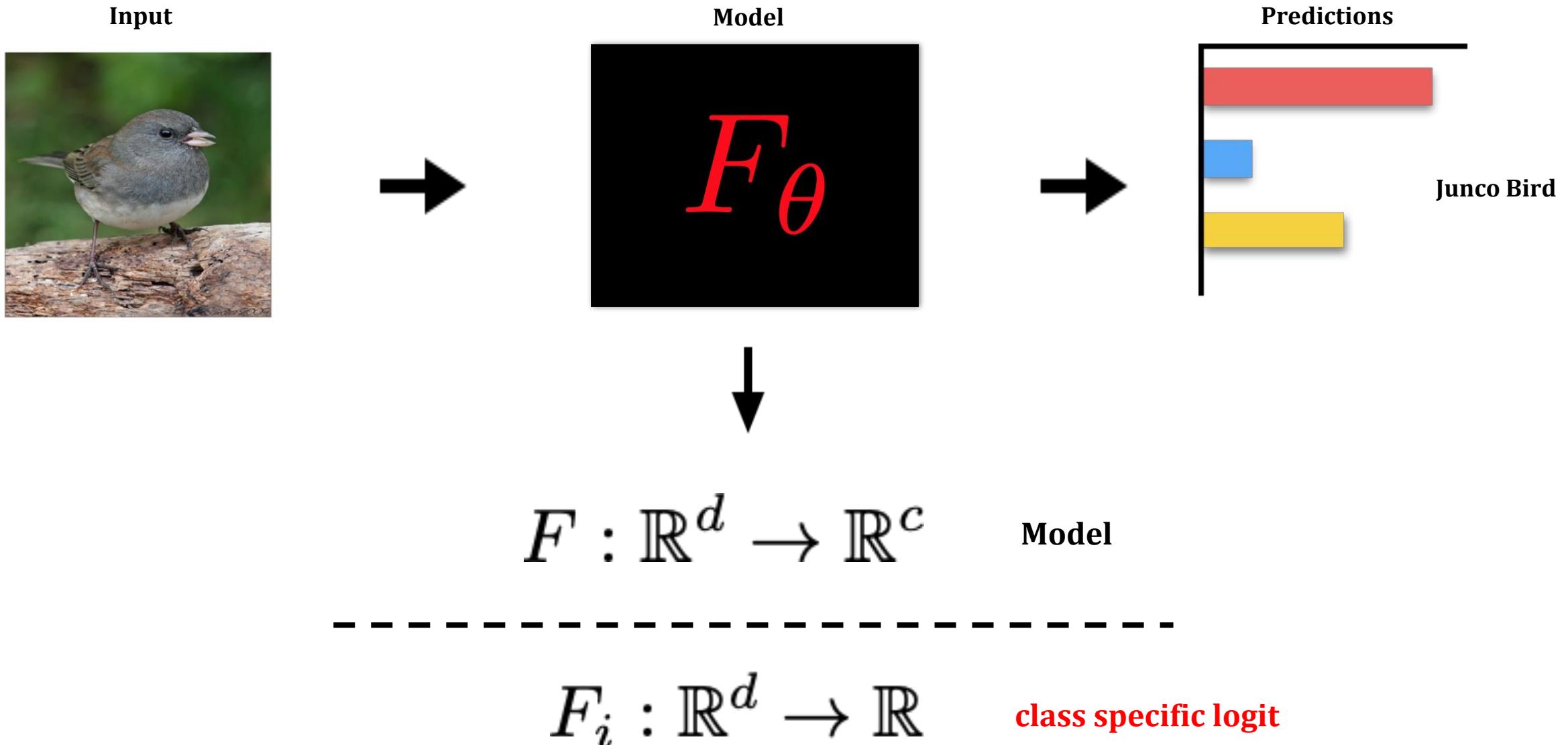
$$y = w_1x_1 + w_2x_2 + \dots + w_dx_d$$

how can we apportion the output across all the input dimensions?

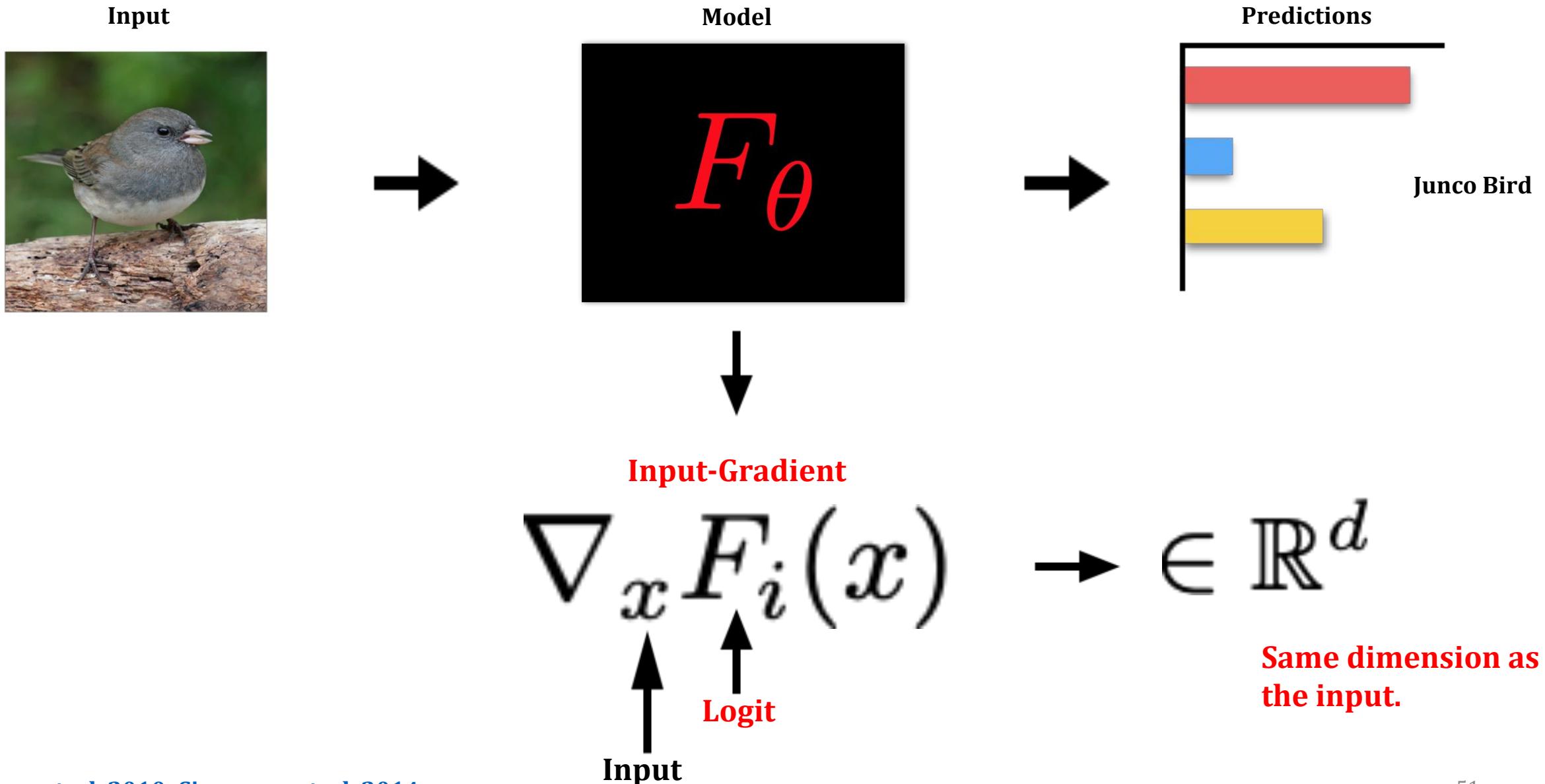


$$(w_1x_1, w_2x_2, \dots, w_dx_d)$$

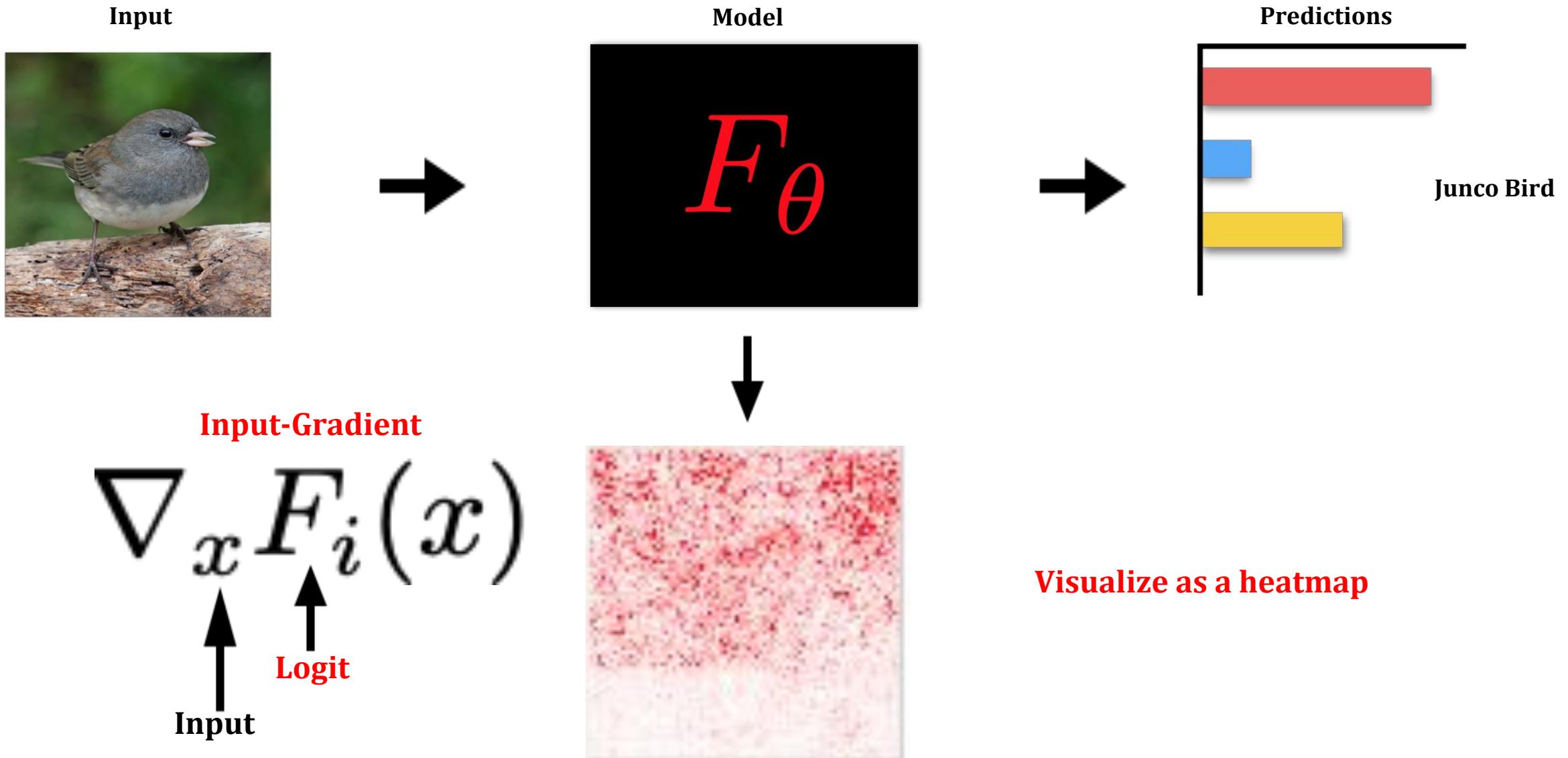
Modern DNN Setting



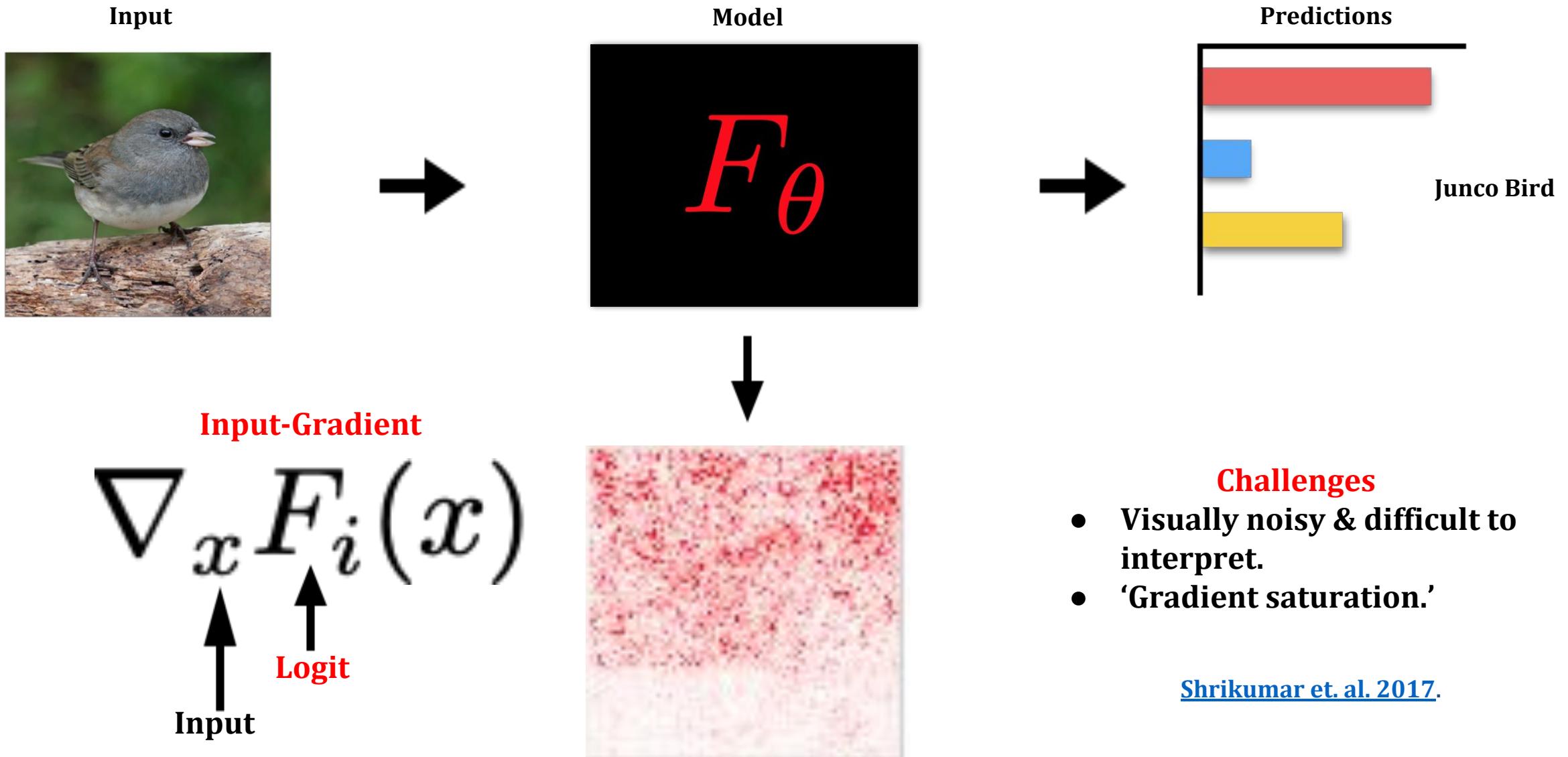
Input-Gradient



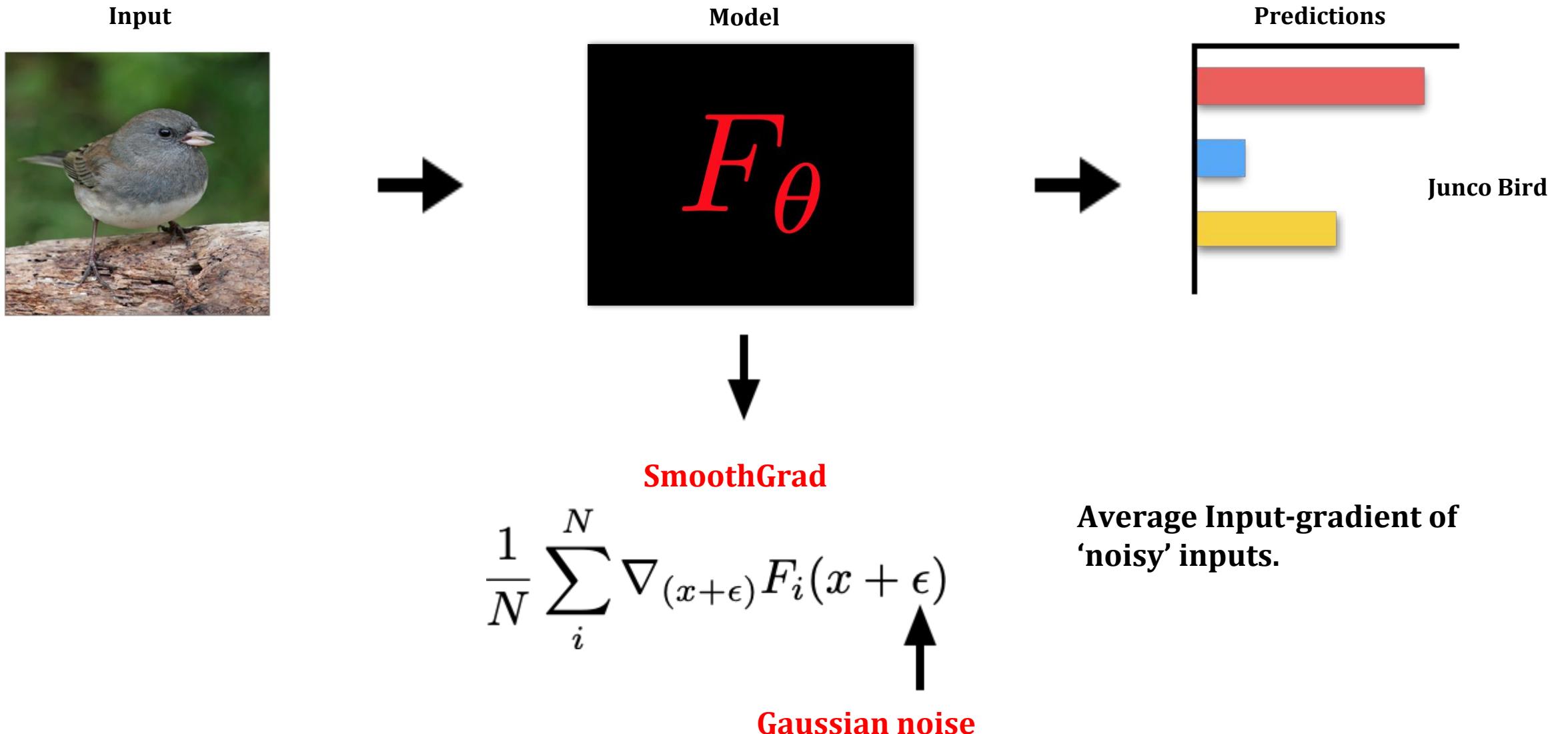
Input-Gradient



Input-Gradient



SmoothGrad



SmoothGrad

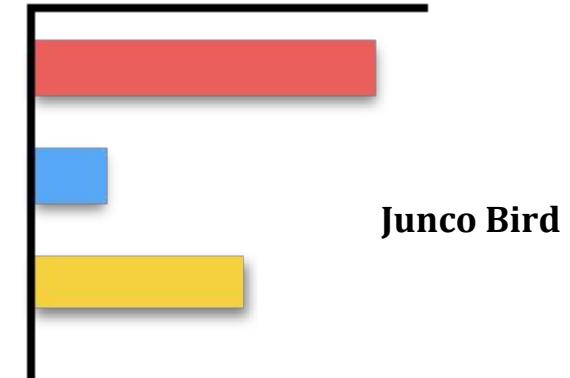
Input



Model



Predictions

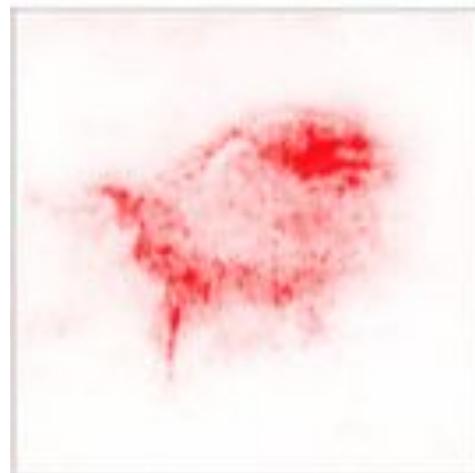


SmoothGrad

$$\frac{1}{N} \sum_i^N \nabla_{(x+\epsilon)} F_i(x + \epsilon)$$



Gaussian noise



Average Input-gradient of
'noisy' inputs.

Integrated Gradients

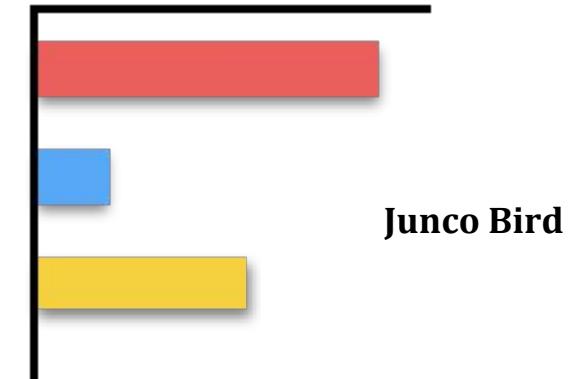
Input



Model



Predictions



$$(x - \tilde{x}) \times \int_{\alpha=0}^1 \frac{\partial F(\tilde{x} + \alpha \times (x - \tilde{x}))}{\partial x}$$

Baseline input

Path integral: 'sum' of interpolated gradients

Integrated Gradients

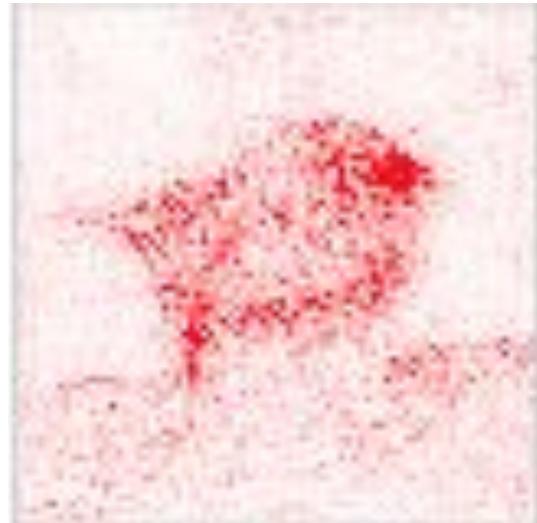
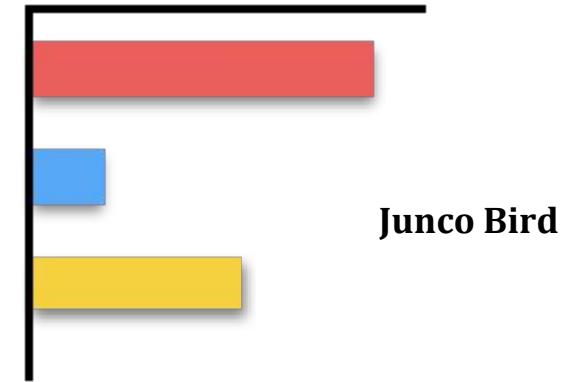
Input



Model



Predictions



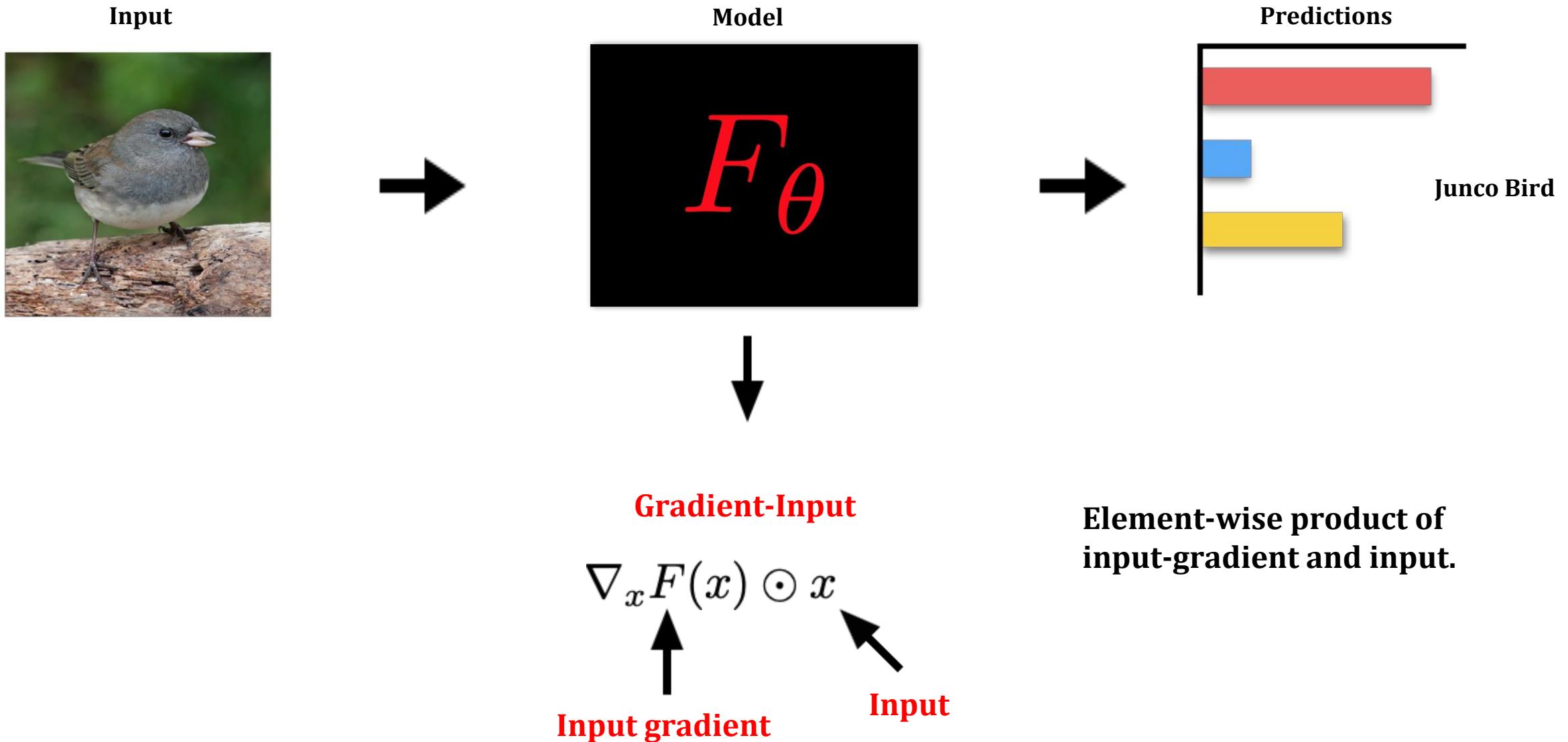
$$(x - \tilde{x}) \times \int_{\alpha=0}^1 \frac{\partial F(\tilde{x} + \alpha \times (x - \tilde{x}))}{\partial x}$$



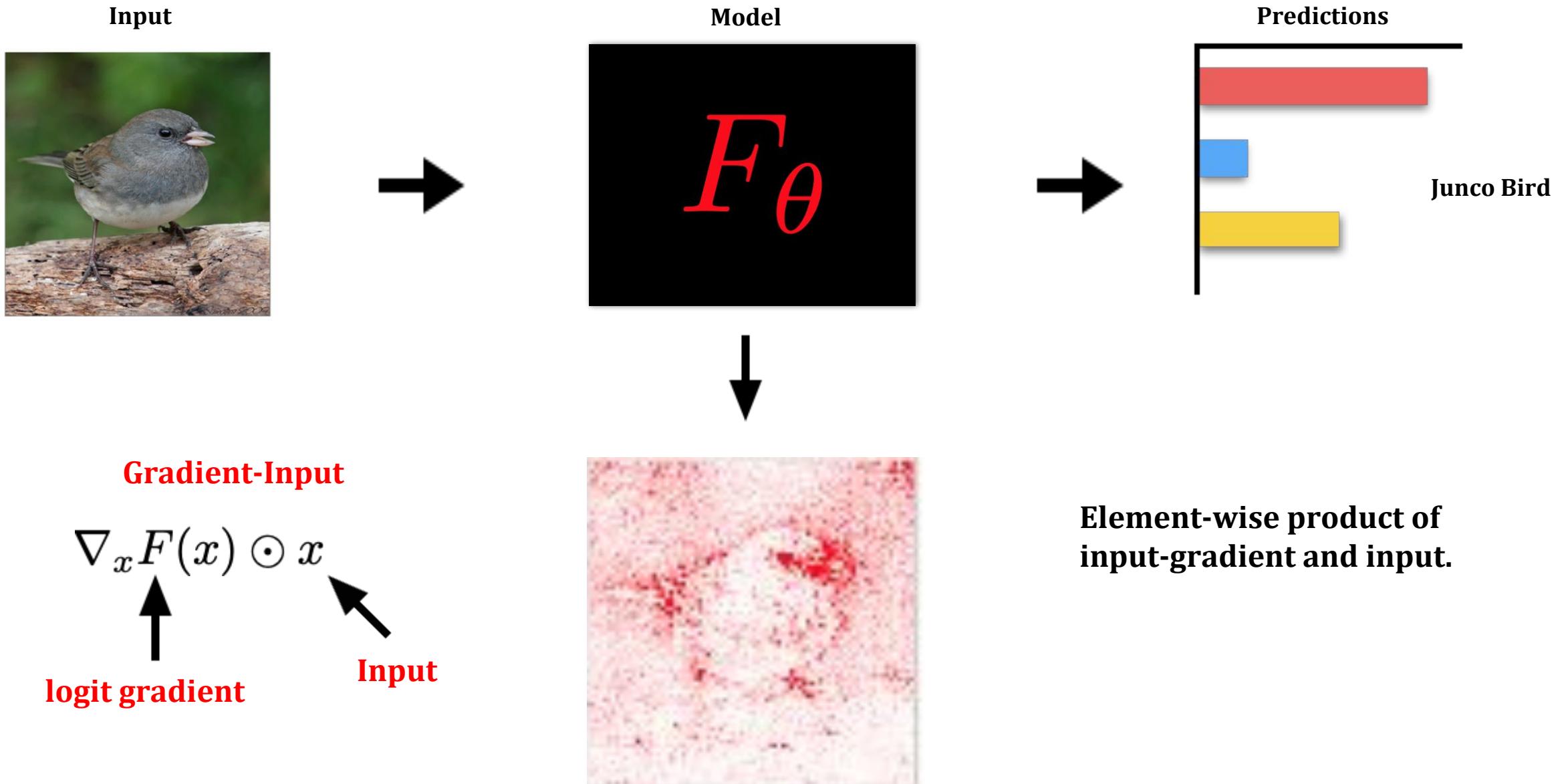
Baseline input

Path integral: 'sum' of interpolated gradients

Gradient-Input



Gradient-Input



‘Modified Backprop’ Approaches

Compute feature relevance by modifying the backpropagation.

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activation: $f_i^{l+1} = \text{relu}(f_i^l) = \max(f_i^l, 0)$

backpropagation: $R_i^l = (\textcolor{red}{f_i^l > 0}) \cdot R_i^{l+1}$, where $R_i^{l+1} = \frac{\partial f^{out}}{\partial f_i^{l+1}}$

‘Modified Backprop’ Approaches

Compute feature relevance by modifying the backpropagation.

activation: $f_i^{l+1} = \text{relu}(f_i^l) = \max(f_i^l, 0)$

backpropagation: $R_i^l = (f_i^l > 0) \cdot R_i^{l+1}$, where $R_i^{l+1} = \frac{\partial f^{out}}{\partial f_i^{l+1}}$

guided
backpropagation: $R_i^l = (f_i^l > 0) \cdot (R_i^{l+1} > 0) \cdot R_i^{l+1}$

Attribution: Guided BackProp

Input

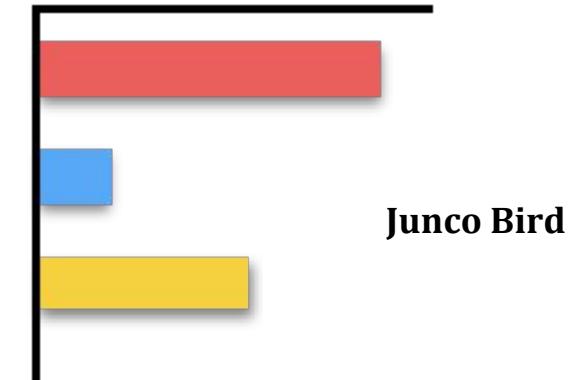


Model

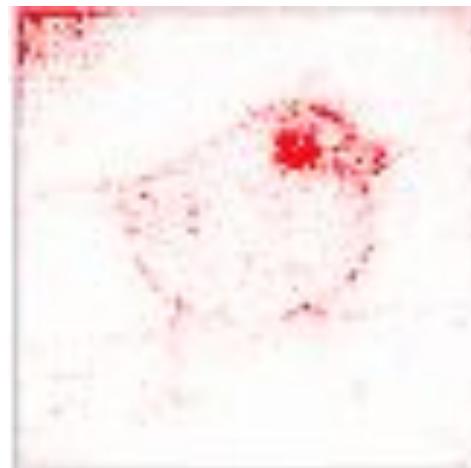
$$F_{\theta}$$



Predictions



Guided BackProp



Attribution: Guided BackProp

Input

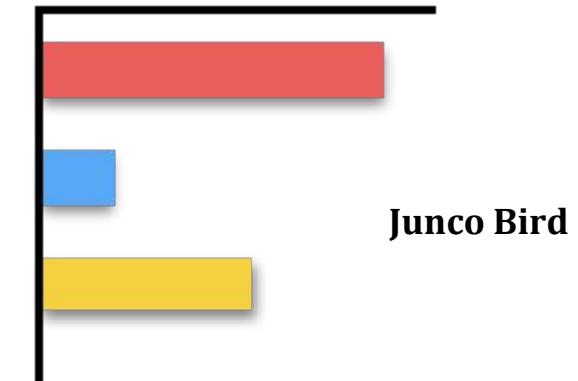


Model

$$F_{\theta}$$



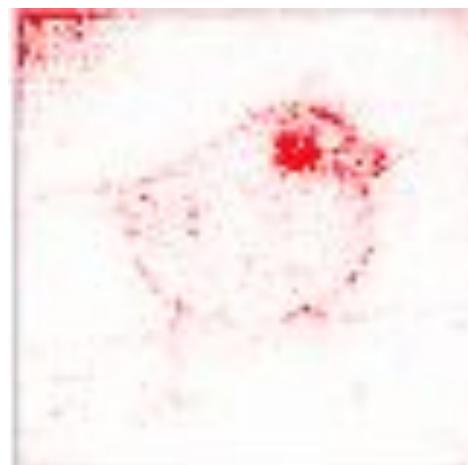
Predictions



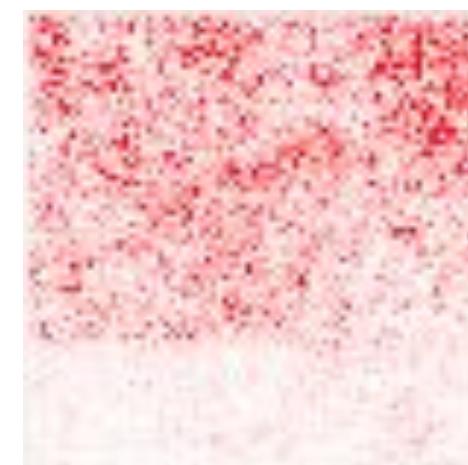
Junco Bird



Guided BackProp

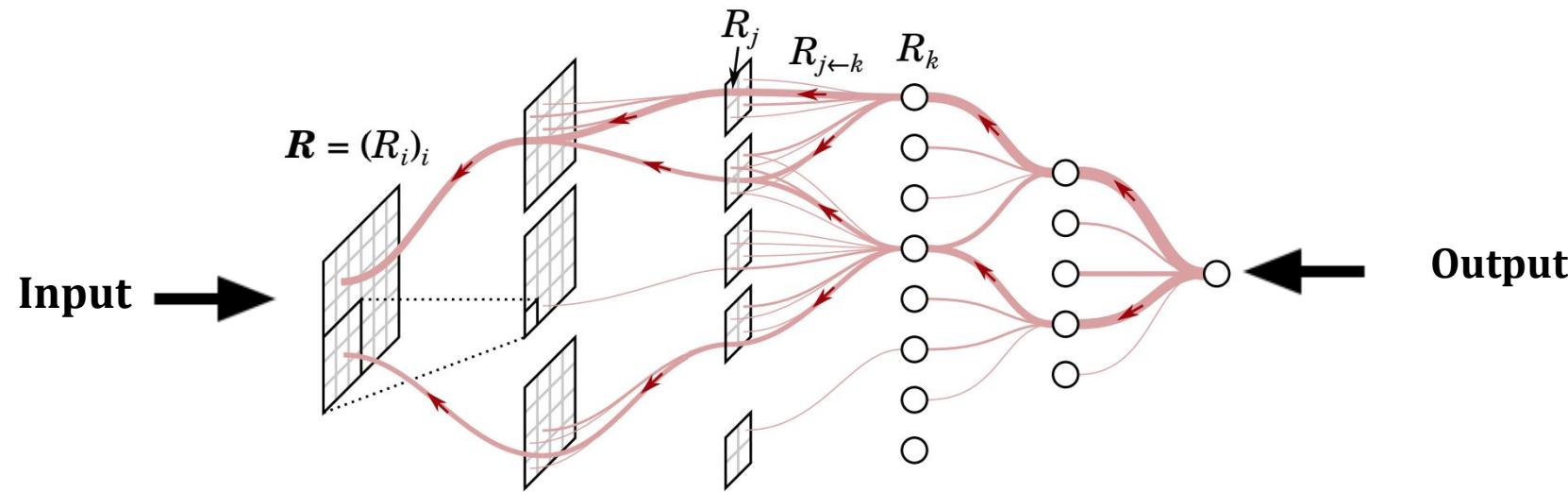


Input Gradient



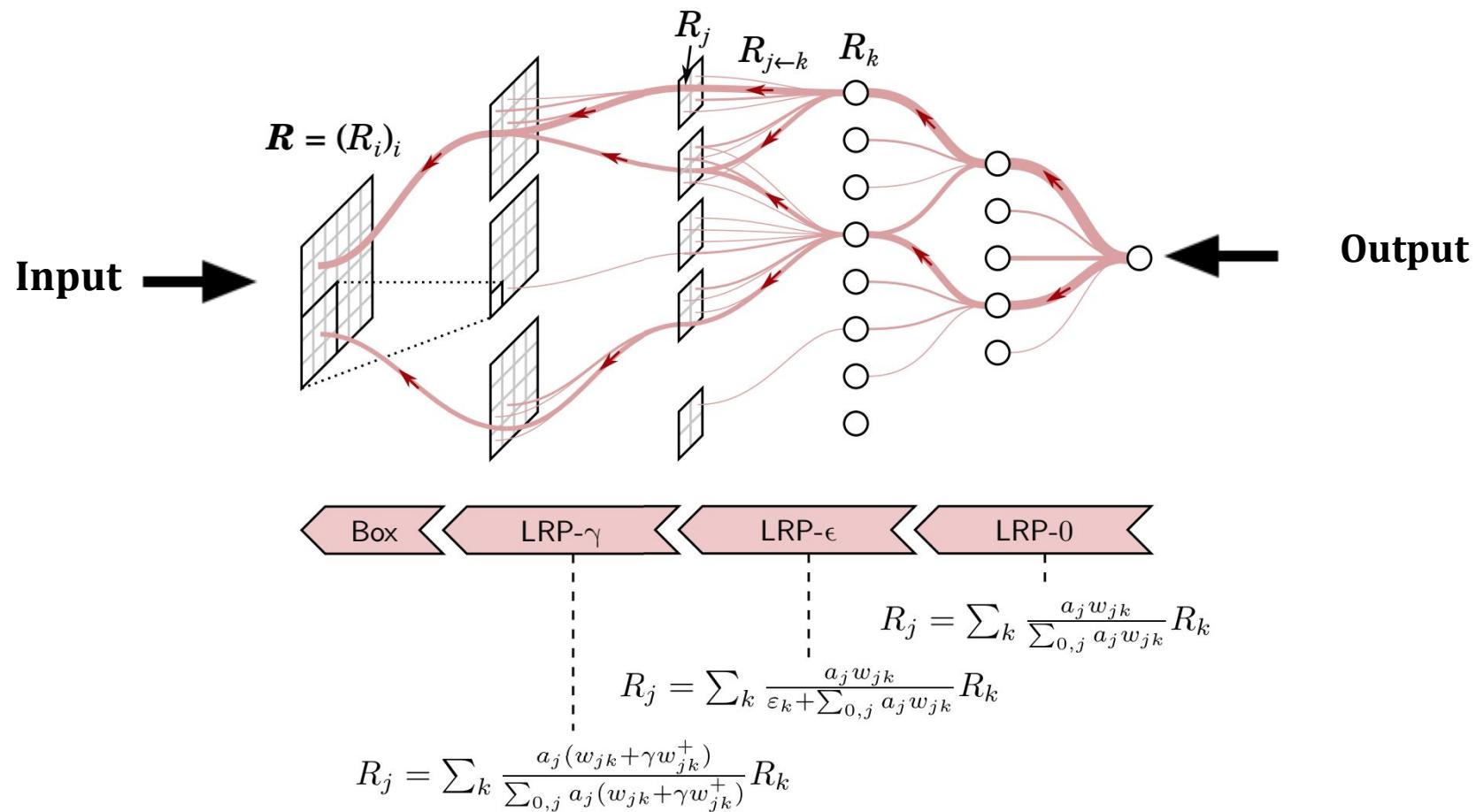
Layer Relevance Propagation (LRP)

Compute feature relevance iteratively and propagate. Different **propagation rules** can be specified.

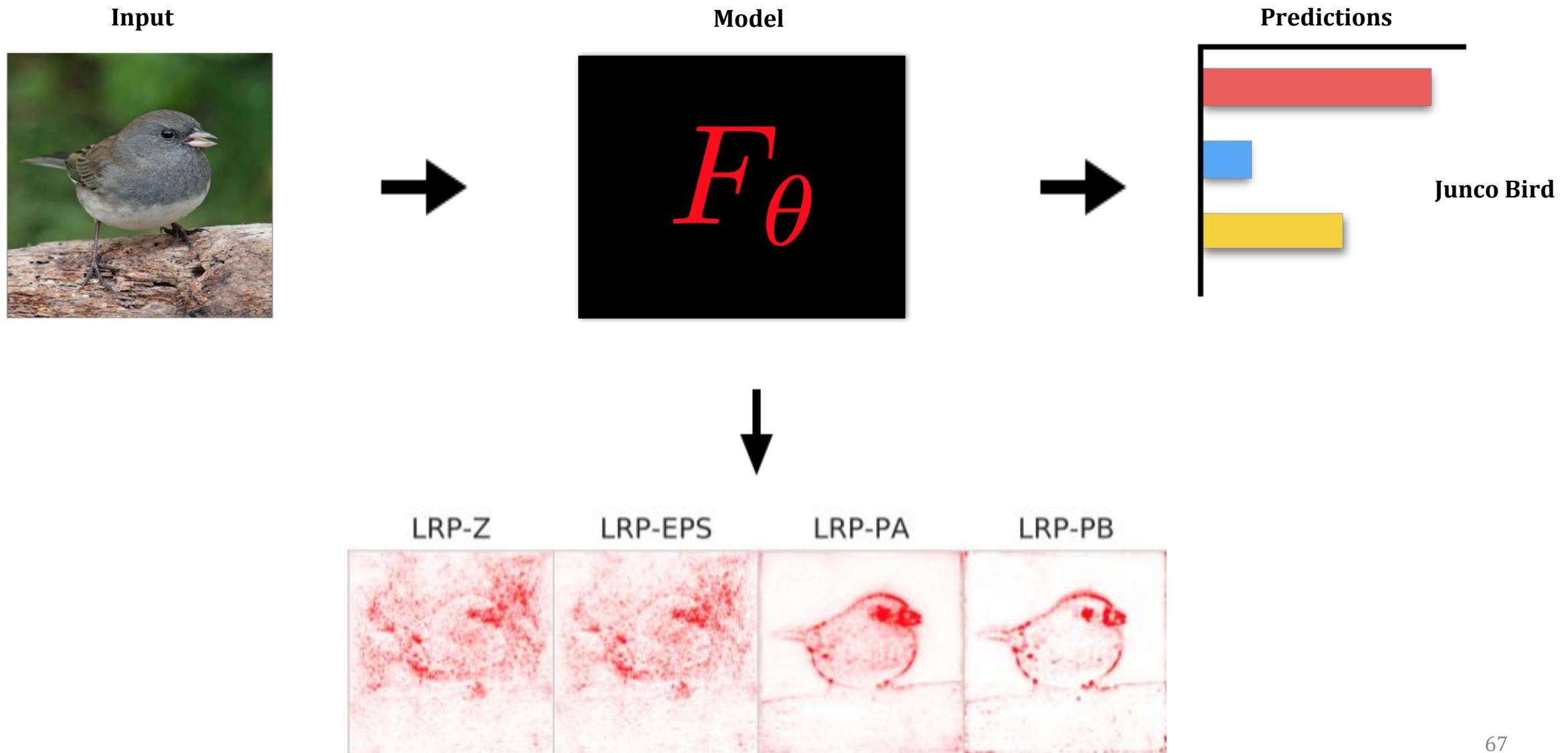


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Layer Relevance Propagation (LRP)



Recap

Input

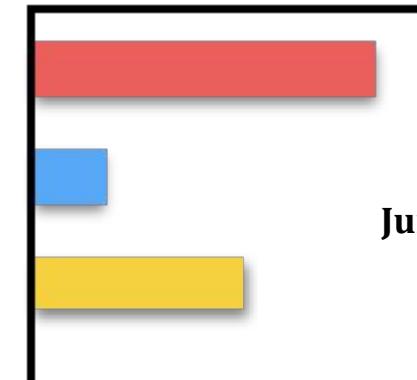


Model

$$F_{\theta}$$



Predictions



Junco Bird

Recap

Input

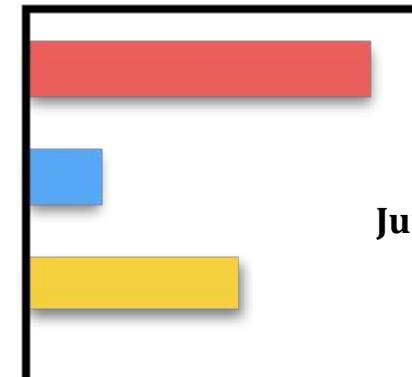


Model

$$F_{\theta}$$

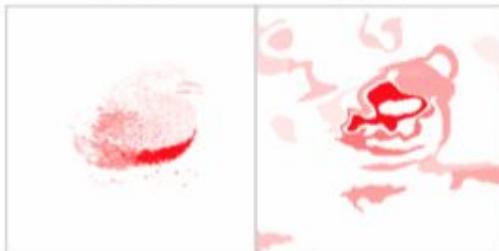


Predictions



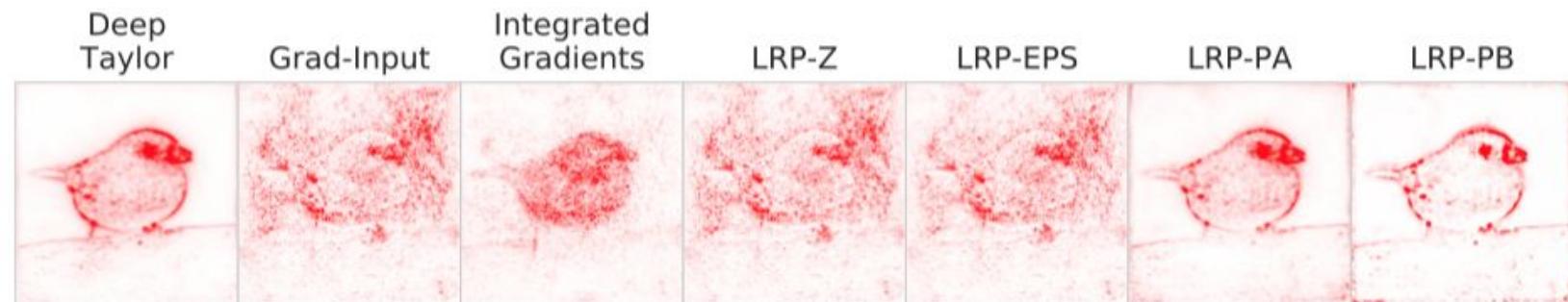
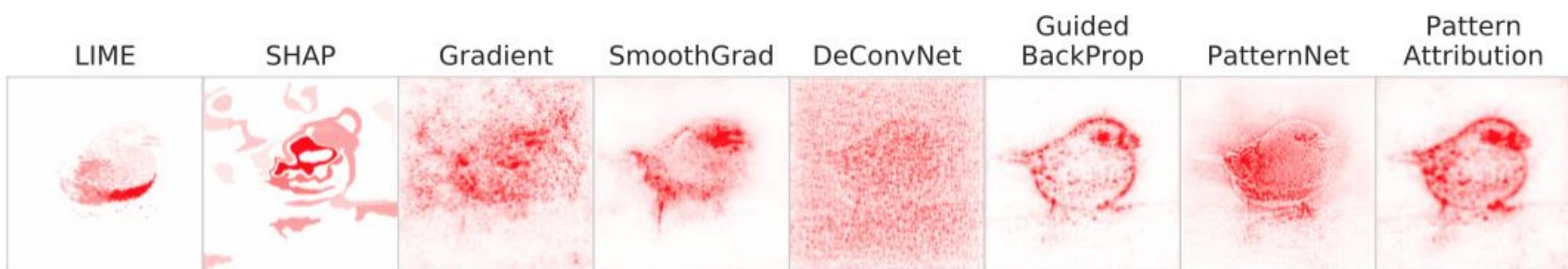
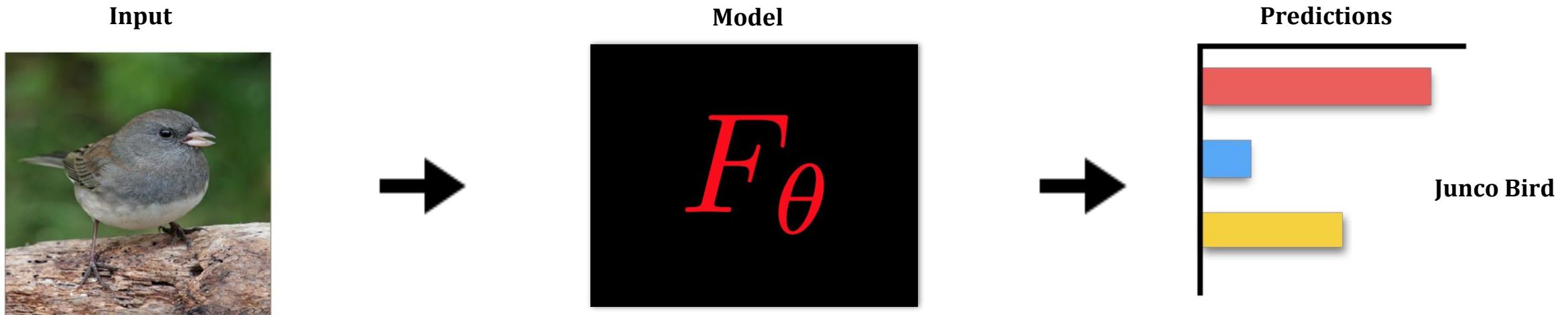
Junco Bird

LIME



SHAP

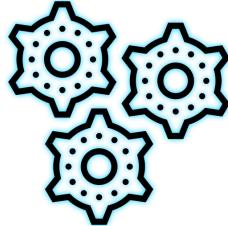
Recap



Additional Methods

- **Class Activation Mapping** (Zhou et. al. 2016).
- **Meaningful Perturbation** (Fong et. al. 2017).
- **RISE** (Petsuik et. al. 2018).
- **Extremal Perturbations** (Fong & Patrick 2019).
- **DeepLift** (Shrikumar et. al. 2018).
- **Expected Gradients** (Erion et. al. 2019)
- **Excitation Backprop** (Zhang et. al. 2016)
- **GradCAM** (Selvaraju et. al. 2016)
- **Guided GradCAM** (Selvaraju et. al. 2016)
- **Occlusion** (Zeiler et. al. 2014).
- **Prediction Difference Analysis** (Gu. et. al. 2019).
- **Internal Influence** (Leino et. al. 2018).

See for additional methods: [Samek & Montavon et. al. 2020](#)



Approaches for Post hoc Explainability

Local Explanations

- Feature Importances
- Rule Based
- Saliency Maps
- Prototypes/Example Based
- Counterfactuals

Global Explanations

- Collection of Local Explanations
- Representation Based
- Model Distillation
- Summaries of Counterfactuals

Prototype Approaches

Explain a model with synthetic or natural input ‘examples’.

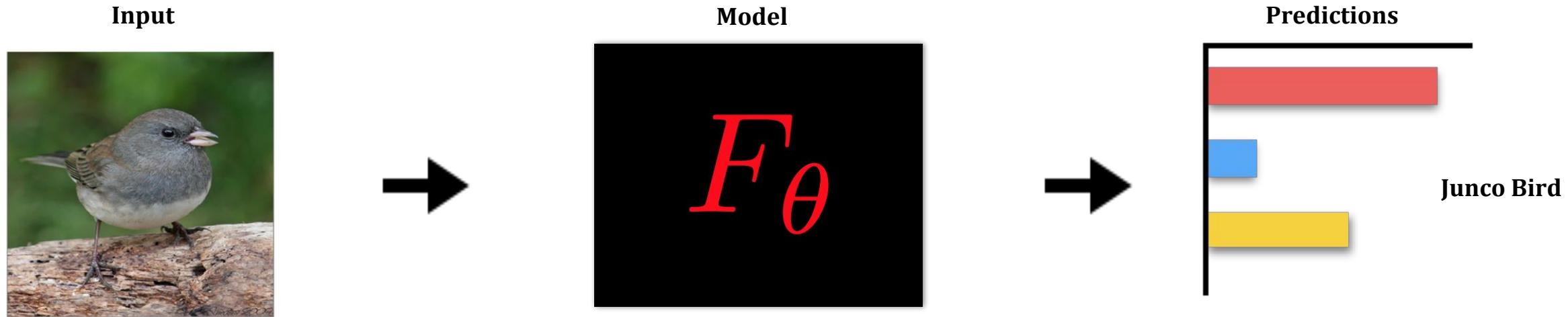
Prototype Approaches

Explain a model with synthetic or natural input ‘examples’.

Insights

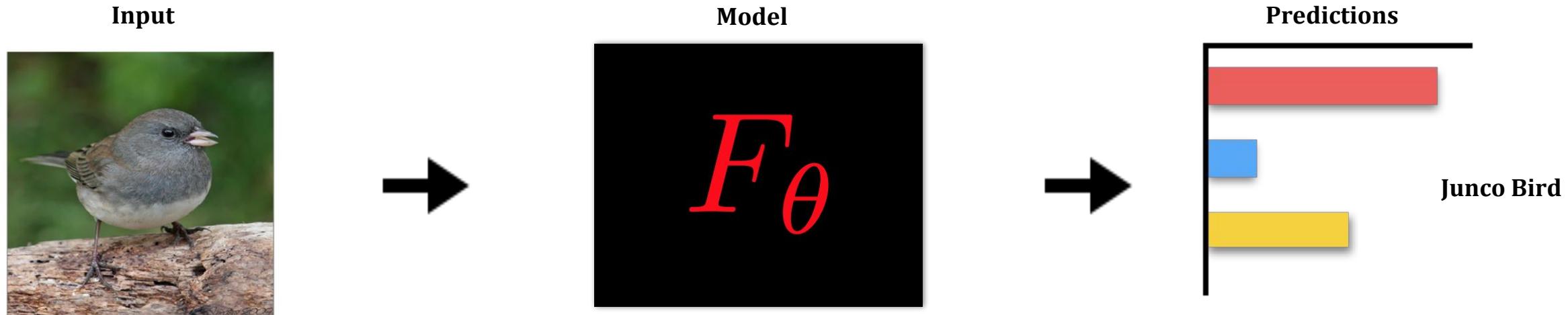
- What kind of input is the model **most likely to misclassify?**
- Which training samples are **mislabeled?**
- Which input **maximally activates** an intermediate neuron?

Training Point Ranking via Influence Functions



Which training data points have the most '*influence*' on the test loss?

Training Point Ranking via Influence Functions

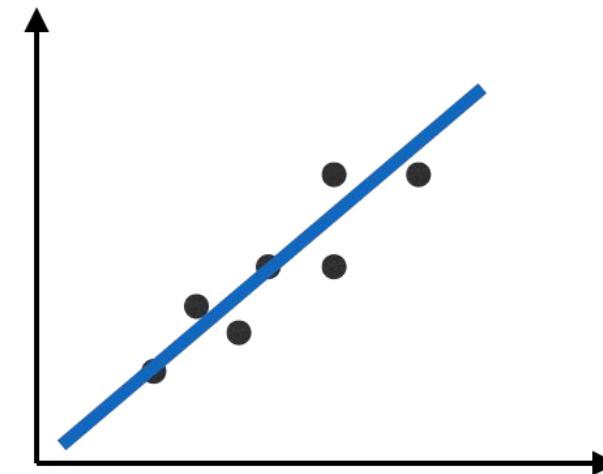
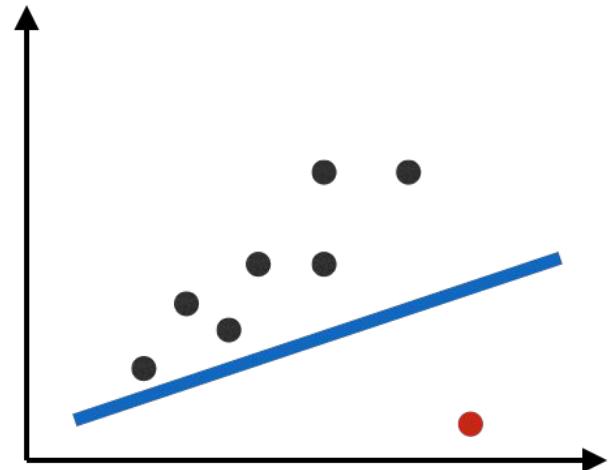


Which training data points have the most '*influence*' on the test loss?



Training Point Ranking via Influence Functions

Influence Function: classic tool used in robust statistics for assessing the effect of a sample on regression parameters ([Cook & Weisberg, 1980](#)).



Instead of refitting model for every data point, **Cook's distance** provides analytical alternative.

Training Point Ranking via Influence Functions

[Koh & Liang \(2017\)](#) extend the ‘Cook’s distance’ insight to modern machine learning setting.

$$z_i = (x_i, y_i) \in \mathcal{X} \times \mathcal{Y} \quad z_j = (x_j, y_j) \leftarrow \text{Training sample point} \quad z_{\text{test}}$$

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ERM Solution

$$\hat{\theta} := \arg \min_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^n \ell(z_i; \theta)$$

UpWeighted ERM Solution

$$\hat{\theta}_{\epsilon, z_j} := \arg \min_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^n \ell(z_i; \theta) + \epsilon \ell(z_j; \theta) \quad \epsilon = -\frac{1}{n}$$

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Influence of Training Point on Parameters

$$\mathcal{I}_{z_j} = \left. \frac{d\hat{\theta}_{\epsilon, z_j}}{d\epsilon} \right|_{\epsilon=0} = -H_{\hat{\theta}}^{-1} \nabla_{\theta} \ell(z_j, \hat{\theta})$$

Influence of Training Point on Test-Input’s loss

$$\mathcal{I}_{z_j, z_{\text{test}}, \text{loss}} = -\nabla_{\theta} \ell(z_{\text{test}}, \hat{\theta})^\top H_{\hat{\theta}}^{-1} \nabla_{\theta} \ell(z_j, \hat{\theta})$$

Training Point Ranking via Influence Functions

Applications:

- compute self-influence to identify mislabelled examples;
- diagnose possible domain mismatch;
- craft training-time poisoning examples.

Training Point Ranking: NLP Application

[Han et. al. \(2020\)](#) use influence-based training point ranking to study spurious training artifacts in NLP setting.

Test input

P: The manager was encouraged by the secretary. *H*: The secretary encouraged the manager. {entail}

Most supporting training examples

P: Because you're having fun. *H*: Because you're having fun. [entail]

P: I don't know if I was in heaven or hell, said Lillian Carter, the president's mother, after a visit. *H*: The president's mother visited. [entail]

P: Inverse price caps. *H*: Inward caps on price. [entail]

P: Do it now, think 'bout it later. *H*: Don't think about it now, just do it. [entail]

Most opposing training examples

P: H'm, yes, that might be, said John. *H*: [non-entail] Yes, that might be the case, said John.

P: This coalition of public and private entities undertakes initiatives aimed at raising public awareness about personal finance and retirement planning. *H*: Personal finance and retirement planning are initiatives aimed at raising public awareness. [non-entail]

Challenges and Other Approaches

Influence function Challenges:

1. **scalability**: computing hessian-vector products can be tedious in practice.
2. **non-convexity**: possibly loose approximation for deeper networks ([Basu et. al. 2020](#)).

Challenges and Other Approaches

Influence function Challenges:

1. **scalability**: computing hessian-vector products can be tedious in practice.
2. **non-convexity**: possibly loose approximation for ‘deeper’ networks ([Basu et. al. 2020](#)).

Alternatives:

- **Representer Points** ([Yeh et. al. 2018](#)).
- **TracIn** ([Pruthi et. al.](#) appearing at NeuRIPs 2020).

‘Activation Maximization’

These approaches identify examples, synthetic or natural, that **strongly activate a function (neuron) of interest.**

‘Activation Maximization’

These approaches identify examples, synthetic or natural, that **strongly activate a function (neuron) of interest.**

Implementation Flavors:

- Search for **natural examples within a specified set** (training or validation corpus) that strongly activate a neuron of interest;
- **Synthesize examples**, typically via gradient descent, that strongly activate a neuron of interest.

Feature Visualization

Dataset Examples show us what neurons respond to in practice



Optimization isolates the causes of behavior from mere correlations. A neuron may not be detecting what you initially thought.

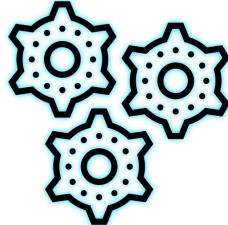


Baseball—or stripes?
mixed4a, Unit 6

Animal faces—or snouts?
mixed4a, Unit 240

Clouds—or fluffiness?
mixed4a, Unit 453

Buildings—or sky?
mixed4a, Unit 492



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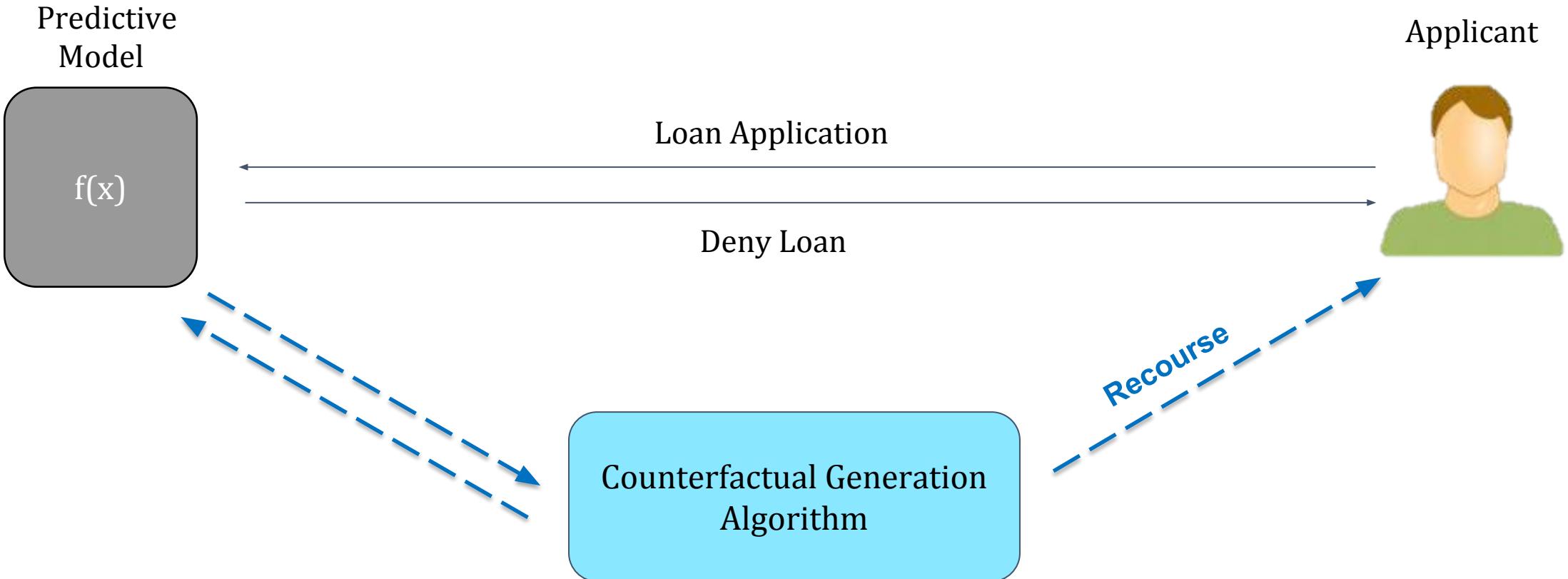
Counterfactual Explanations

As ML models increasingly deployed to make high-stakes decisions (e.g., loan applications), it becomes important to provide **recourse** to affected individuals.

Counterfactual Explanations

*What features need to be changed and by how much to flip a model's prediction ?
(i.e., to reverse an unfavorable outcome).*

Counterfactual Explanations

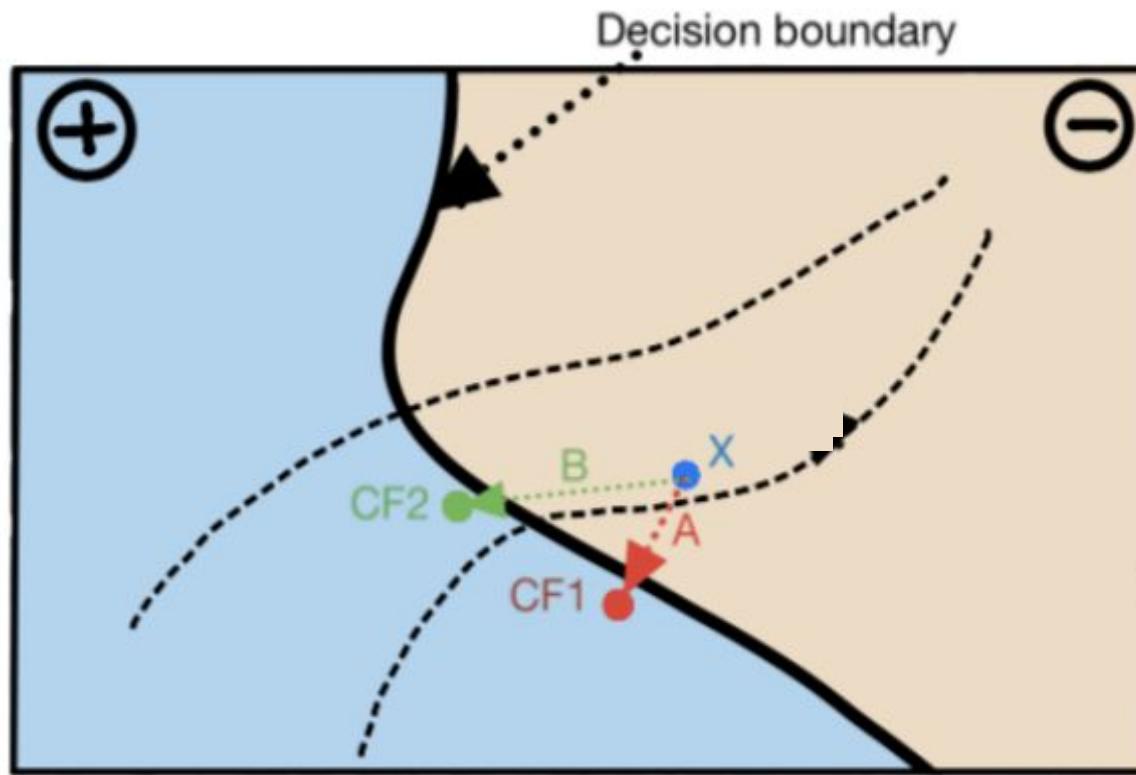


Recourse: Increase your salary by 50K & pay your credit card bills on time for next 3 months

Counterfactual Explanations

- Important to provide “recourse” to affected individuals (GDPR)
- Counterfactual Explanations:
 - *What features need to be changed and by how much to flip a model's prediction (i.e., to reverse an unfavorable outcome).*

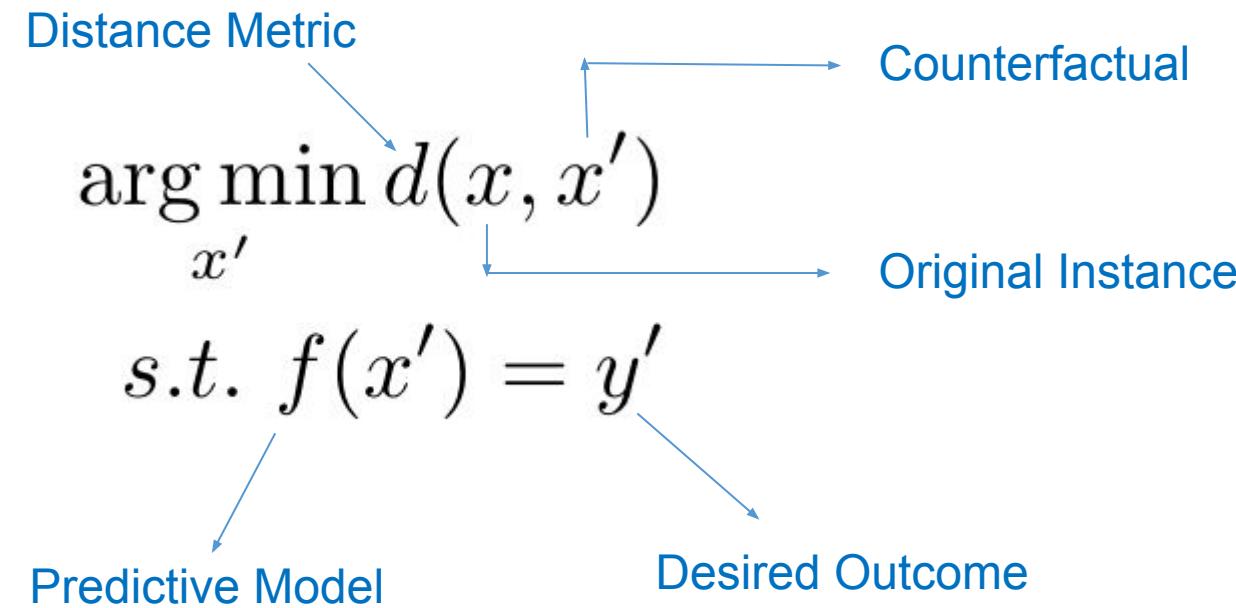
Generating Counterfactual Explanations: Intuition



Proposed solutions differ on:

1. How to choose among candidate counterfactuals?
2. How much access is needed to the underlying predictive model?

Take 1: Minimum Distance Counterfactuals



Choice of **distance metric** dictates what kinds of counterfactuals are chosen.

Wachter et. al. use normalized Manhattan distance.

Take 1: Minimum Distance Counterfactuals

$$\begin{aligned} & \arg \min_{x'} d(x, x') \\ & \text{s.t. } f(x') = y' \end{aligned} \quad \longrightarrow \quad \arg \min_{x'} \lambda (f(x') - y')^2 + d(x, x')$$

Wachter et. al. solve a differentiable, unconstrained version of the objective using ADAM optimization algorithm with random restarts.

This method **requires access to gradients** of the underlying predictive model.

Take 1: Minimum Distance Counterfactuals

Person 1: If your LSAT was 34.0, you would have an average predicted score (0).

Person 2: If your LSAT was 32.4, you would have an average predicted score (0).

Person 3: If your LSAT was 33.5, and you were 'white', you would have an average predicted score (0).

Person 4: If your LSAT was 35.8, and you were 'white', you would have an average predicted score (0).

Person 5: If your LSAT was 34.9, you would have an average predicted score (0).

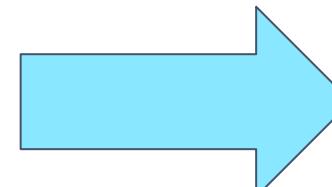


Not feasible to act upon these features!

Take 2: Feasible and Least Cost Counterfactuals

$$\arg \min_{x'} d(x, x')$$

$$s.t. f(x') = y'$$



$$\arg \min_{x' \in \mathcal{A}} \text{cost}(x, x')$$

$$s.t. f(x') = y'$$

- \mathcal{A} is the set of **feasible** counterfactuals (input by end user)
 - E.g., changes to race, gender are not feasible
- **Cost** is modeled as **total log-percentile shift**
 - Changes become **harder** when starting off from a **higher percentile value**

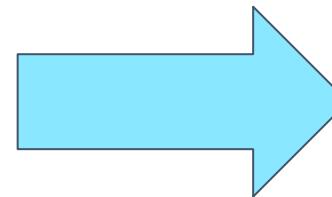
Take 2: Feasible and Least Cost Counterfactuals

$$\begin{array}{c} \arg \min_{x'} d(x, x') \\ s.t. f(x') = y' \end{array} \quad \xrightarrow{\hspace{1cm}} \quad \begin{array}{c} \arg \min_{x' \in \mathcal{A}} cost(x, x') \\ s.t. f(x') = y' \end{array}$$

- Ustun et. al. **only** consider the case where the model is a **linear classifier**
 - Objective formulated as an IP and optimized using CPLEX
- Requires ***complete access*** to the linear classifier i.e., weight vector

Take 2: Feasible and Least Cost Counterfactuals

$$\begin{aligned} \arg \min_{x'} d(x, x') \\ s.t. \quad f(x') = y' \end{aligned}$$



$$\begin{aligned} \arg \min_{x' \in \mathcal{A}} cost(x, x') \\ s.t. \quad f(x') = y' \end{aligned}$$

Question: What if we have a black box or a non-linear classifier?

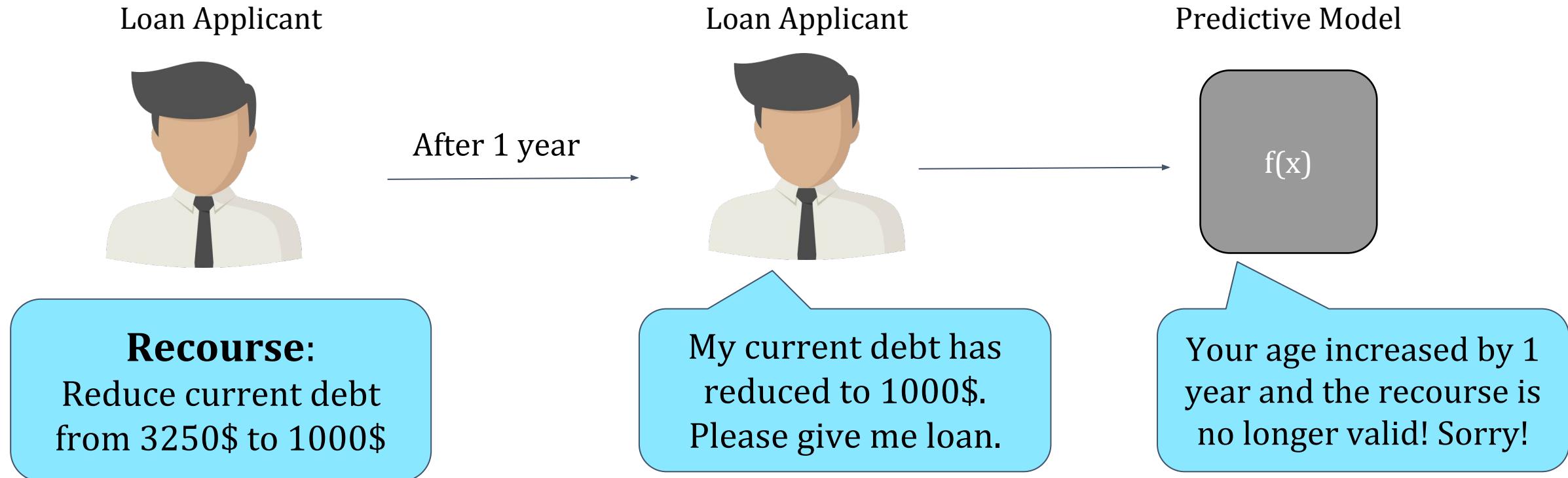
Answer: generate a local linear model approximation (e.g., using LIME) and then apply Ustun et. al.'s framework

Take 2: Feasible and Least Cost Counterfactuals

FEATURES TO CHANGE	CURRENT VALUES	→	REQUIRED VALUES
<i>n_credit_cards</i>	5	→	3
<i>current_debt</i>	\$3,250	→	\$1,000
<i>has_savings_account</i>	FALSE	→	TRUE
<i>has_retirement_account</i>	FALSE	→	TRUE

Changing one feature without affecting another might not be possible!

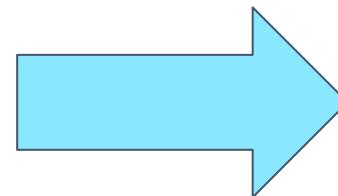
Take 3: Causally Feasible Counterfactuals



Important to account for *feature interactions* when generating counterfactuals!
But how?!

Take 3: Causally Feasible Counterfactuals

$$\begin{aligned} & \arg \min_{x'} d(x, x') \\ & s.t. f(x') = y' \end{aligned}$$



$$\begin{aligned} & \arg \min_{x'} d_{causal}(x, x') \\ & s.t. f(x') = y' \end{aligned}$$

Leverage Structural Causal Model (SCM) to define this new distance metric

Take 3: Causally Feasible Counterfactuals

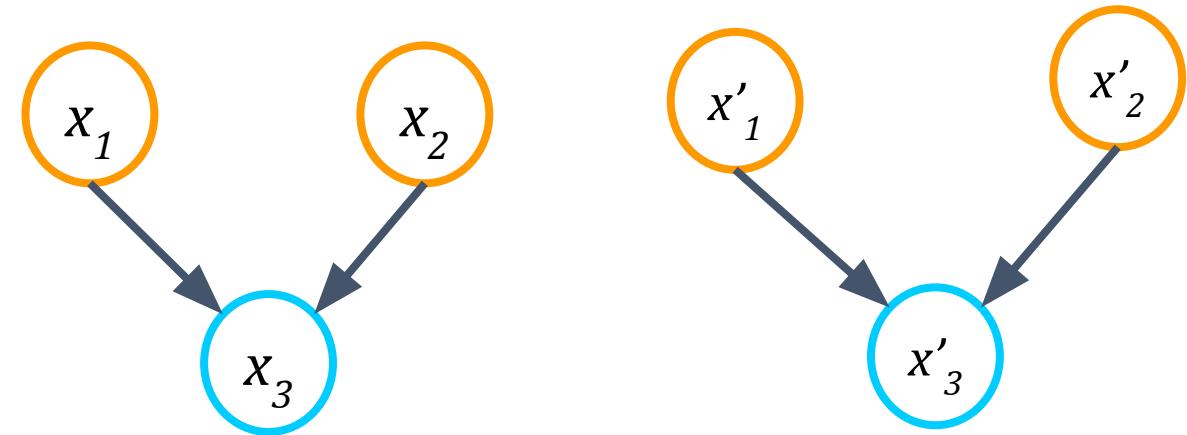
$$d_{causal}(x, x') =$$

$$\sum_{u \in U} \underbrace{d(x_u, x'_u)}_{\text{Standard L1/L2 distance for each variable } u \text{ with no parents}} +$$

Standard L1/L2 distance for each variable u with no parents

$$\sum_{v \in V} \underbrace{d(x_v, \mathbb{E}[x'_v | x'_{v_{p1}}, x'_{v_{p2}}, \dots x'_{v_{pM}}])}_{\text{For variables } v \text{ with parents, compute L1/L2 distance between value of } v \text{ for original instance and expected value of } v \text{ given its parents for counterfactual}}$$

For variables v with parents, compute L1/L2 distance between value of v for original instance and *expected value of v* given its parents for counterfactual



Original
Instance

Counterfactual

U is set of nodes without parents in the graph;
V is set of nodes with parents in the graph

Take 3: Causally Feasible Counterfactuals

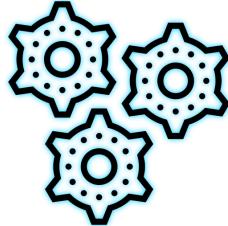
- Requires knowledge of full causal graph
 - *Empirically*, partial knowledge also seems to work fine
 - Learn about feasibility constraints/partial causal graph from user inputs
- Solving the objective: Leverage a Variational Autoencoder (VAE)
 - *requires access to gradients* of the underlying predictive model.

Other Takes on Feasible Counterfactuals

- **Data Manifold Closeness:** Generated counterfactual should be “close to” the original data distribution.
- **Sparsity:** Ideal to change small number of features in the counterfactual

Other Takes on Feasible Counterfactuals

- **Data Manifold Closeness:** Generated counterfactual should be “close to” the original data distribution.
 - Include term to minimize the distance (e.g., averaged Euclidean distance) between counterfactual and all original data instances
- **Sparsity:** Ideal to change small number of features in the counterfactual
 - Include term to minimize the total number of features being changed to obtain desired outcome (e.g., L0/L1 norm)



Approaches for Post hoc Explainability

Local Explanations

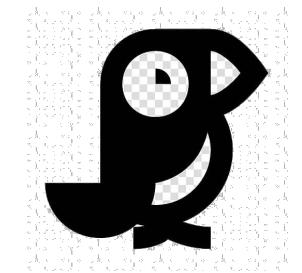
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Global Explanations

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Global Explanations

- Explain the **complete behavior** of a given (black box) **model**
 - Provide a *bird's eye view* of model behavior
- Help **detect *big picture* model biases** persistent across larger subgroups of the population
 - Impractical to manually inspect local explanations of several instances to ascertain big picture biases!
- Global explanations are **complementary** to local explanations



Local vs. Global Explanations

Explain individual predictions

Help unearth biases in the *local neighborhood* of a given instance

Help vet if individual predictions are being made for the right reasons

Explain complete behavior of the model

Help shed light on *big picture biases* affecting larger subgroups of the population

Help vet if the model, at a high level, is suitable for deployment

Local vs. Global Explanations

Explain individual predictions

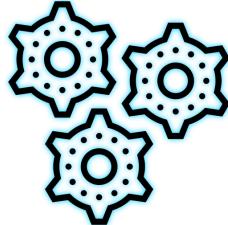
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Global Explanation as a Collection of Local Explanations

How to generate a global explanation of a (black box) model?

- Generate a local explanation for every instance in the data using one of the approaches discussed earlier
- Pick a **subset of k local explanations** to constitute the **global explanation**

What local explanation technique to use?

How to choose the subset of k local explanations?

Global Explanations from Local Feature Importances: SP-LIME

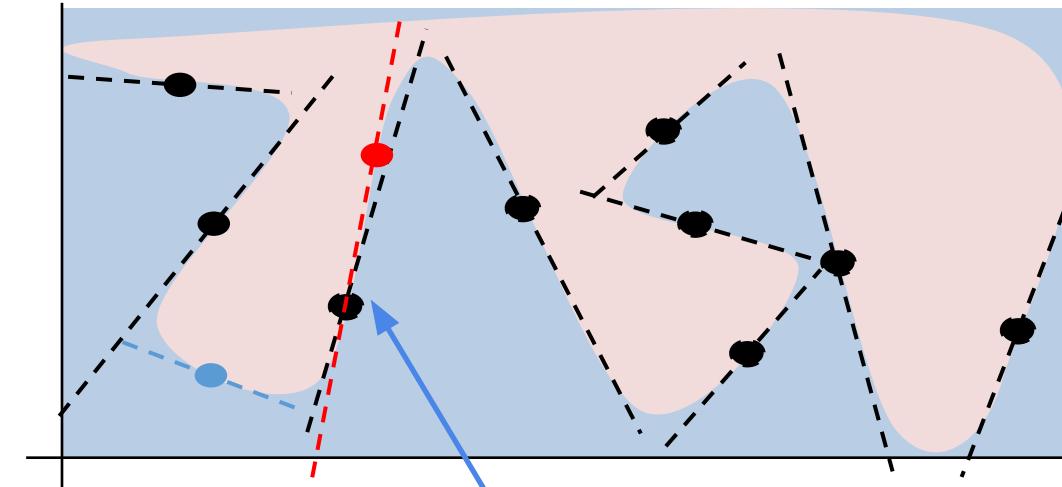
LIME explains a single prediction
local behavior for a single instance

Can't examine all explanations
Instead pick k explanations to show to the user

Representative
Should summarize the
model's global behavior

Diverse
Should not be redundant in
their descriptions

SP-LIME uses submodular optimization
and *greedily* picks k explanations

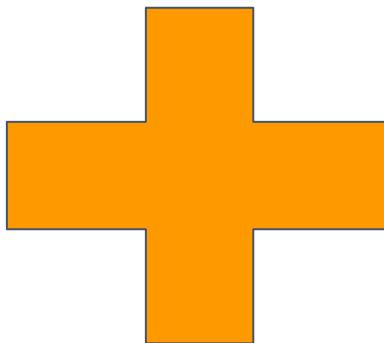


Single explanation

Model Agnostic

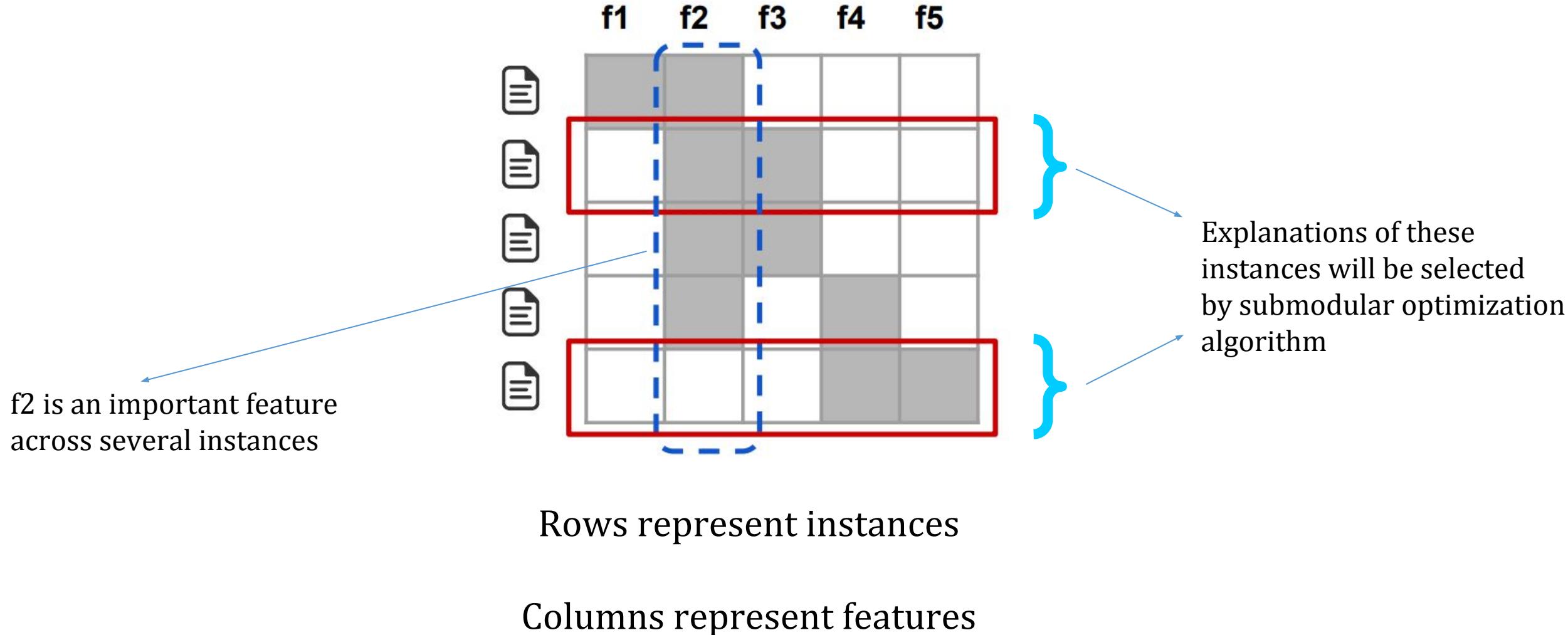
Picking k Explanations: Intuition

Aggregate
Feature Importances
across all instances



“Coverage” of
Features

Global Explanations from Local Feature Importances: SP-LIME



Global Explanations from Local Rule Sets: SP-Anchor

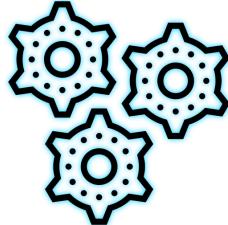
Model Agnostic

Use the same approach as above with Anchors algorithm (instead of LIME) which produces local rule sets as explanations.

Global Explanations from Local Rule Sets: SP-Anchor

- Use Anchors algorithm discussed earlier to obtain local rule sets for every instance in the data
- Use the same procedure to *greedily select a subset of k local rule sets* to correspond to the global explanation

Model Agnostic



Approaches for Post hoc Explainability

Local Explanations

- Feature Importances
- Rule Based
- Saliency Maps
- Prototypes/Example Based
- Counterfactuals

Global Explanations

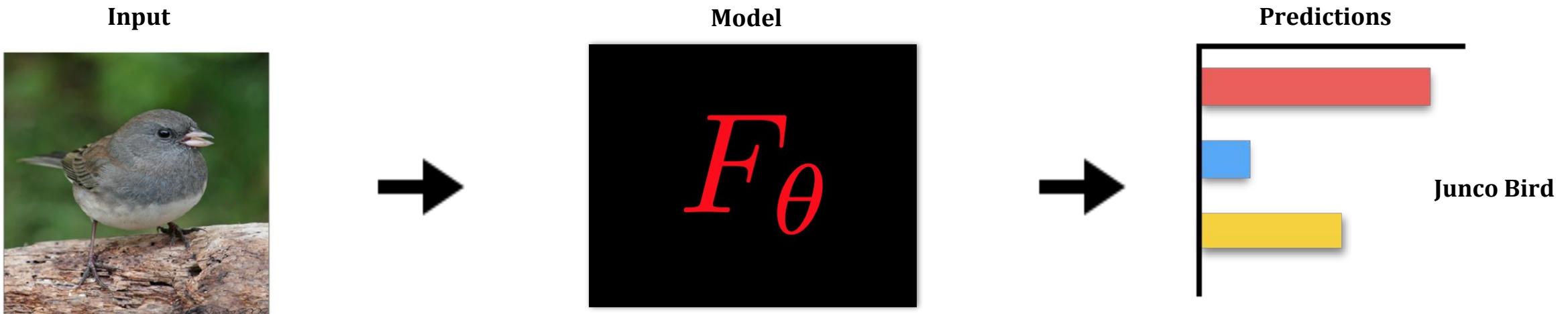
- Collection of Local Explanations
- Representation Based
- Model Distillation
- Summaries of Counterfactuals

Representation Based Approaches

- Derive model understanding by analyzing intermediate representations of a DNN.
- Determine model's reliance on 'concepts' that are semantically meaningful to humans.

Representation Based Approaches

- Derive model understanding by analyzing intermediate representations of a DNN.
- Determine model's reliance on 'concepts' that are semantically meaningful to humans.



Does the model rely on the '**green background**'?

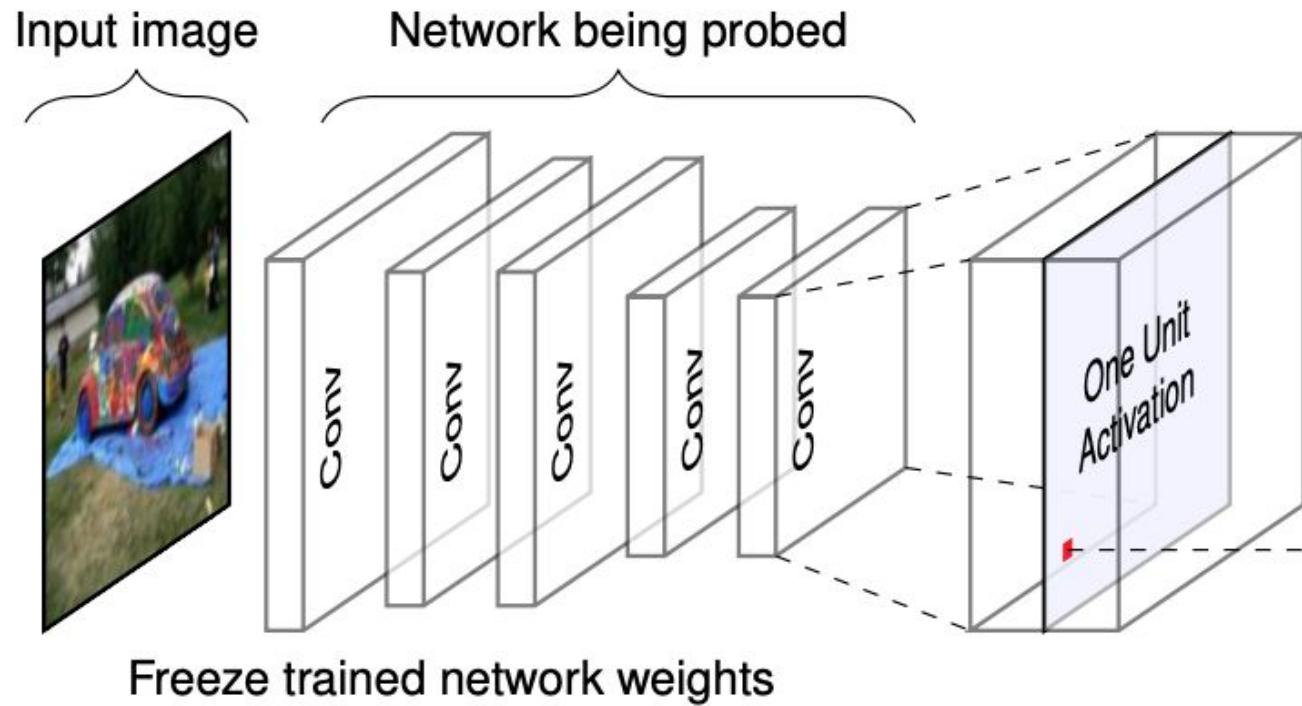
Network Dissection

Input image



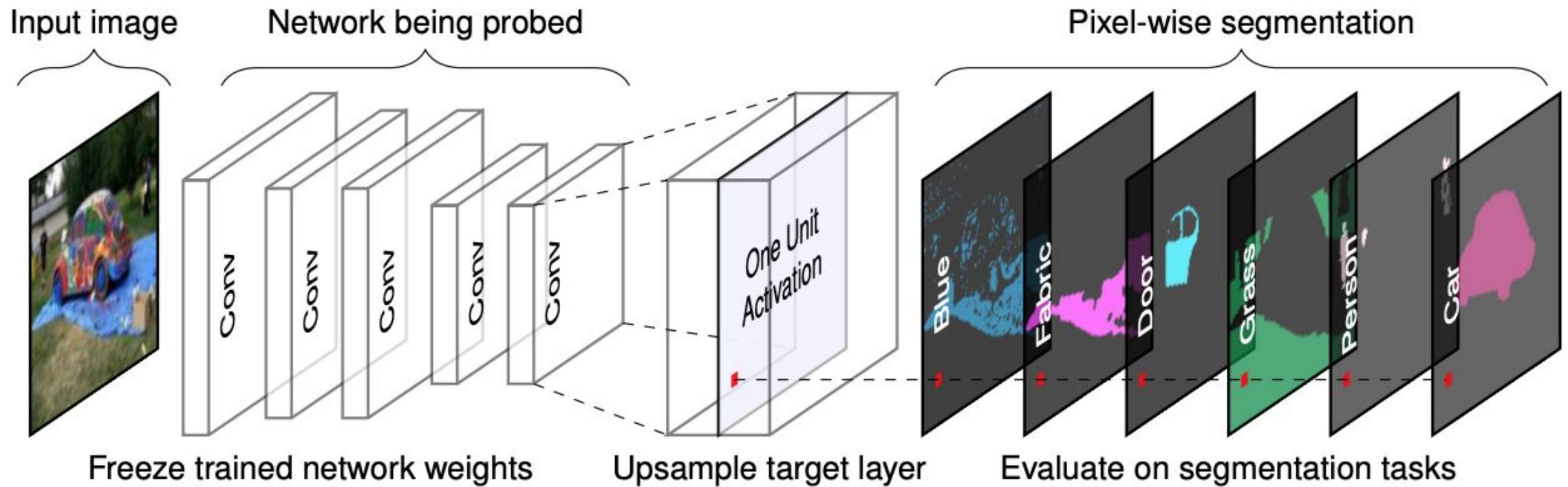
1. Identify a broad set of human-labeled visual concepts.

Network Dissection



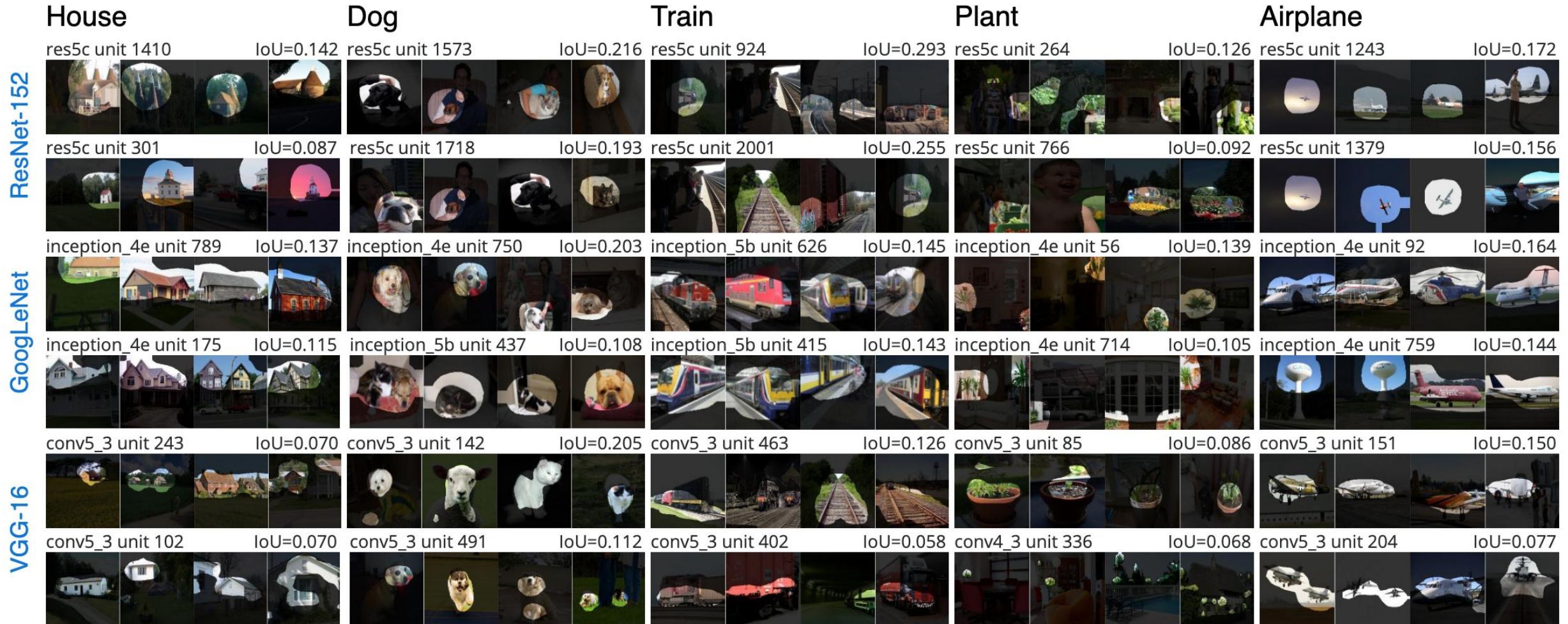
1. Identify a broad set of human-labeled visual concepts.
2. Gather the response of hidden variables (convolutional filters) to known concepts.

Network Dissection



1. Identify a broad set of human-labeled visual concepts.
2. Gather the response of hidden variables (convolutional filters) to known concepts.
3. Quantify alignment of hidden variable-concept pairs

Network Dissection



Compositional Extension

Natural Language Inference

Unit 870 (gender-sensitive)

((NOT hyp:man) AND pre:man) OR hyp:eating
AND (NOT pre:woman)) OR hyp:dancing
IoU 0.123 W entail -0.046 W neutral -0.021 W contra 0.040

Pre A guy pointing at a giant blackberry.

Hyp A woman tearing down a giant display.

Act 29.31 True **contra** Pred **contra**

Pre A man in a hat is working with...flowers.

Hyp Women are working with flowers.

Act 27.64 True **contra** Pred **contra**

Unit 99 (high overlap)

((NOT hyp:JJ) AND overlap-75% AND (NOT
pre:people)) OR pre:basket OR pre:tv
IoU 0.118 W entail 0.043 W neutral -0.029 W contra -0.021

Pre A woman in a light blue jacket is riding a bike.

Hyp A women in a jacket riding a bike.

Act 19.13 True **entail** Pred **entail**

Pre A girl in a pumpkin dress sitting at a table.

Hyp There is a girl in a pumpkin dress sitting at a table.

Act 17.84 True **entail** Pred **entail**

Vision

Unit 192 skyscraper OR lighthouse OR water tower
IoU 0.06

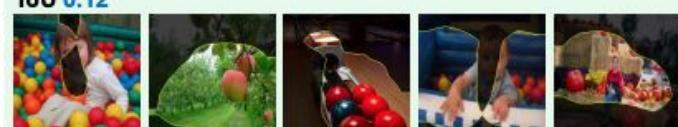


Unit 310 sink OR bathtub OR toilet
IoU 0.16



(a) abstraction (lexical and perceptual)

Unit 321 ball pit OR orchard OR bounce game
IoU 0.12



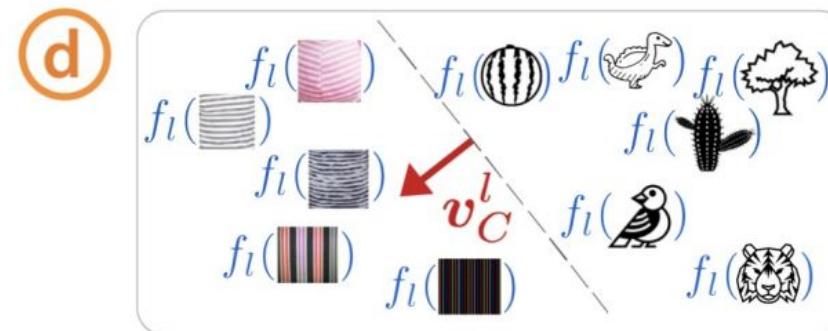
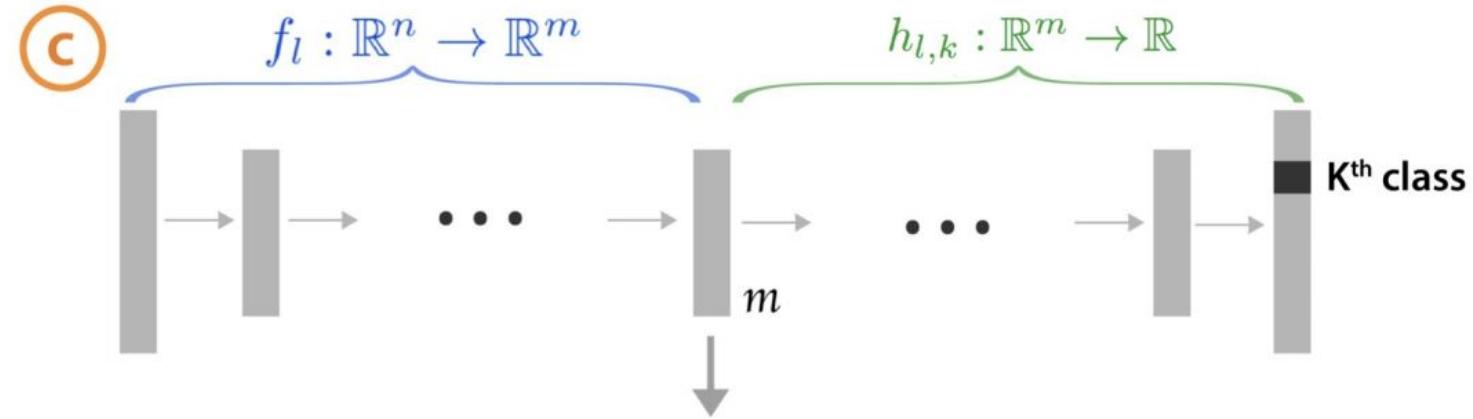
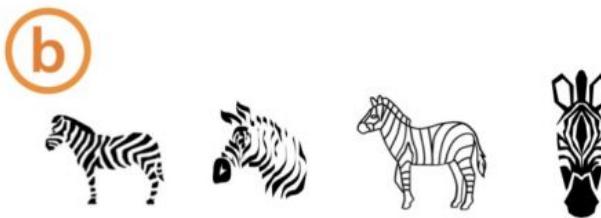
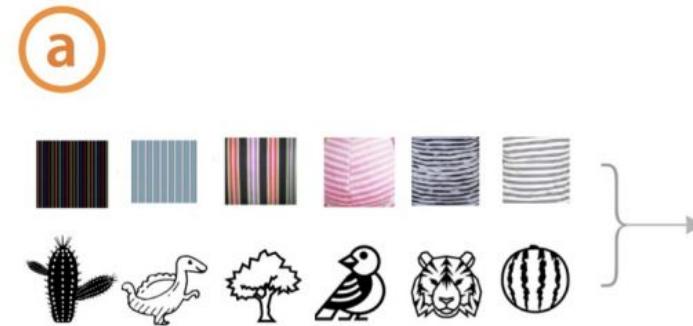
Unit 102 cradle OR autobus OR fire escape
IoU 0.12



(b) abstraction (perceptual only)

Quantitative Testing with Concept Activation Vectors (TCAV)

TCAV measures the sensitivity of a model's prediction to **user provided concept** using the model **internal representations**.

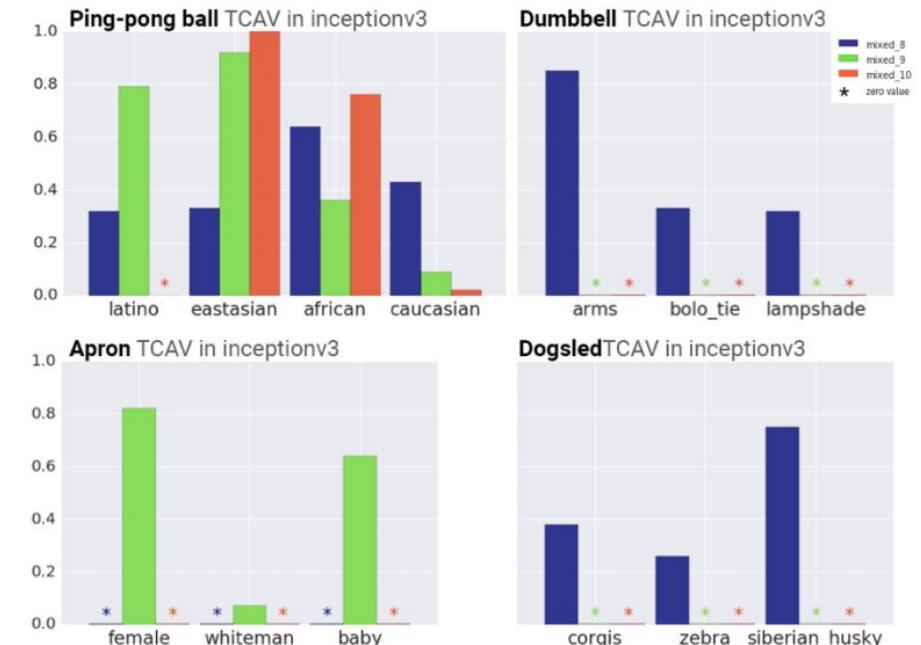
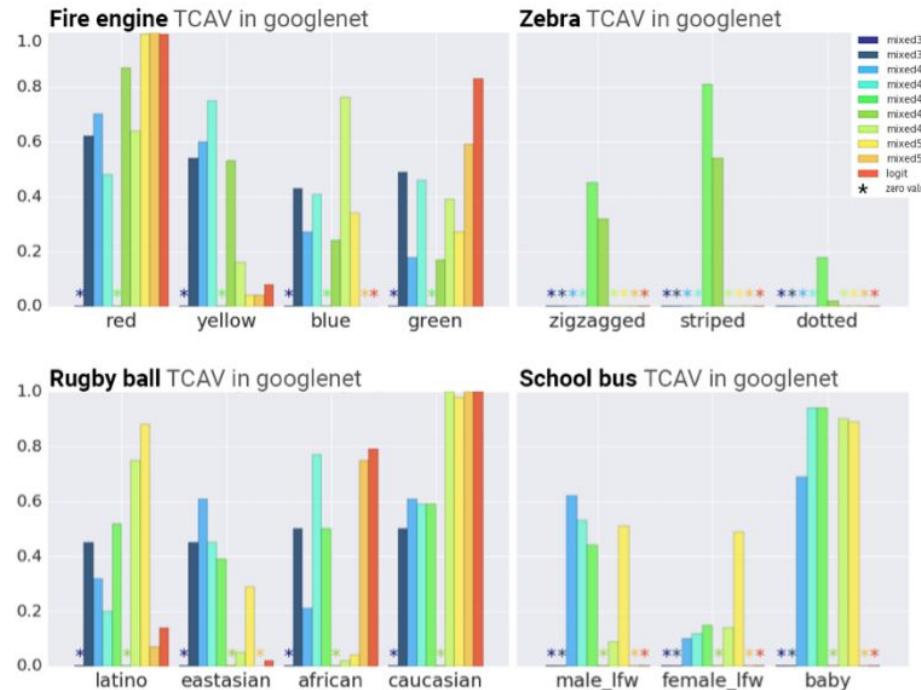


e

$$S_{C,k,l}(^\circ\text{zebra}) = \nabla h_{l,k}(f_l(\text{zebra})) \cdot v_C^l$$

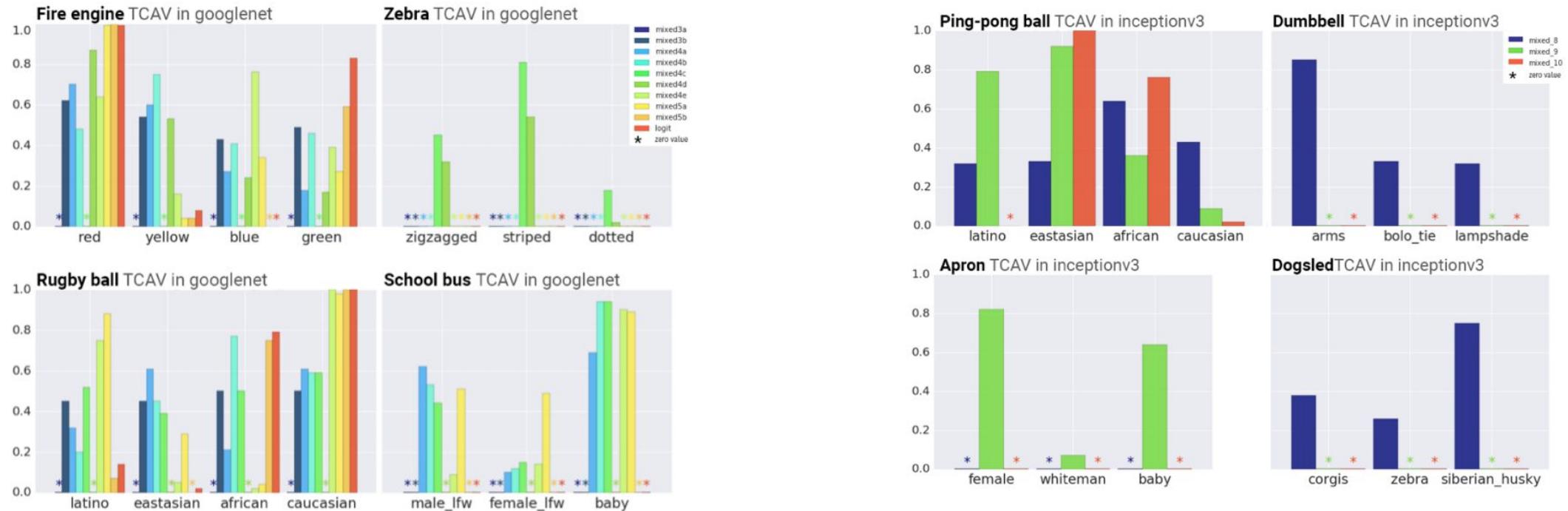
Quantitative Testing with Concept Activation Vectors (TCAV)

Insights from Googlenet and Inceptionv3



Quantitative Testing with Concept Activation Vectors (TCAV)

Insights from Googlenet and Inceptionv3



Additional Variants:

- Regression problems in medical domain ([Graziani et. al. 2019](#)).
- Automatic extraction of visual concepts ([Ghorbani et. al. 2019](#)).

Connections to **Probing** and **Representational Similarity**

- The line of work presented has connections to the literature on **probing** in **NLP**.
- See [recent tutorial](#) by [Belinkov, Gehrmann, & Pavlick at ACL 2020](#) for additional discussion

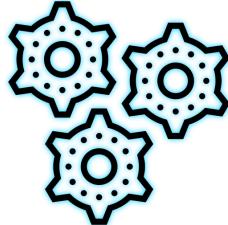
Connections to **Probing** and **Representational Similarity**

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Representational Similarity

1. How similar are the representations at the lower layers of a model compared to its higher layers.
2. How similar are the representations of one model to another?

See: [Raghu et. al. 2017](#) & [Kornblith et. al. 2019](#) for techniques that can provide insights on the questions above.



Approaches for Post hoc Explainability

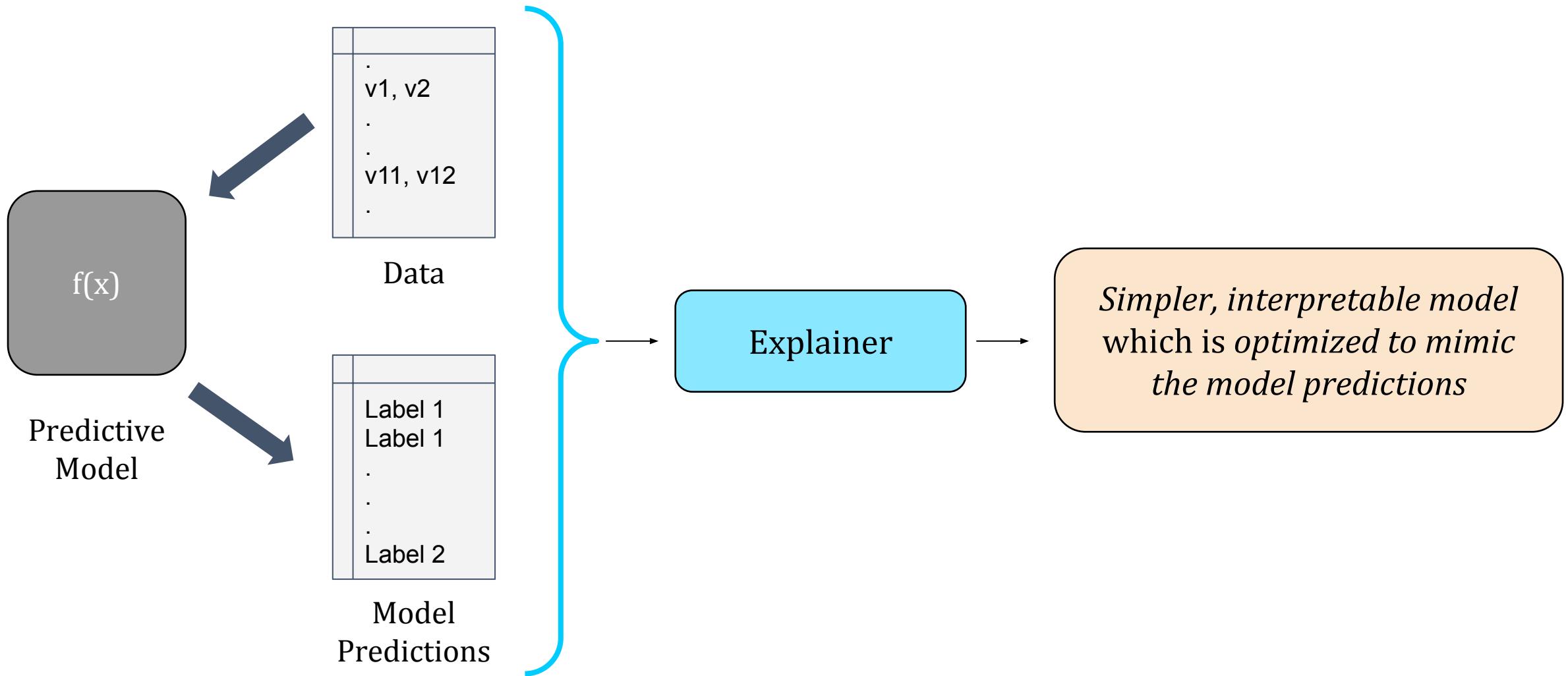
Local Explanations

- Feature Importances
- Rule Based
- Saliency Maps
- Prototypes/Example Based
- Counterfactuals

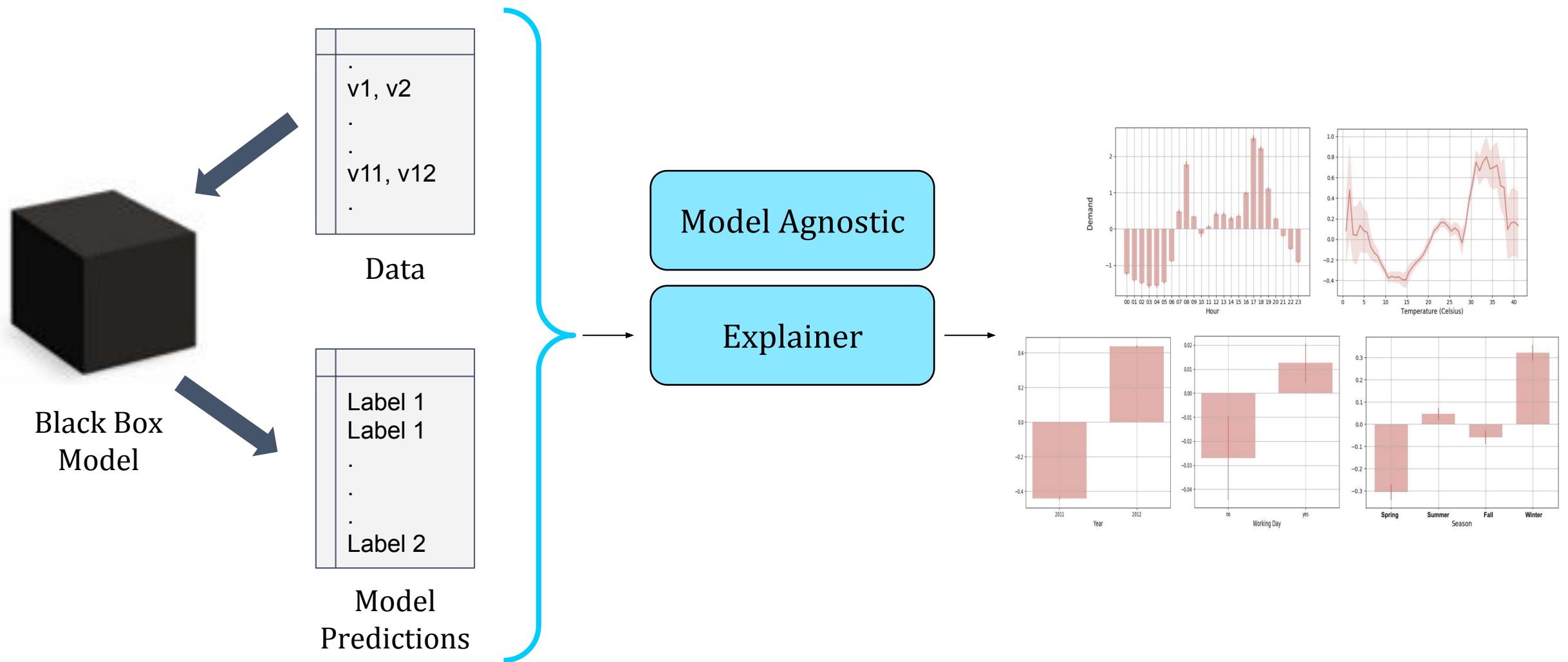
Global Explanations

- Collection of Local Explanations
- Representation Based
- Model Distillation
- Summaries of Counterfactuals

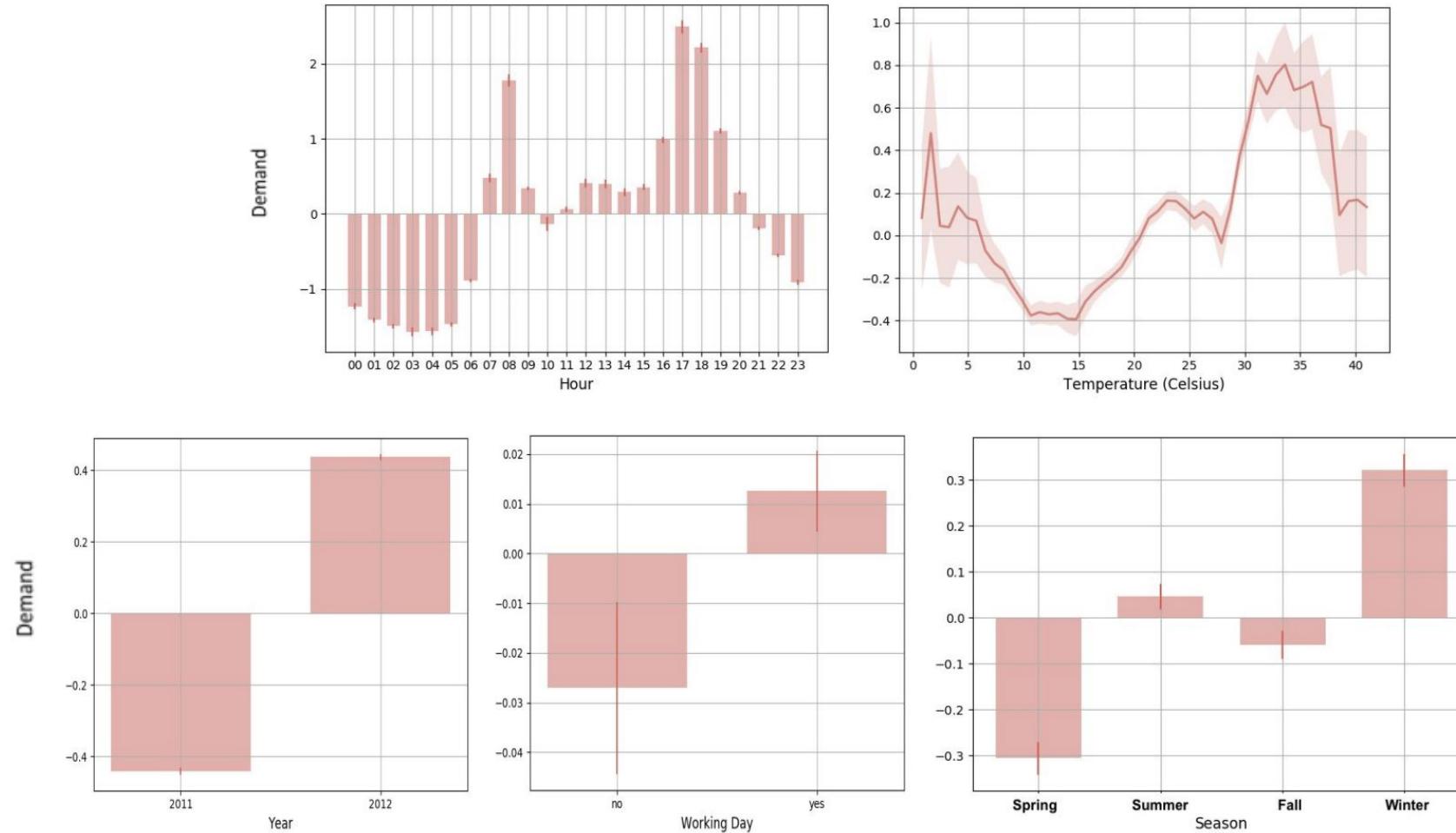
Model Distillation for Generating Global Explanations



Generalized Additive Models as Global Explanations

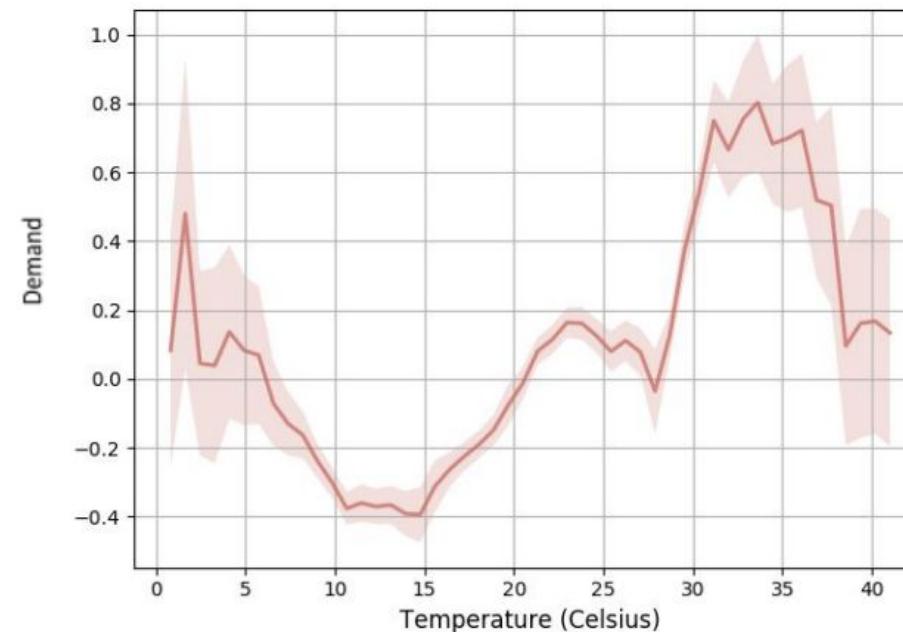


Generalized Additive Models as Global Explanations: *Shape Functions* for Predicting Bike Demand



Generalized Additive Models as Global Explanations: *Shape Functions* for Predicting Bike Demand

How does bike demand vary as a function of temperature?



Generalized Additive Models as Global Explanations

Generalized Additive Model (GAM) :

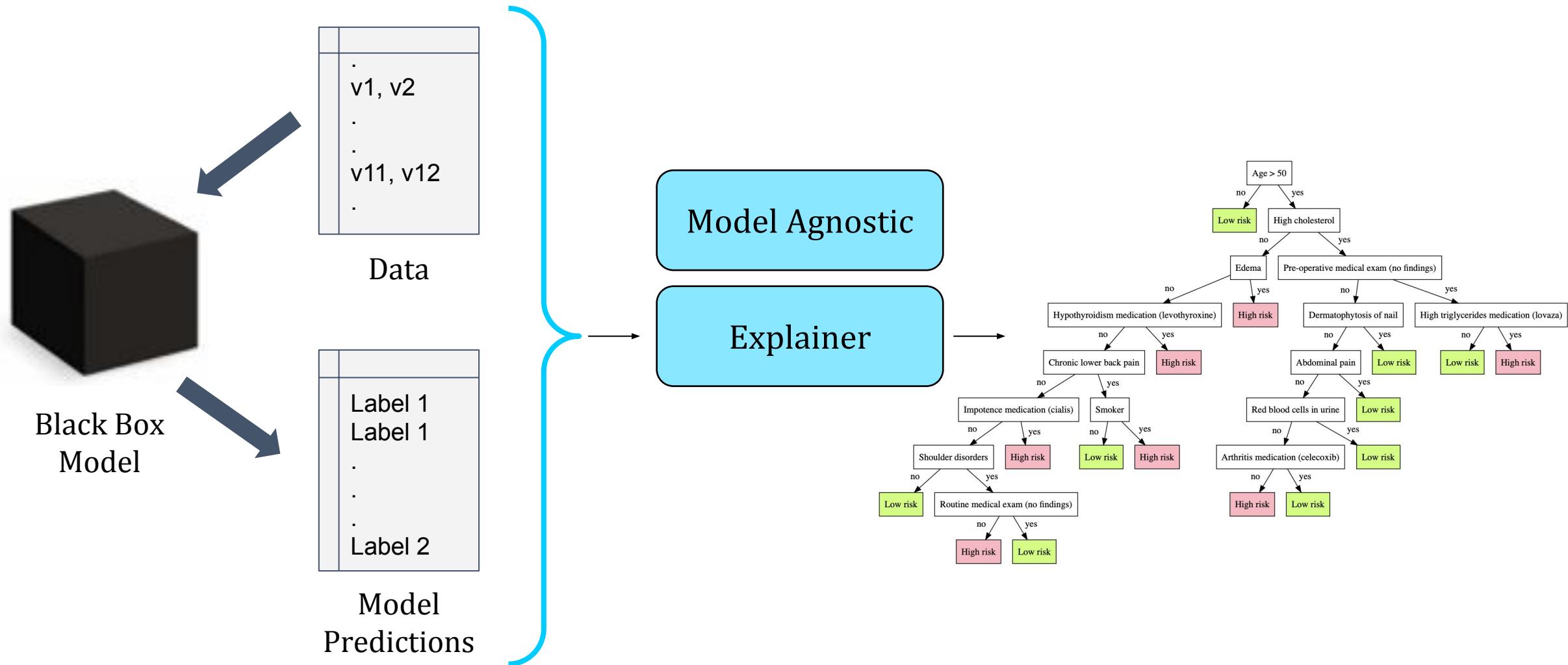
$$\hat{y} = h_0 + \sum_i h_i(x_i) + \sum_{i \neq j} h_{ij}(x_i, x_j) + \sum_{i \neq j} \sum_{j \neq k} h_{ijk}(x_i, x_j, x_k) + \dots$$


Shape functions of
individual features

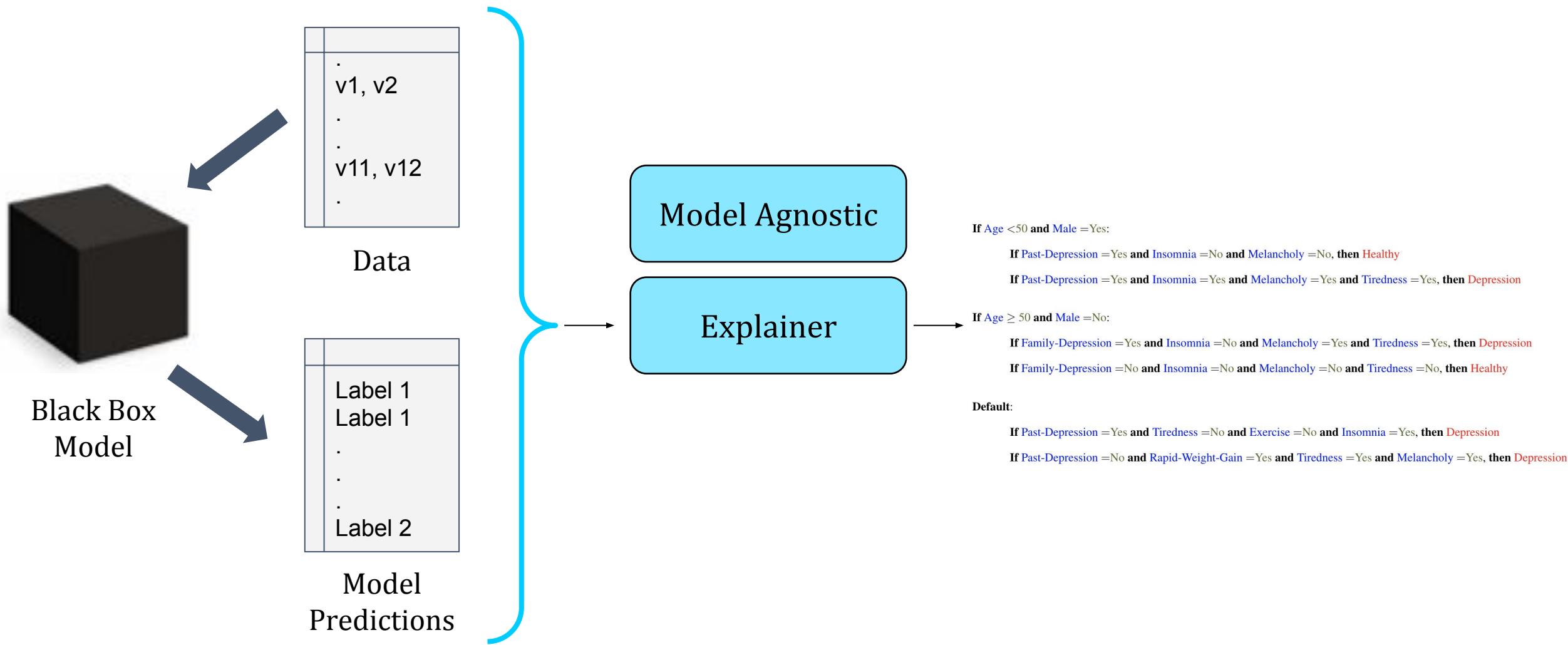
Higher order
feature interaction
terms

Fit this model to the predictions of the black box to obtain the shape functions.

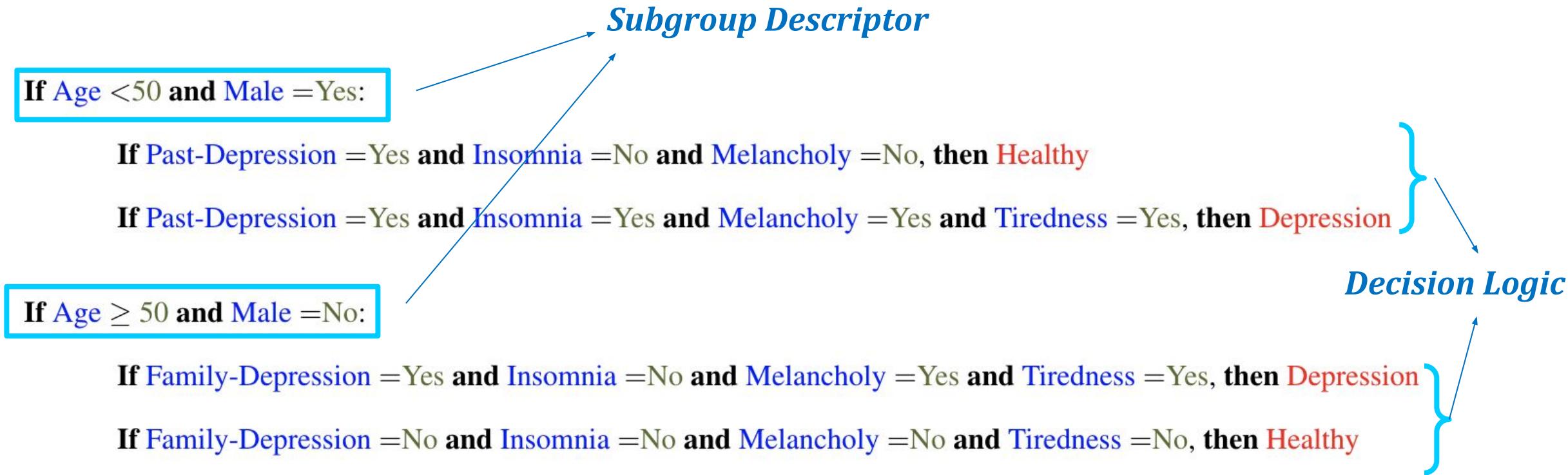
Decision Trees as Global Explanations



Customizable Decision Sets as Global Explanations



Customizable Decision Sets as Global Explanations



Default:

If Past-Depression = Yes and Tiredness = No and Exercise = No and Insomnia = Yes, then Depression

If Past-Depression = No and Rapid-Weight-Gain = Yes and Tiredness = Yes and Melancholy = Yes, then Depression

Customizable Decision Sets as Global Explanations

If Exercise =Yes and Smoking =No:

If Rapid-Weight-Gain =Yes and Tiredness =Yes and Melancholy =Yes and Insomnia =Yes and Age <50, then Depression

If Tiredness =Yes and Melancholy =Yes and Age ≥ 50 , then Depression

If Tiredness =No and Melancholy =No, then Healthy

If Smoking =Yes:

If Rapid-Weight-Gain =Yes and Melancholy =Yes, then Depression

If Tiredness =No and Insomnia =No and Melancholy =No and Rapid-Weight-Gain =No, then Healthy

If Insomnia =Yes and Past-Depression =Yes and Tiredness =Yes, then Depression

Default:

If Past-Depression =Yes and Tiredness =Yes and Melancholy =Yes, then Depression

If Past-Depression =No and Rapid-Weight-Gain =Yes and Tiredness =No and Melancholy =Yes, then Depression

If Family-Depression =Yes and Age ≥ 50 and Male =No and Tiredness =Yes, then Depression



Customizable Decision Sets as Global Explanations: Desiderata & Optimization Problem

Fidelity

Describe model behavior accurately

Fidelity

Minimize number of instances for which explanation's label \neq model prediction

Unambiguity

No contradicting explanations

Unambiguity

Minimize the number of duplicate rules applicable to each instance

Simplicity

Users should be able to look at the explanation and reason about model behavior

Simplicity

Minimize the number of conditions in rules;
Constraints on number of rules & subgroups;

Customizability

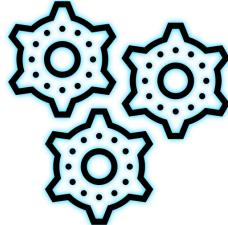
Users should be able to understand model behavior across various subgroups of interest

Customizability

Outer rules should only comprise of features of user interest (candidate set restricted)

Customizable Decision Sets as Global Explanations

- The complete optimization problem is *non-negative*, *non-normal*, *non-monotone*, and *submodular* with *matroid constraints*
- Solved using the well-known *smooth local search* algorithm (Feige et. al., 2007) with best known optimality guarantees.



Approaches for Post hoc Explainability

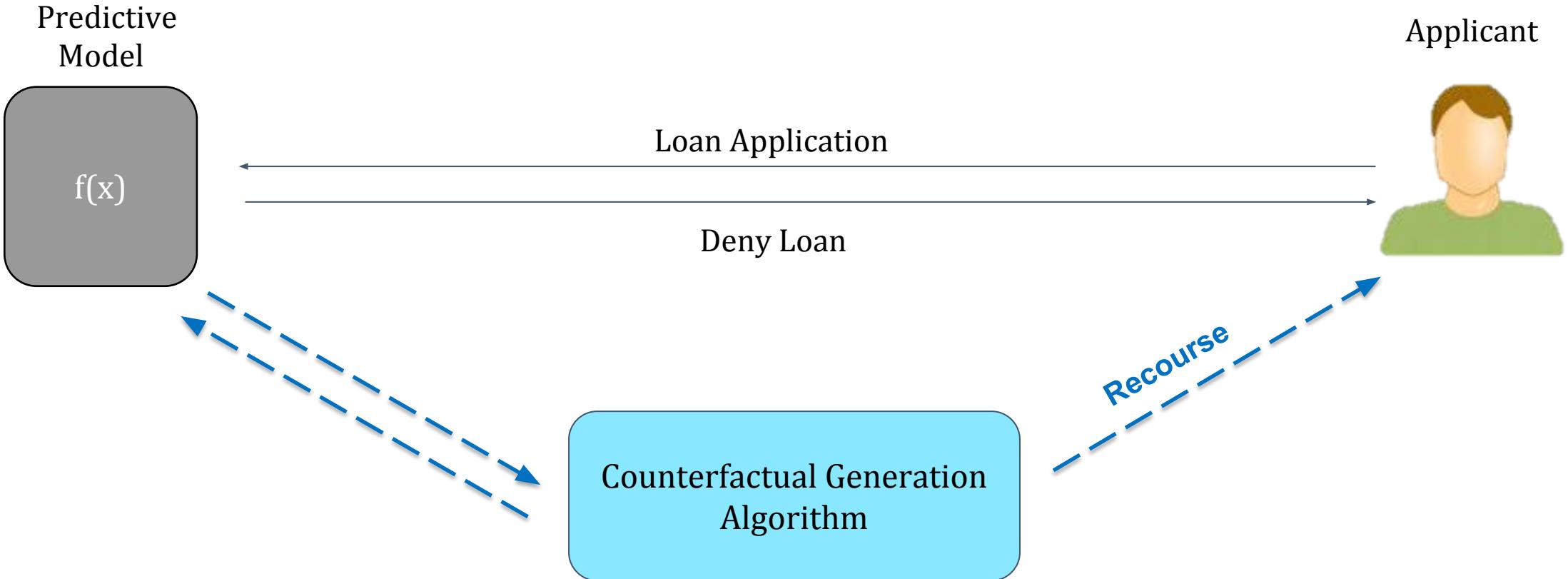
Local Explanations

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Global Explanations

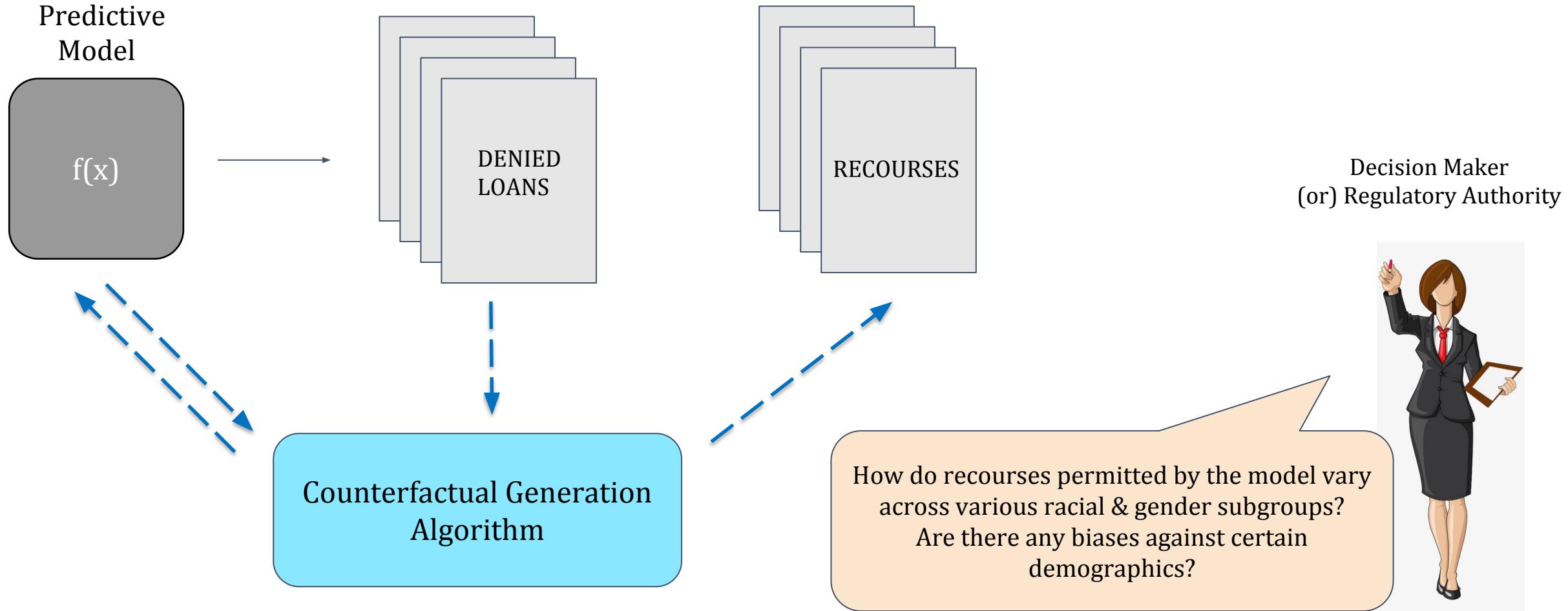
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Counterfactual Explanations

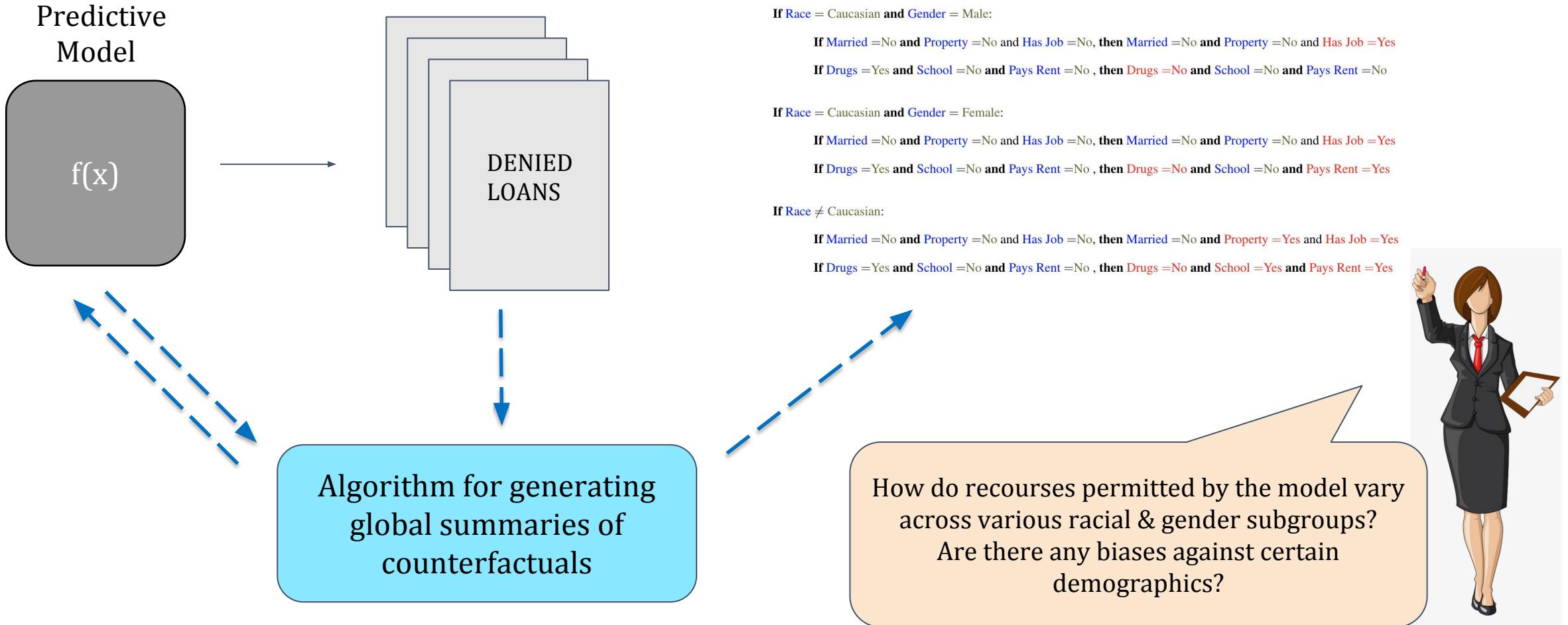


Recourse: Increase your salary by 50K & pay your credit card bills on time for next 3 months

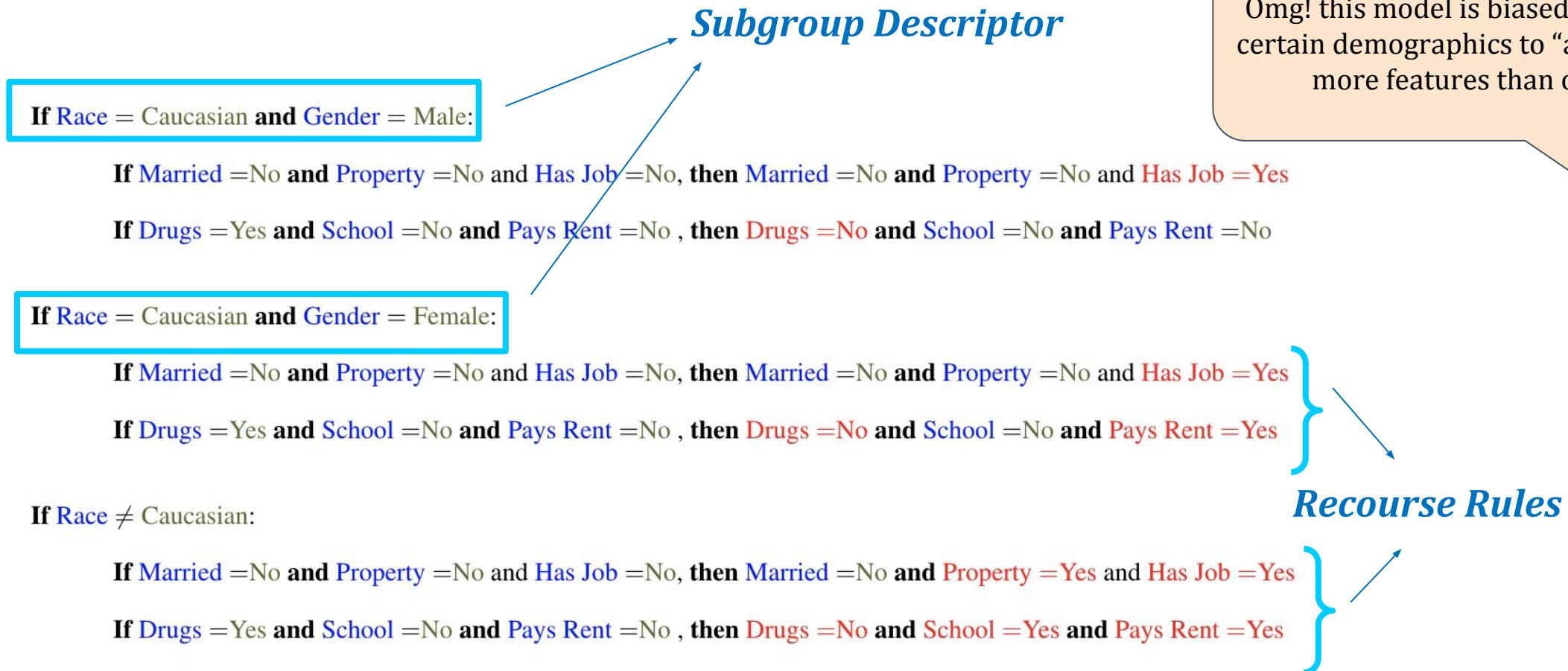
Counterfactual Explanations



Customizable Global Summaries of Counterfactuals



Customizable Global Summaries of Counterfactuals



Customizable Global Summaries of Counterfactuals: Desiderata & Optimization Problem

Recourse Correctness

Prescribed recourses should obtain desirable outcomes

Recourse Coverage

(Almost all) applicants should be provided with recourses

Minimal Recourse Costs

Acting upon a prescribed recourse should not be impractical or terribly expensive

Interpretability of Summaries

Summaries should be readily understandable to stakeholders (e.g., decision makers/regulatory authorities).

Customizability

Stakeholders should be able to understand model behavior across various subgroups of interest

Recourse Correctness

Minimize number of applicants for whom prescribed recourse does not lead to desired outcome

Recourse Coverage

Minimize number of applicants for whom recourse does not exist (i.e., satisfy no rule).

Minimal Recourse Costs

Minimize total ***feature costs*** as well as ***magnitude of changes*** in feature values

Interpretability of Summaries

Constraints on # of rules, # of conditions in rules & # of subgroups

Customizability

Outer rules should only comprise of features of stakeholder interest (candidate set restricted)

Customizable Global Summaries of Counterfactuals: Feature Costs & Magnitude of Changes

- **Feature Costs:** *Each feature is associated with a cost which indicates how hard it is change that feature.*
- **How to obtain feature costs?**
 - Obtain pairwise feature comparison inputs from domain experts
 - Apply Bradley Terry model which connects pairwise feature comparisons to individual feature costs and estimate these costs.
- **Magnitude of Changes:** are penalized via total log percentile shift

Customizable Global Summaries of Counterfactuals: Feature Costs & Magnitude of Changes

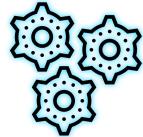
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- **Magnitude of Changes:** are penalized via total log percentile shift

$$p_{ij} = \frac{e^{\beta_i}}{e^{\beta_i} + e^{\beta_j}}$$

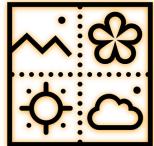
Customizable Global Summaries of Counterfactuals

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Tutorial on Post hoc Explanations



Approaches for Post hoc Explainability



Explanations in Different Modalities



Evaluation of Explanations



Limits of Post hoc Explainability

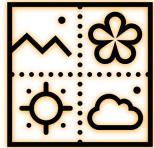


Future of Post hoc Explainability

Tutorial on Post hoc Explanations



Approaches for Post hoc Explainability



Explanations in Different Modalities



Evaluation of Explanations

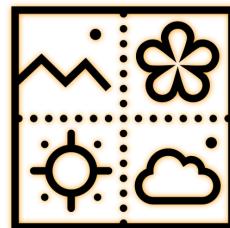


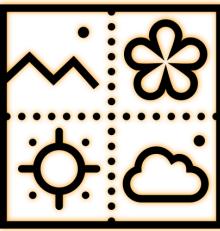
Limits of Post hoc Explainability



Future of Post hoc Explainability

Post hoc Explanations in Different Modalities



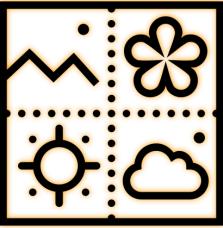


Different Data Modalities

Structured Data

Computer Vision

Natural Language



Different Data Modalities

Structured Data

Computer Vision

Natural Language

Structured Data

NoDefaultNbr	Married	Single	Age_1t_25	Age_in_25_t	Age_in_40_t	Age_geq_60	EducationLevel	MaxBillAmount	MaxPayment	MonthsWith1	MonthsWith2	MonthsWith3	MostRecent1	MostRecent2	TotalOverdue	TotalMonths	HistoryOfOverduePayments
1	1	0	1	0	0	0	2	120	20	0	6	0	120	0	1	4	1
0	0	1	0	1	0	0	2	110	60	0	6	0	80	0	2	4	1
0	1	0	1	0	0	0	2	890	155.32	0	5	0	890	50	0	0	0
1	0	0	1	0	0	0	2	1510	60	0	0	3	1430	60	0	0	0
1	0	0	0	1	0	0	2	1090	1120	1	2	0	260	60	0	0	0
0	1	0	1	0	0	0	3	1970	80	0	0	3	1970	80	0	0	0
0	1	0	1	0	0	0	3	16570	1680	0	0	5	11240	1680	0	0	0
0	1	1	0	0	0	0	2	360	50	4	6	0	360	10	0	0	0
1	0	0	1	0	0	0	1	430	100	0	6	0	340	100	1	2	1
0	1	0	1	0	0	0	1	420	400	1	4	0	0	0	0	0	0
0	1	0	1	0	0	0	1	340	110	1	6	0	340	70	1	2	1
0	1	0	0	1	0	0	3	680	680	2	6	0	370	670	1	2	1
0	1	0	0	1	0	0	2	370	200	0	6	0	370	30	0	0	0
0	1	0	1	0	0	0	2	2060	100	0	0	4	2010	100	2	7	1
0	1	0	1	0	0	0	3	2160	90	0	0	0	2160	90	0	0	0
0	0	1	0	0	0	0	1	1550	50	0	0	1	1550	0	1	3	1
0	1	1	0	0	0	0	3	580	100	0	0	5	470	100	1	8	1
1	0	0	0	1	0	0	3	7730	5970	1	1	0	7730	320	0	0	0
1	0	0	0	1	0	0	3	0	0	0	6	0	0	0	1	1	1
0	1	0	1	0	0	0	3	0	0	0	6	0	0	0	1	1	1
0	1	0	1	0	0	0	1	1170	1030	1	4	0	1170	90	0	0	0

Categorical Data

Ordinal Data

Numerical Data
(Discrete & Continuous)

Structured Data: Why care about explainability?

- Lot of information in various real world settings available as structured data
- Lots of applications deal with structured data
 - Disease diagnosis and treatment (e.g., weight, age, symptoms, glucose level)
 - Risk prediction in education/lending/criminal justice (e.g., credit scores, previous crimes, student GPAs, education level)
 - Recommender systems for movies/products (e.g., list of movies liked in the past)

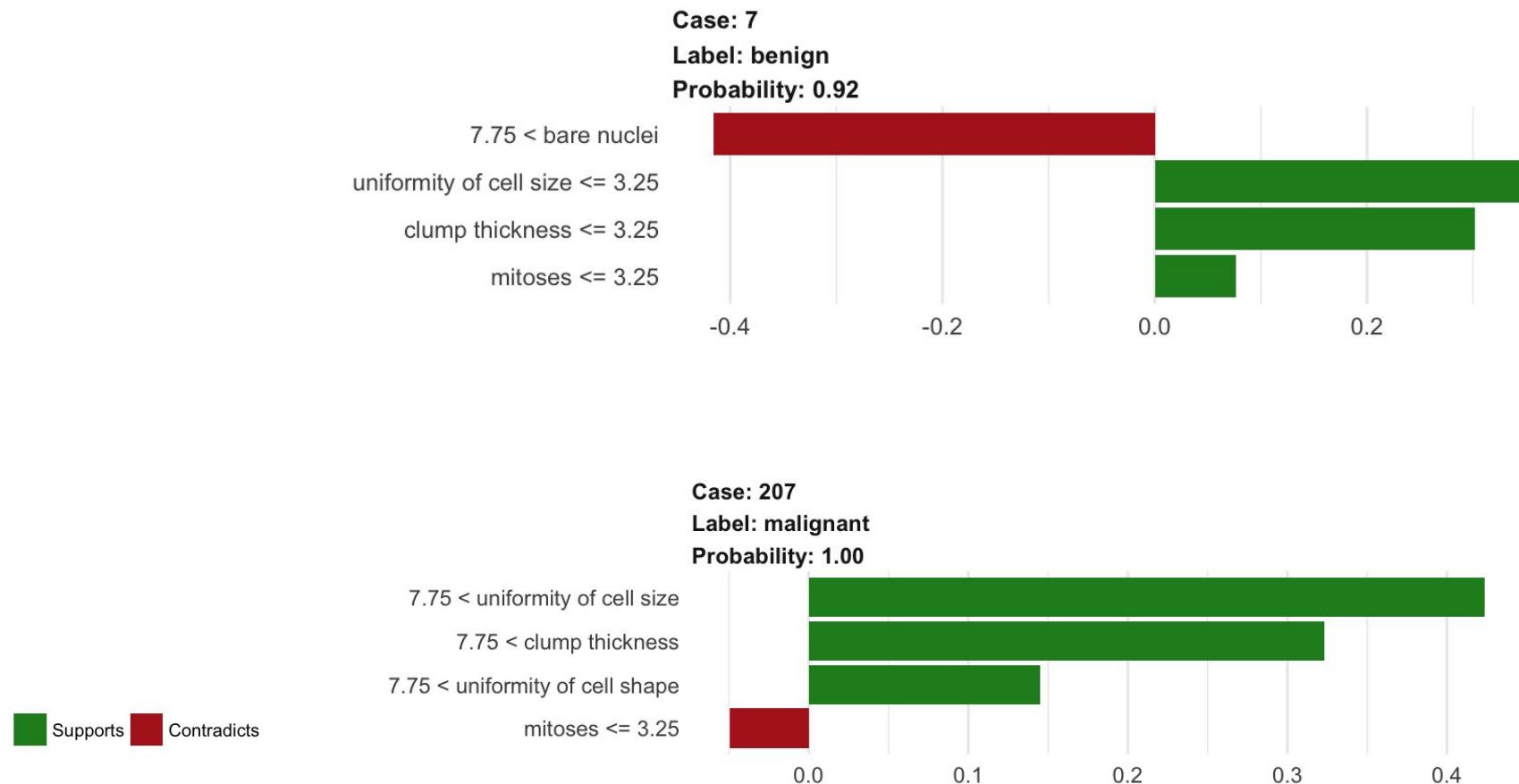
Challenges for Structured Data

- Different types of variables in the data
 - Different types of variables call for different similarity/perturbation functions
 - gradients may not always be meaningful
- Depending on the task/domain, data could be either low or high dimensional
 - E.g., movie recommendations -- user x movie matrix (high dimensional)

Structured Data: Explainability Techniques

- Feature importance based explanations
 - Perturbation methods e.g., LIME/SHAP
 - Saliency maps and other gradient based methods not very meaningful

Feature Importance Based Explanations



Structured Data: Explainability Techniques

- Feature importance based explanations
 - Perturbation methods e.g., LIME/SHAP
 - Saliency maps and other gradient based methods not very meaningful
- Prototype/example based explanations
 - might not always be interpretable
 - e.g., an instance with 100 feature values as prototype

Prototype Based Explanations

Prediction: Not Diabetic

Influential instances driving the prediction:

Instance #	Age	Weight	Smoking	Exercise	Prediction
1	32	153	No	Yes	Not Diabetic
2	27	172	Yes	Yes	Not Diabetic
3	55	163	No	Yes	Not Diabetic
4	18	147	No	No	Not Diabetic

Structured Data: Explainability Techniques

- Feature importance based explanations
 - Perturbation methods e.g., LIME/SHAP
 - Saliency maps and other gradient based methods not very meaningful
- Prototype/example based explanations
 - might not always be interpretable
 - e.g., an instance with 100 feature values as prototype
- Rule based explanations

Rule Based Explanations

If Respiratory-Illness=Yes and Smoker=Yes and Age ≥ 50 then Lung Cancer

If Risk-LungCancer=Yes and Blood-Pressure ≥ 0.3 then Lung Cancer

If Risk-Depression=Yes and Past-Depression=Yes then Depression

If BMI ≥ 0.3 and Insurance=None and Blood-Pressure ≥ 0.2 then Depression

If Smoker=Yes and BMI ≥ 0.2 and Age ≥ 60 then Diabetes

If Risk-Diabetes=Yes and BMI ≥ 0.4 and Prob-Infections ≥ 0.2 then Diabetes

If Doctor-Visits ≥ 0.4 and Childhood-Obesity=Yes then Diabetes

If Respiratory-Illness=Yes and Smoker=Yes and Age ≥ 50 then Lung Cancer

Else if Risk-Depression=Yes then Depression

Else if BMI ≥ 0.2 and Age ≥ 60 then Diabetes

Else if Headaches=Yes and Dizziness=Yes, then Depression

Else if Doctor-Visits ≥ 0.3 then Diabetes

Else if Disposition-Tiredness=Yes then Depression

Else Diabetes

Structured Data: Explainability Techniques

- Feature importance based explanations
 - Perturbation methods e.g., LIME/SHAP
 - Saliency maps and other gradient based methods not very meaningful
- Prototype/example based explanations
 - might not always be interpretable
 - e.g., an instance with 100 feature values as prototype
- Rule based explanations
- Counterfactual explanations

Counterfactual Explanations

FEATURES TO CHANGE	CURRENT VALUES	REQUIRED VALUES
<i>MostRecentPaymentAmount</i>	\$0	→ \$500
<i>MonthsWithLowSpendingOverLast6Months</i>	6	→ 5
<i>MonthsWithZeroBalanceOverLast6Months</i>	1	→ 2

If Female =No and Foreign Worker =No:

If Missed Payments =Yes and Critical Loans =Yes, then Missed Payments =Yes and Critical Loans =No

If Unemployed =Yes and Critical Loans =Yes and Has Guarantor =No,

then Unemployed =Yes and Critical Loans =No and Has Guarantor =Yes

If Female =No and Foreign Worker =Yes:

If Skilled Job =No and Years at Job ≤ 1 , then Skilled Job =Yes and Years at Job ≥ 4

If Unemployed =Yes and Has Guarantor =No and Has CoApplicant =No,

then Unemployed =No and Has Guarantor =Yes and Has CoApplicant =Yes

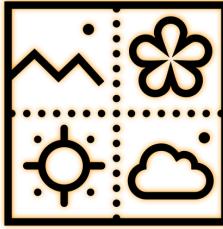
If Female =Yes:

If Married =No and Owns House =No, then Married =Yes and Owns House =Yes

If Unemployed =No and Has Guarantor =Yes and Has CoApplicant =No,

then Unemployed =No and Has Guarantor =Yes and Has CoApplicant =Yes

Different Data Modalities

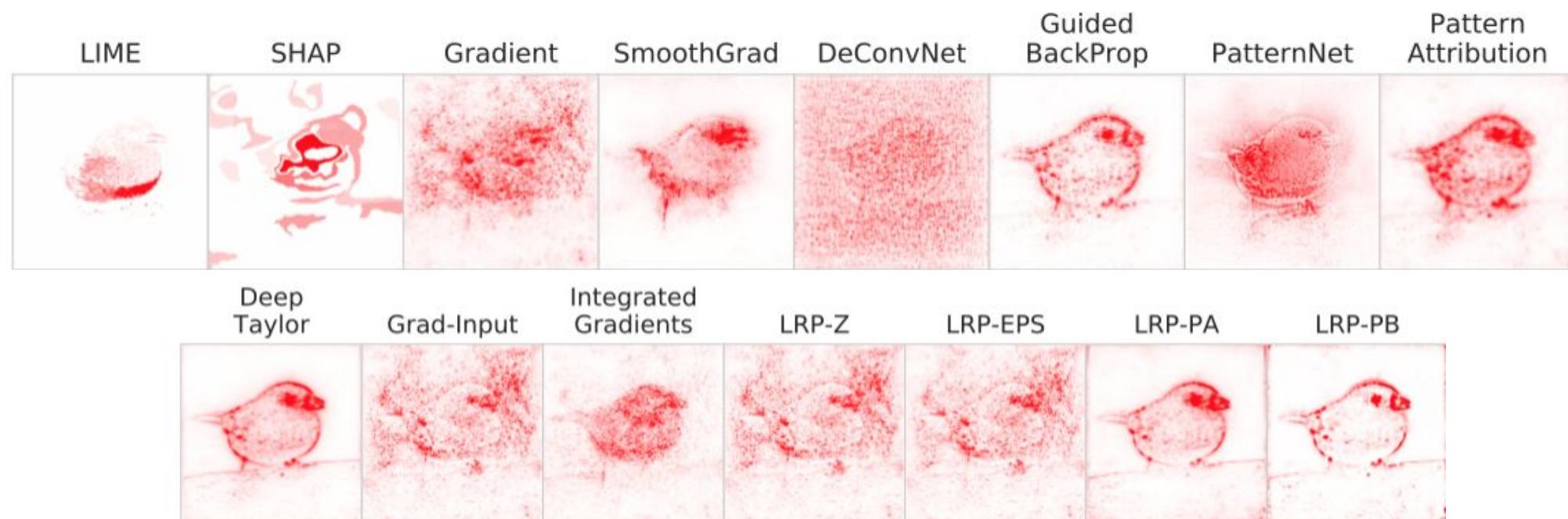
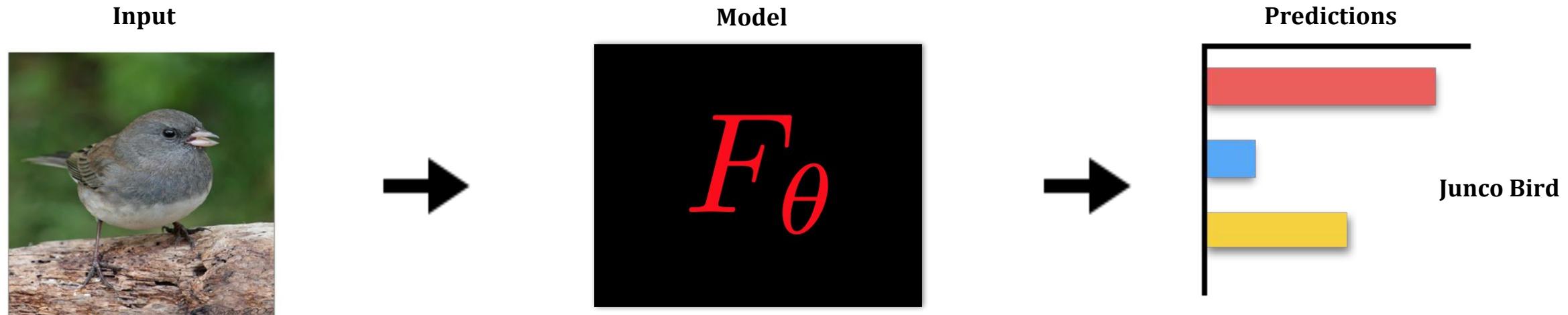


Structured Data

Computer Vision

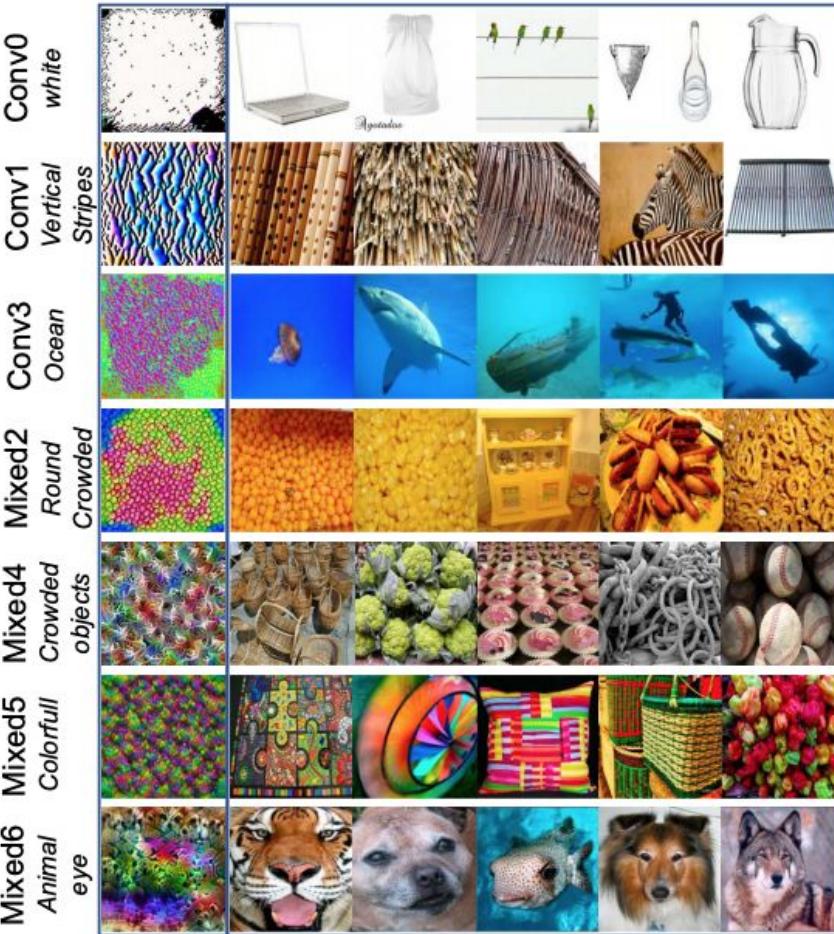
Natural Language

Feature Importance Approaches on VGG-16

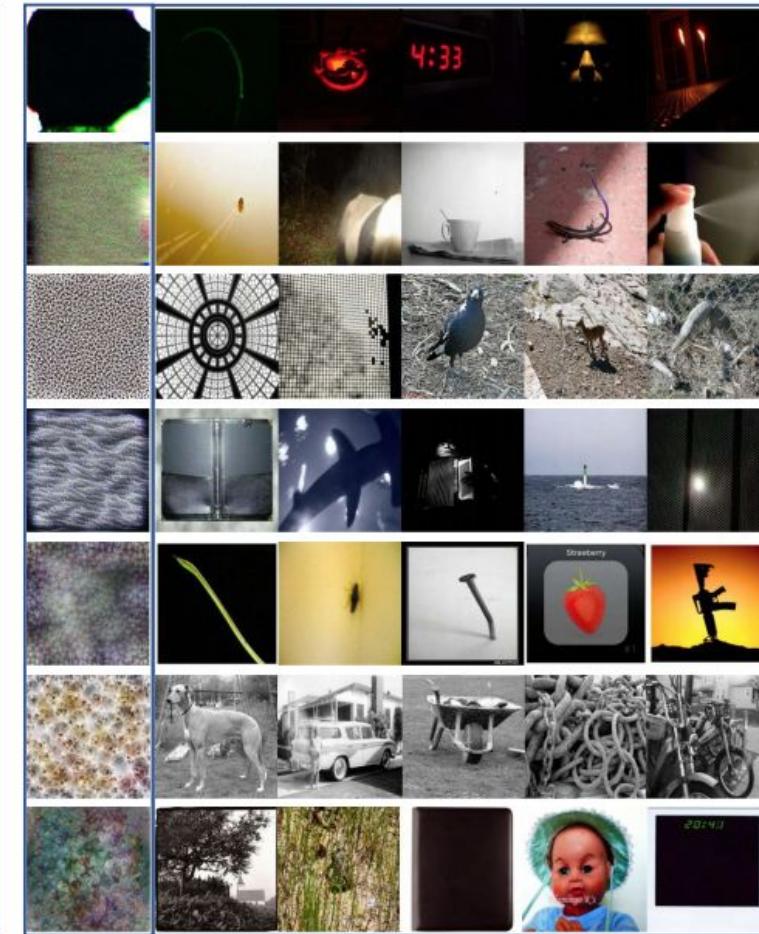


Neuron Shapley Importance for Inception-V3 Trained on ImageNet

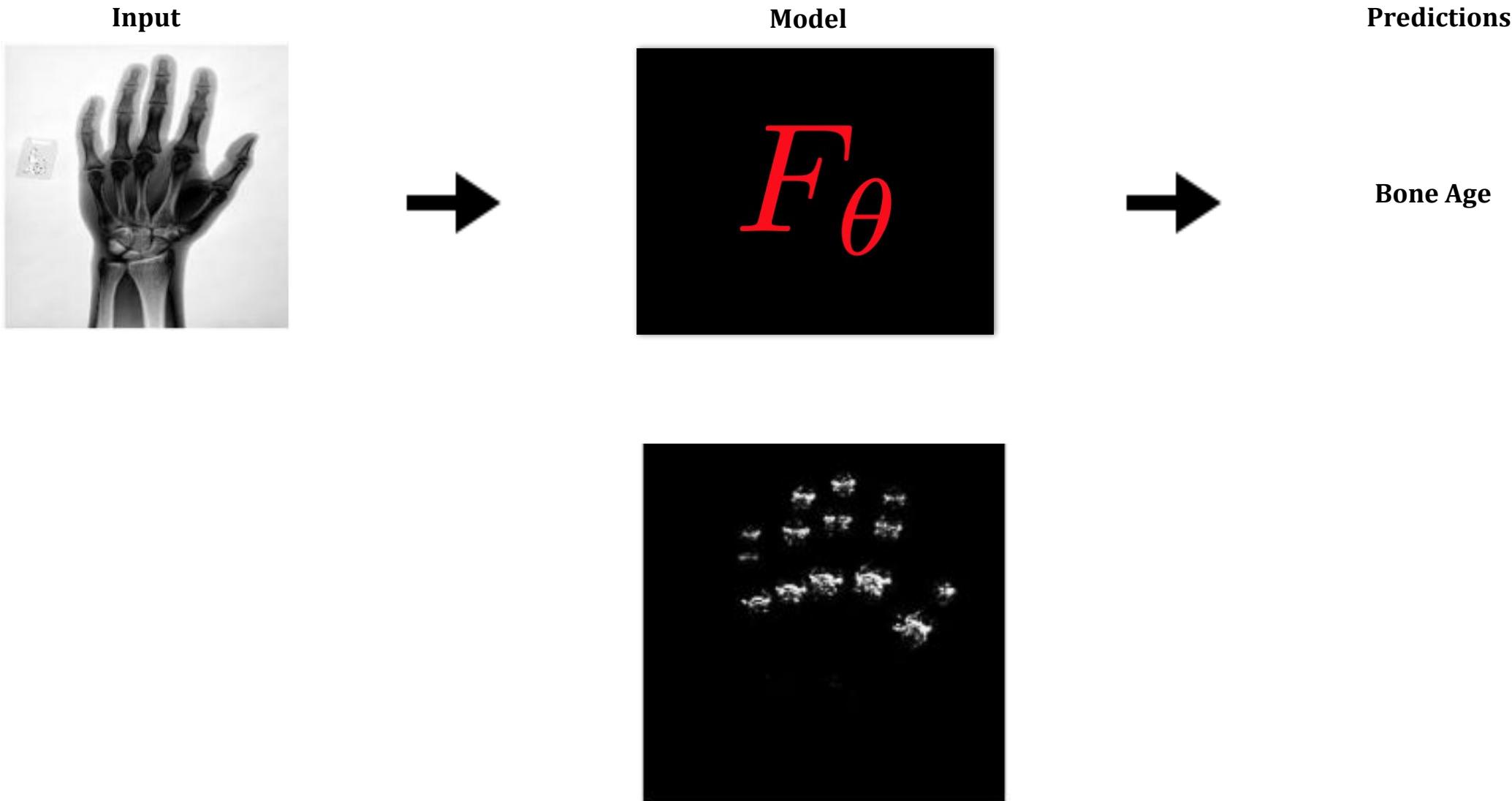
Positive Activation



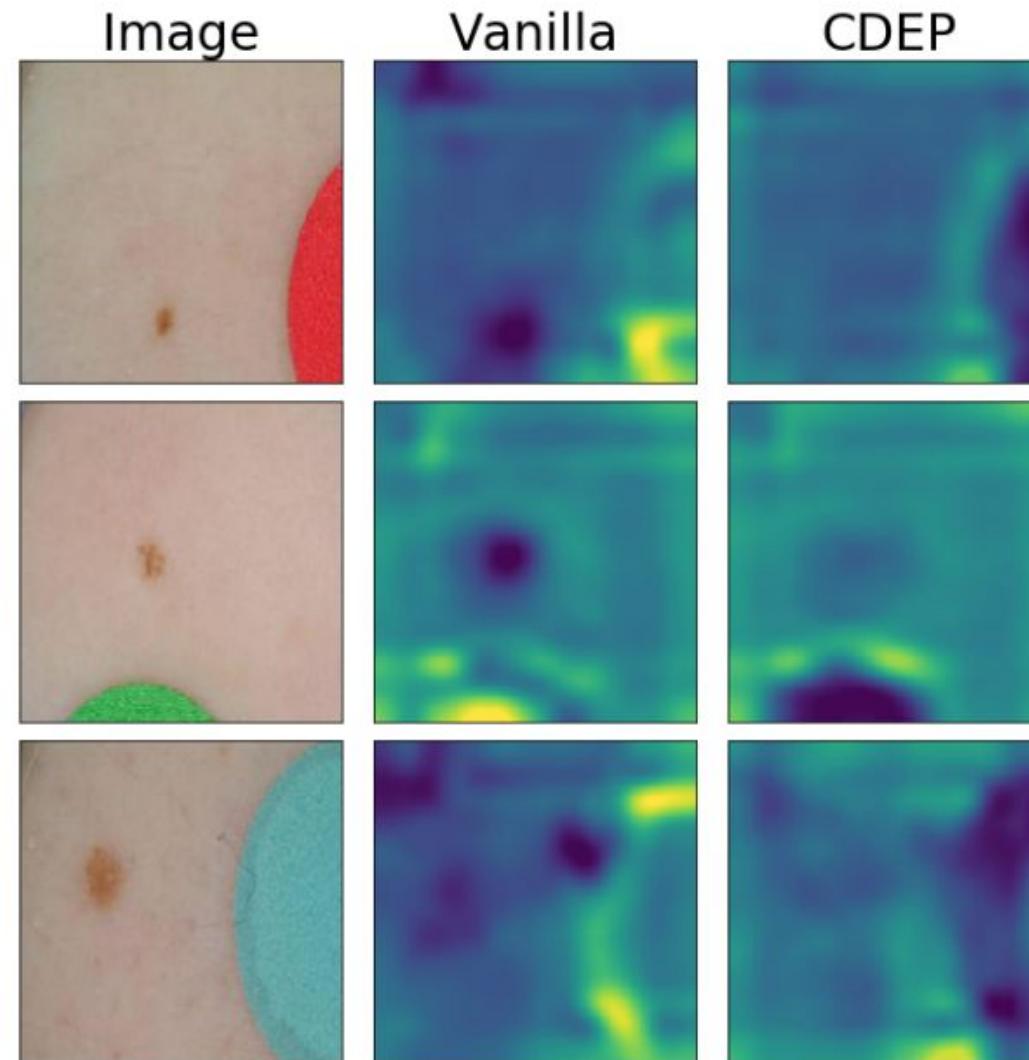
Negative Activation



Saliency Map for Bone Age Model



Contextual Decomposition for a Skin Cancer Prediction Model



Integrated Gradients for Diabetic Retinopathy Model

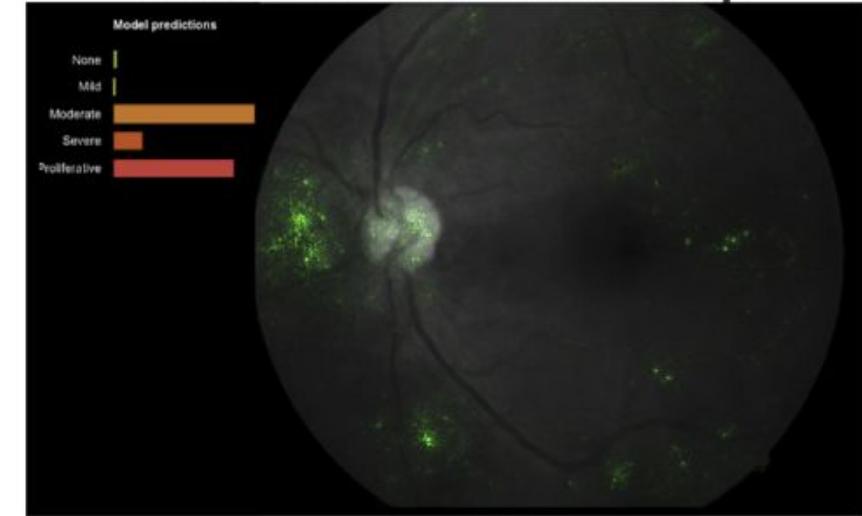
Unassisted



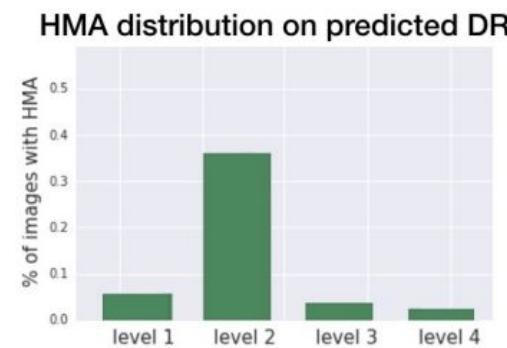
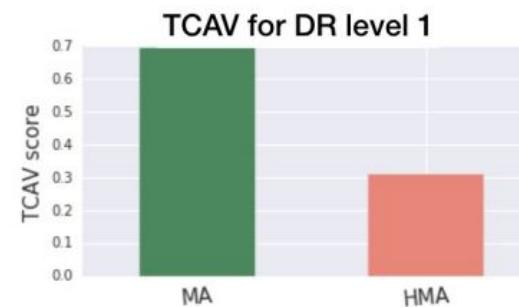
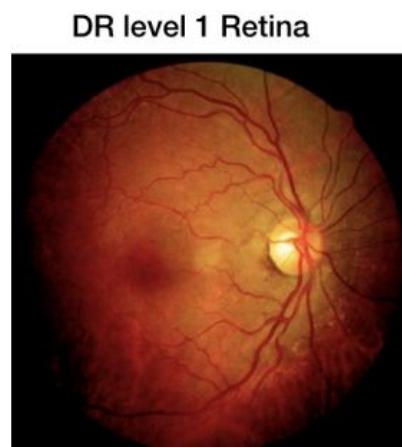
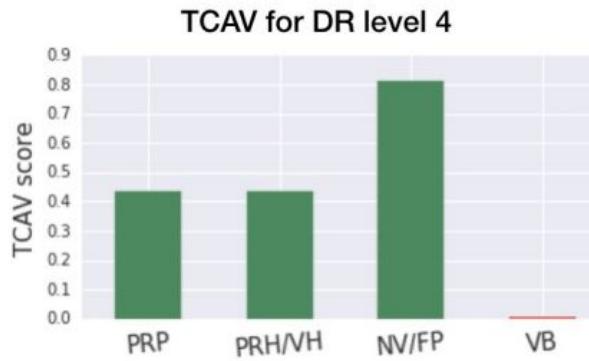
Grades Only



Grades + Heatmap



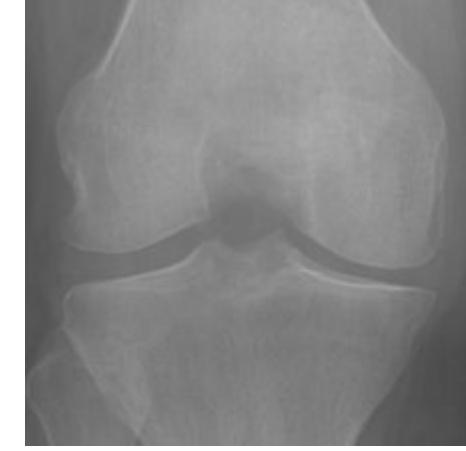
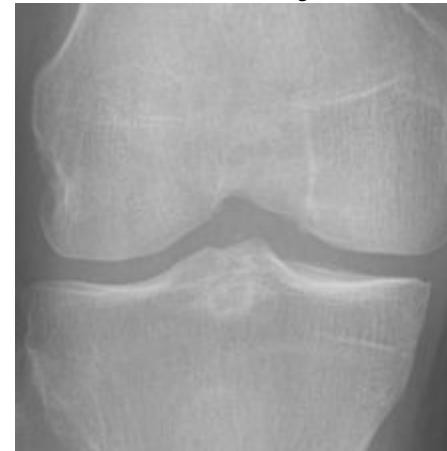
TCAV for Diabetic Retinopathy Model

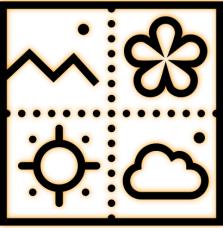


Challenges Transferring Approaches to Medical Setting

Adapting explanation methods developed for benchmark tasks like ImageNet and CIFAR to medical imaging setting is challenging in practice due to input **homogeneity**.

Knee Xray





Different Data Modalities

Structured Data

Computer Vision

Natural Language

Natural Language Processing

- Why should we care about interpretability for NLP?
 - Lots of **NLP applications** everywhere
 - Translation, Social Media Analysis, Hate Speech Filtering, Digital Assistants, ...
 - Quickly evolving, **in major ways**, last few years
 - Word Embeddings, ELMo, BERT, GPT-2/3, T5, ...
 - Gap between what the benchmarks show and how good they are is **vast**
 - Lots of question answering, classification, textual entailment, etc. are “solved”
 - Brings up **unique and additional challenges** (that are more general)
 - Domains with discrete/structured/combinatorial inputs...

Challenges for NLP

- Discrete space of inputs
 - E.g. gradients are not directly applicable (or as meaningful)
- Not all combinations are well defined
 - They need not to be nonsense, ungrammatical
- Difficult to write a similarity/perturbation functions
- Format is not fixed: not everything is classification
 - structured prediction, text generation, span selection, ...
- Language does not lend itself to “simple explanations”

Word Attribution for NLP

Sentiment

an intelligent fiction about learning through cultural clash.

QA

What company won free advertisement due to QuickBooks contest ?

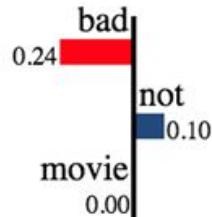
MLM

[CLS] The [MASK] ran to the emergency room to see her patient . [SEP]

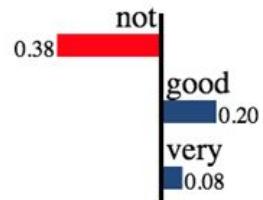
Perturbation-based Explanations for NLP

LIME

+ This movie is not bad.



— This movie is not very good.



This movie is **not bad**



Anchors

This audio is not bad

This novel is not bad

This footage is not bad

What is the mustache made of? **banana**

Input Reduction

A puzzling man named NLP Cool

PER

went to buy some

organic fruit at

Grandpa Joe 's

ORG

in downtown

Deep Learning

LOC

Input Reduction

A puzzling man named NLP Cool went to buy some

PER

organic fruit at Grandpa Joe 's in downtown Deep Learning

ORG

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Reduced input for NLP Cool named NLP Cool

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LOC

Reduced input for NLP Cool named NLP Cool

PER

Reduced input for Grandpa Joe 's at Grandpa Joe 's

ORG

Reduced input for Deep Learning in downtown Deep Learning

LOC

Prototypes for NLP

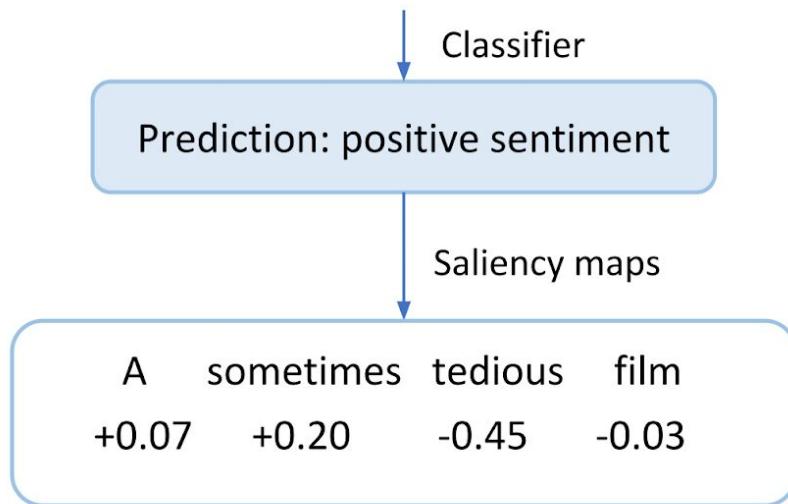
A sometimes tedious film.



Prediction: positive sentiment

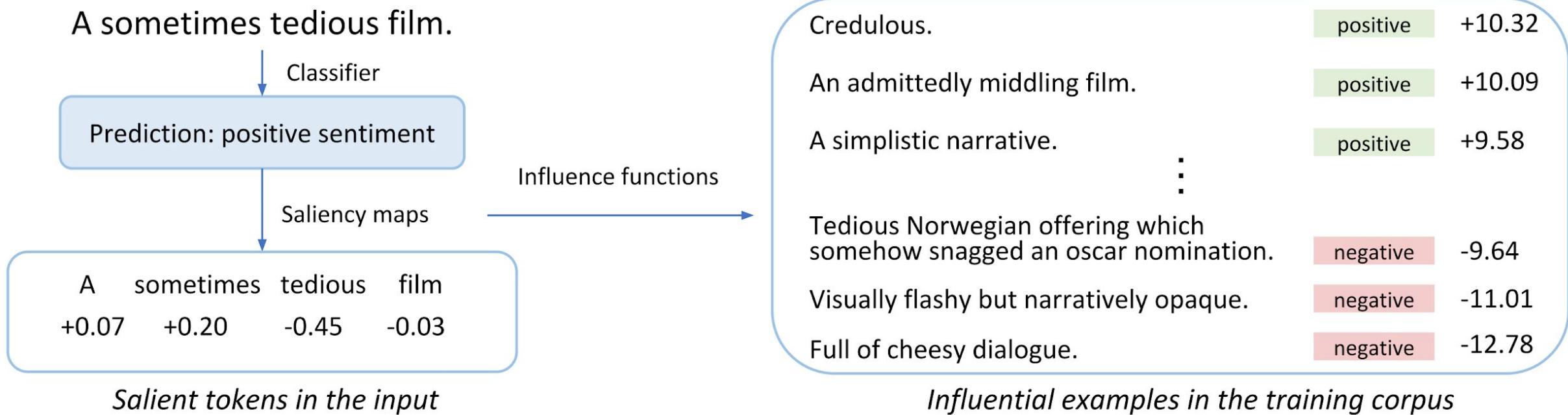
Prototypes for NLP

A sometimes tedious film.



Salient tokens in the input

Prototypes for NLP



Useful Implementations

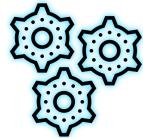
Lots of code available (in no particular order):

- https://captum.ai/tutorials/Bert_SQuAD_Interpret
- <https://github.com/PAIR-code/lit>
- <https://allennlp.org/interpret>
- <https://github.com/QData/TextAttack>
- <https://github.com/interpretml/interpret-text>
- Influence functions for text
- Triggers Code
- Anchors Code
- LIME Code

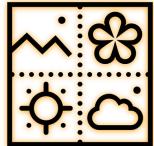


GitHub

Tutorial on Post hoc Explanations



Approaches for Post hoc Explainability



Explanations in Different Modalities



Evaluation of Explanations

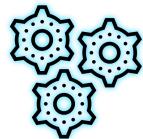


Limits of Post hoc Explainability

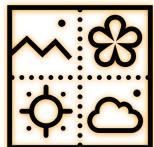


Future of Post hoc Explainability

Tutorial on Post hoc Explanations



Approaches for Post hoc Explainability



Explanations in Different Modalities



Evaluation of Explanations



Limits of Post hoc Explainability



Future of Post hoc Explainability

Evaluation of Post hoc Explanations



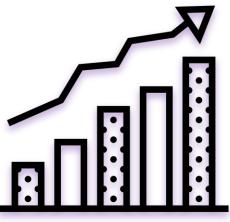
How we evaluate explanations?



Two Different Factors

		What are you evaluating?		
		Understand the Behavior	Useful for Debugging	Help make decisions
How we evaluate it?	Application-grounded			
	Human-grounded			
	Functionally-grounded			

Evaluating Post hoc Explanations

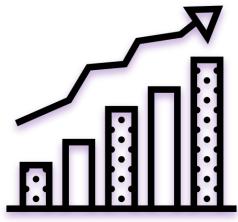


Understand the Behavior

Help make decisions

Useful for Debugging

Evaluating Post hoc Explanations



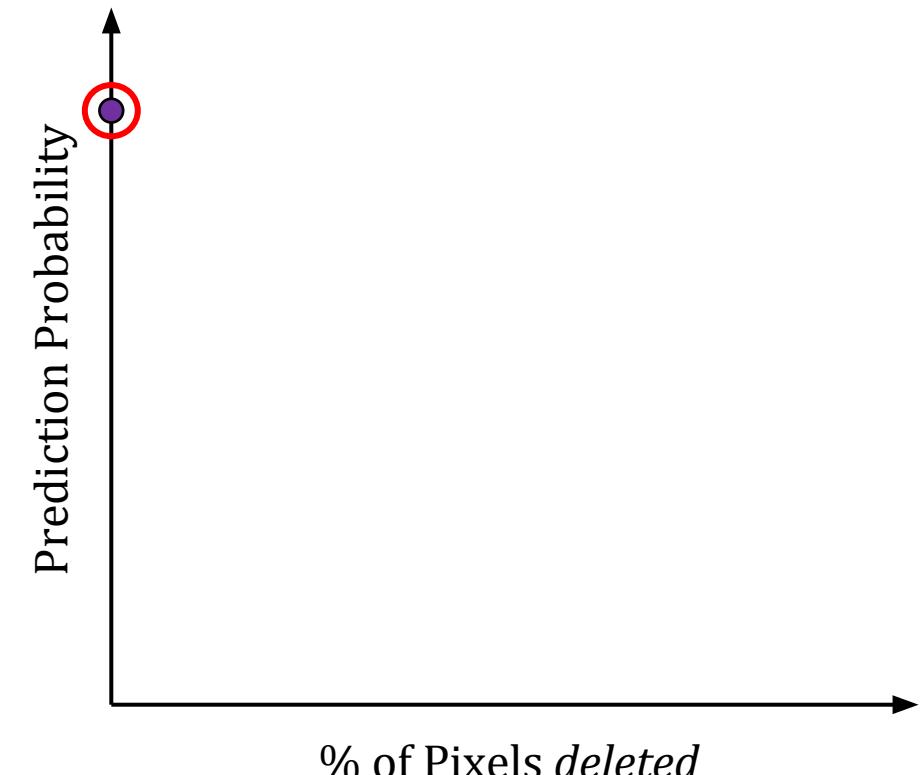
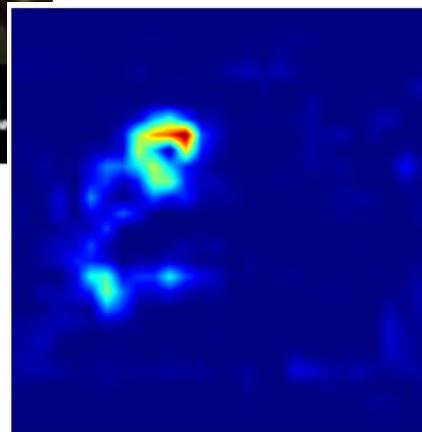
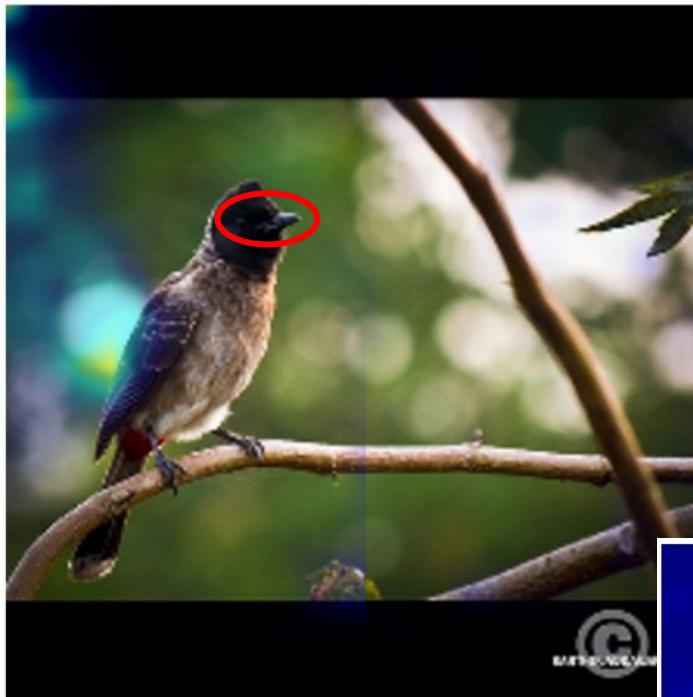
Understand the Behavior

Help make decisions

Useful for Debugging

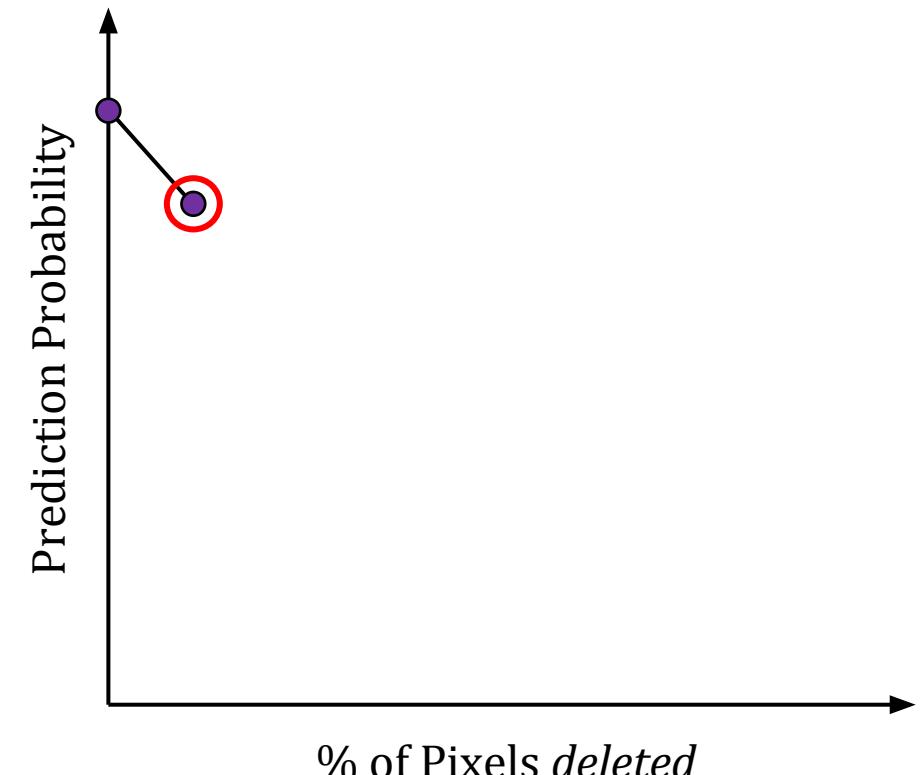
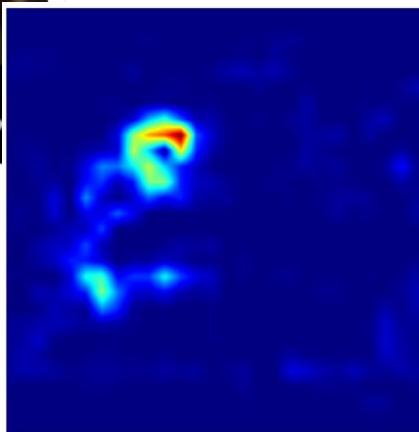
How important are selected features?

- **Deletion:** remove important features and see what happens..



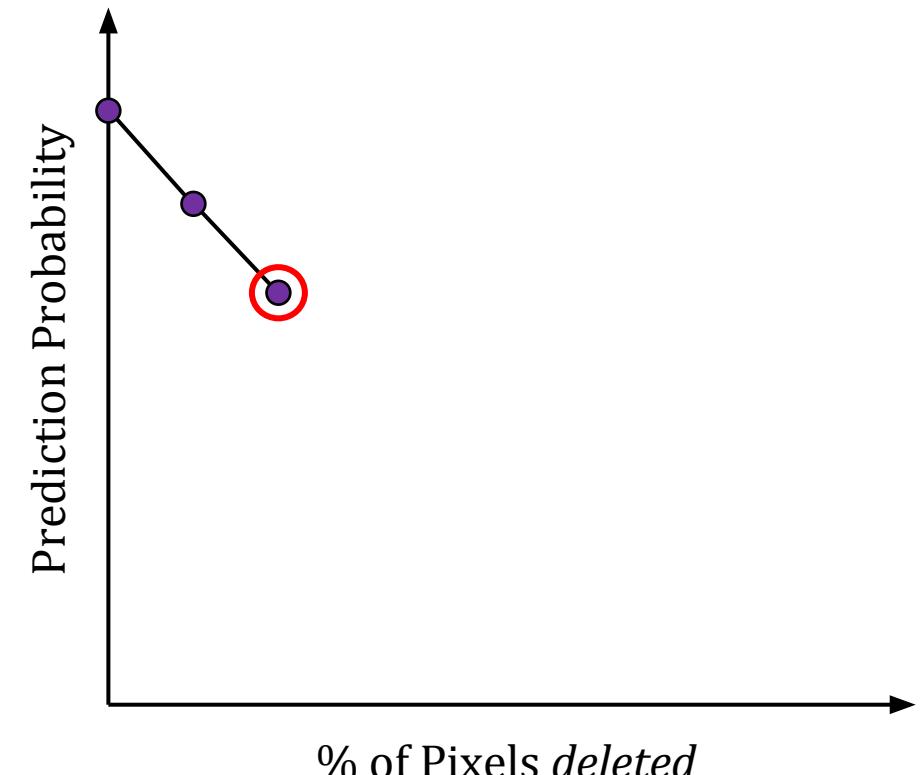
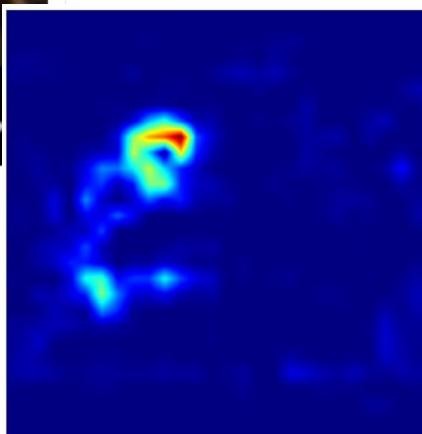
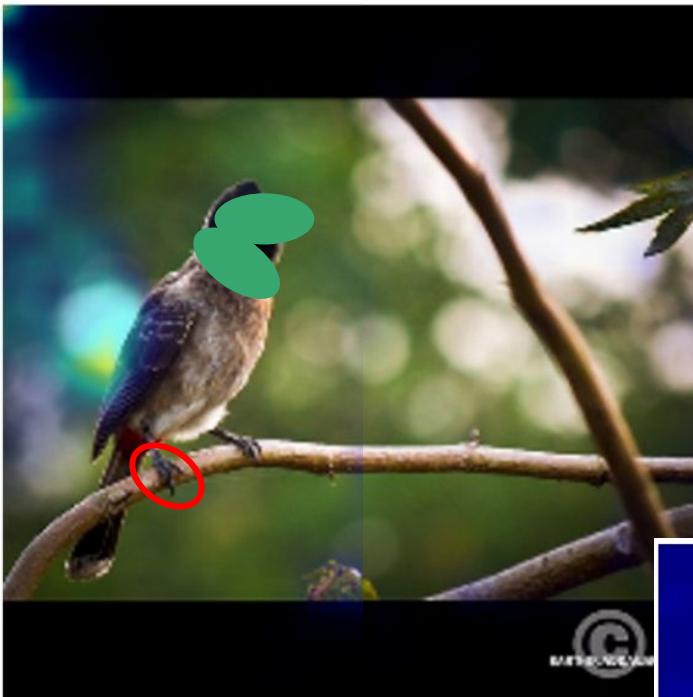
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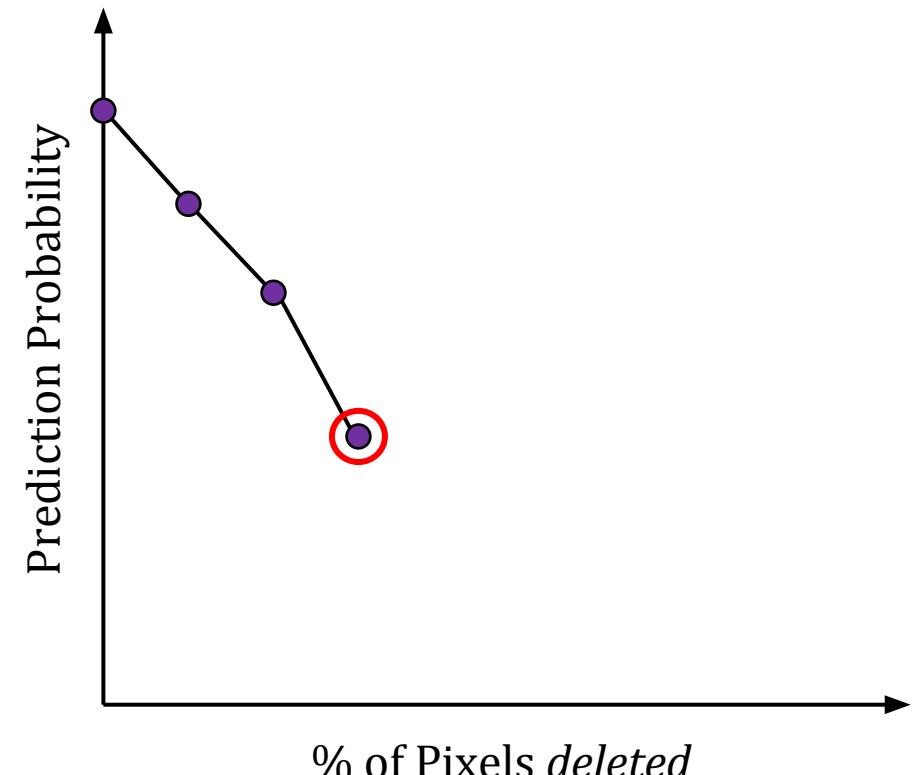
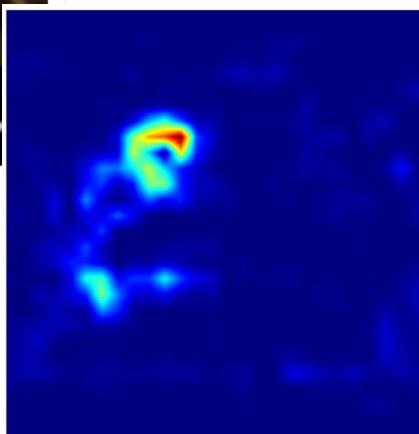
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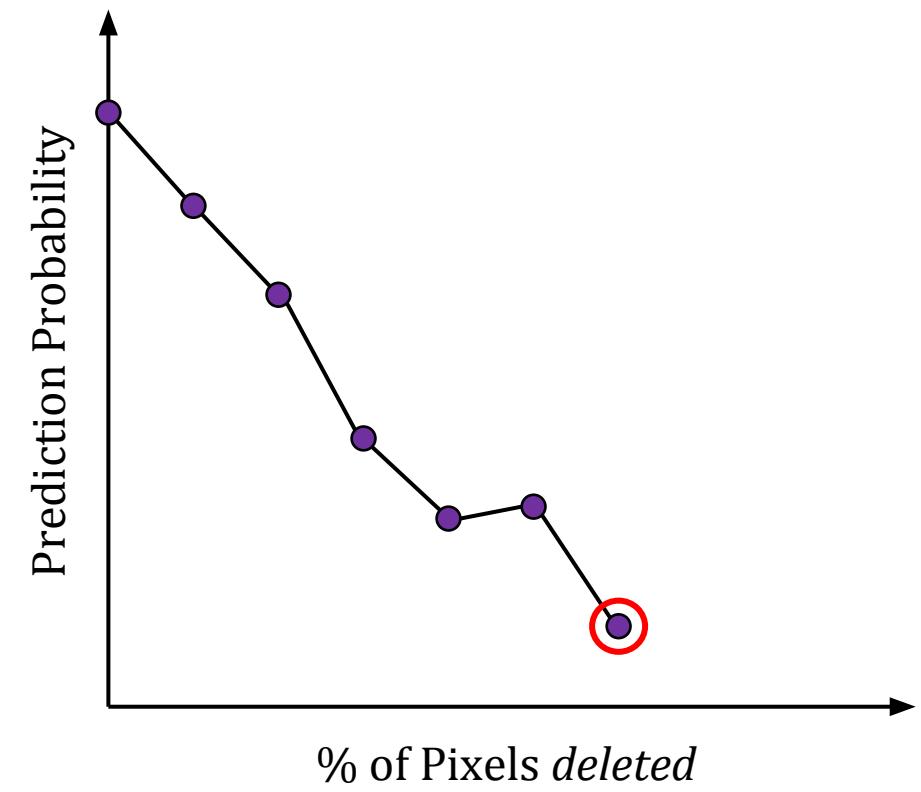
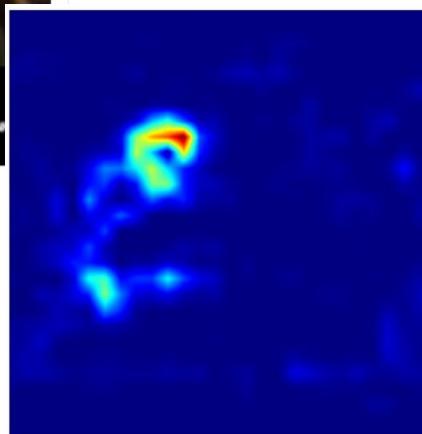
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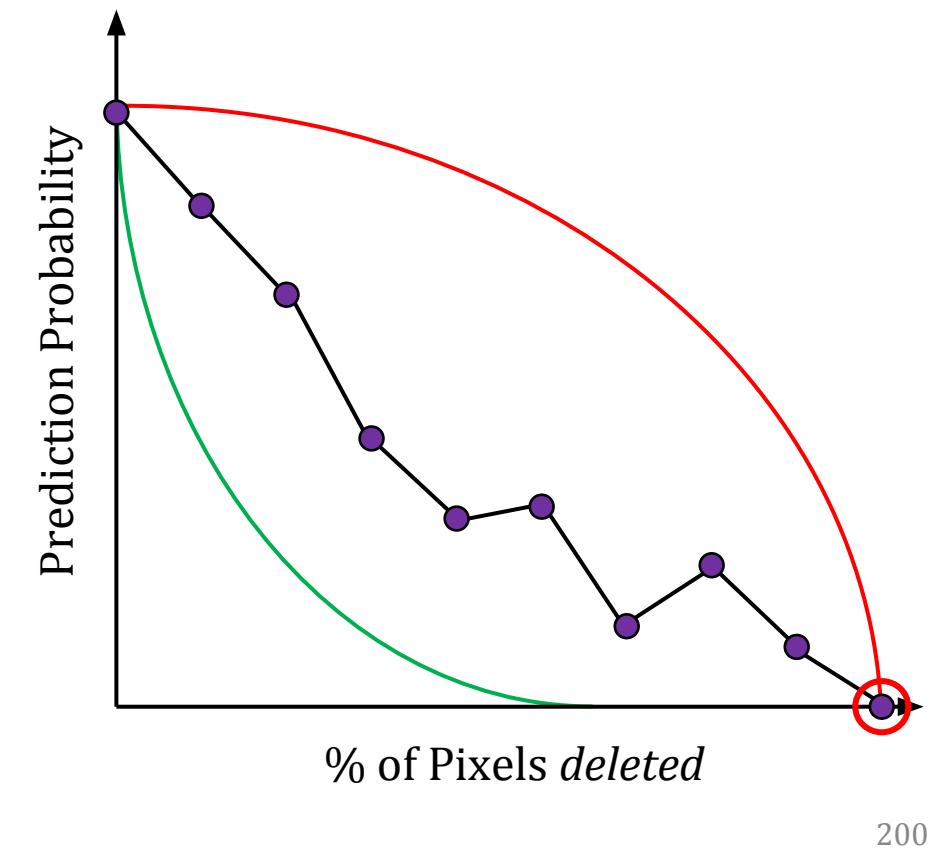
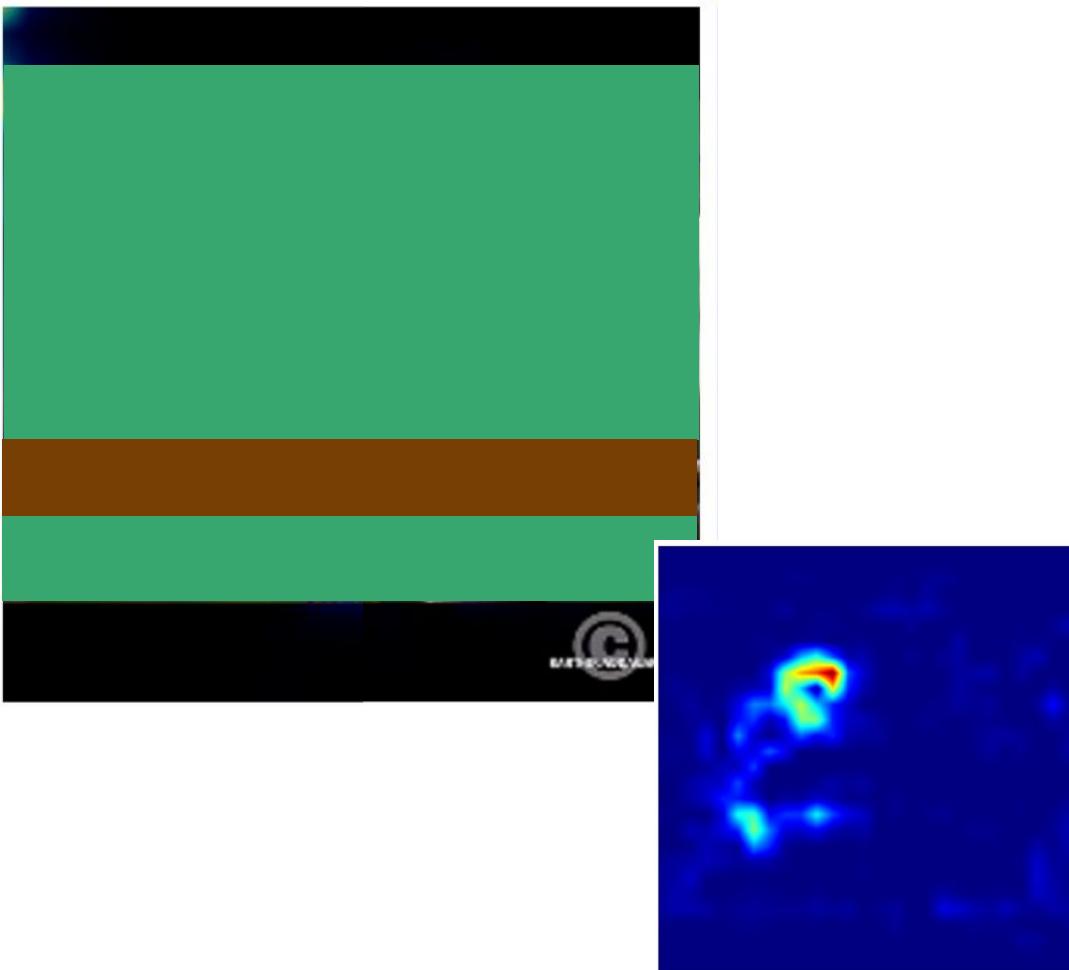
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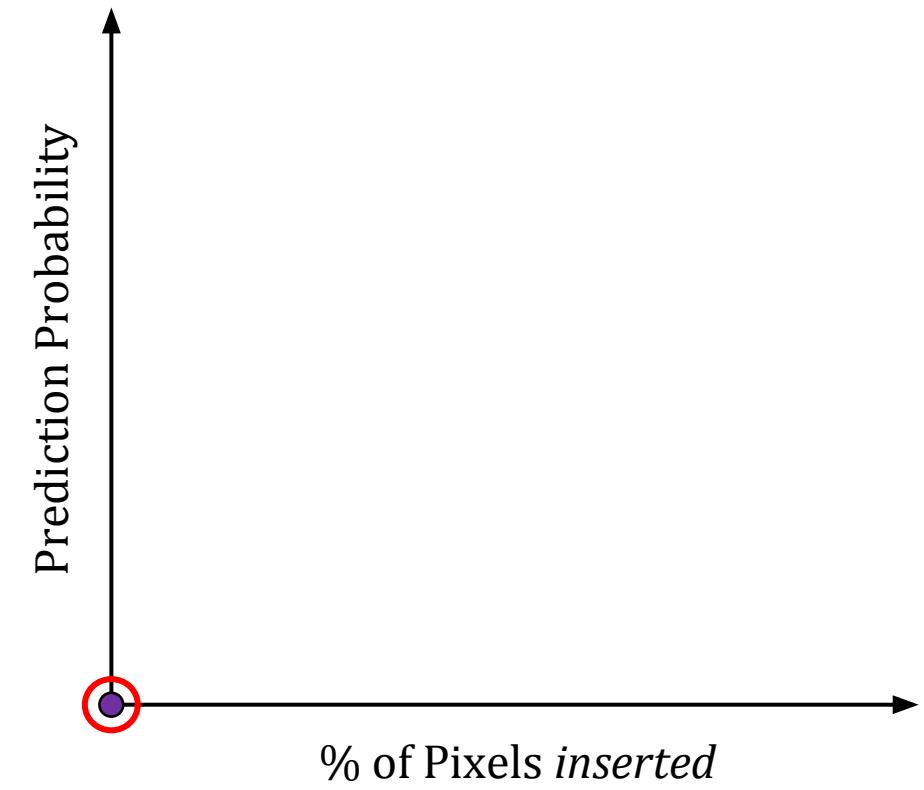
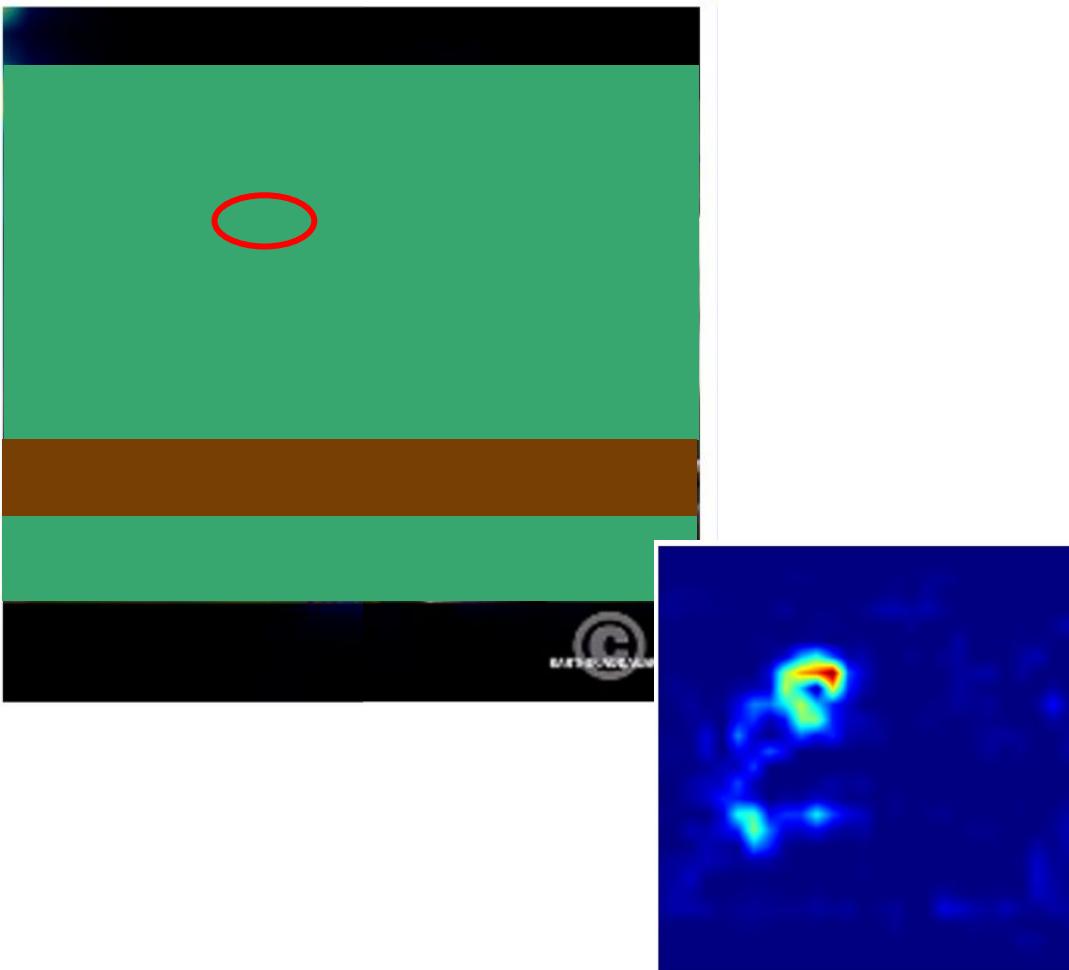
How important are selected features?

- **Deletion:** remove important features and see what happens..



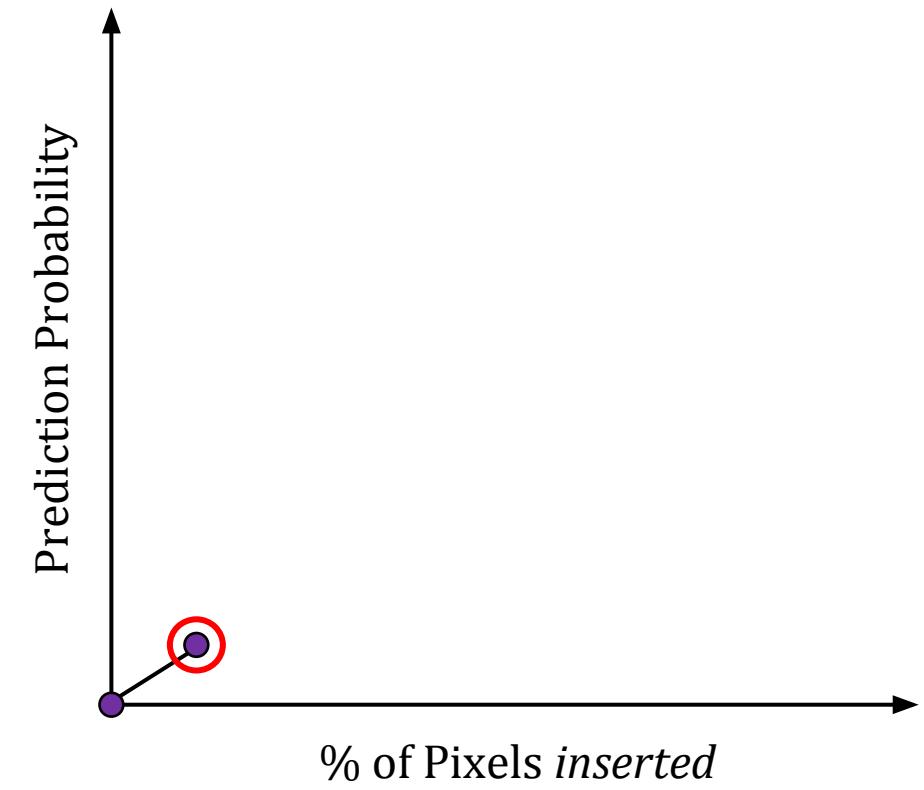
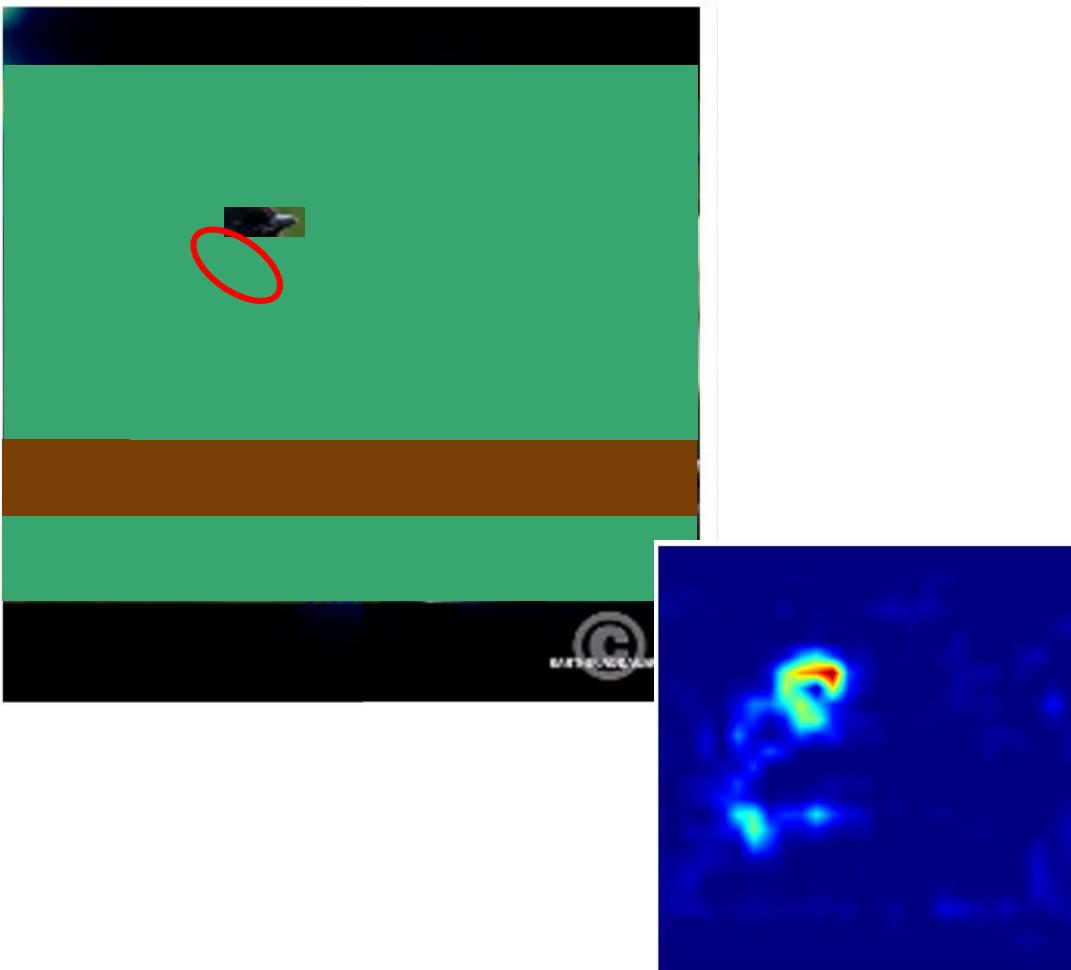
How important are selected features?

- **Insertion:** add important features and see what happens..



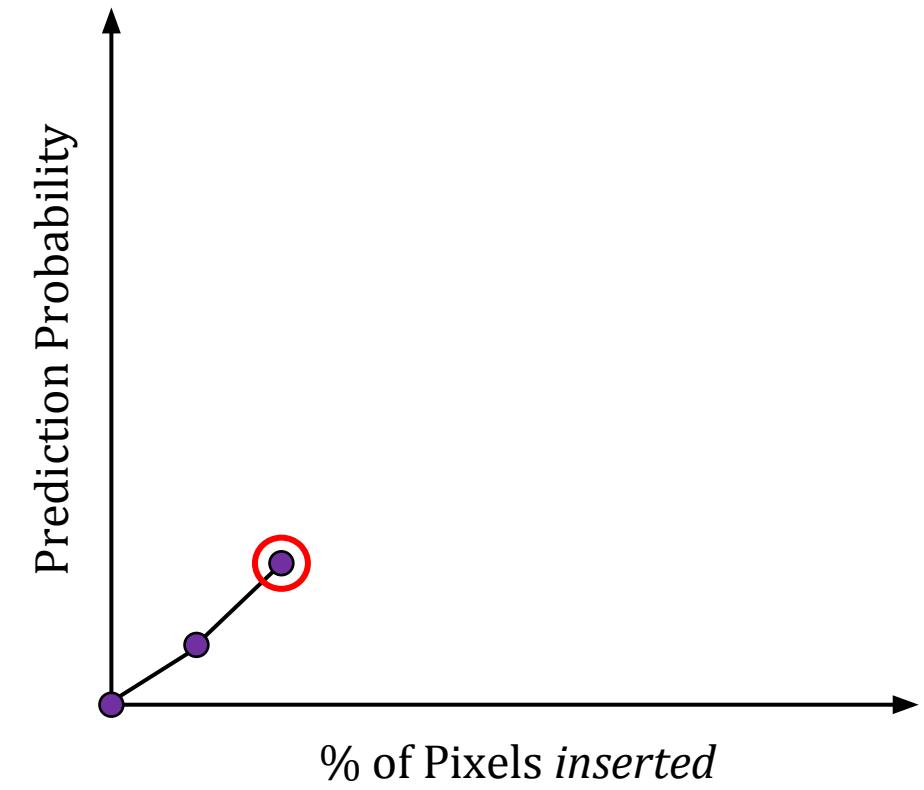
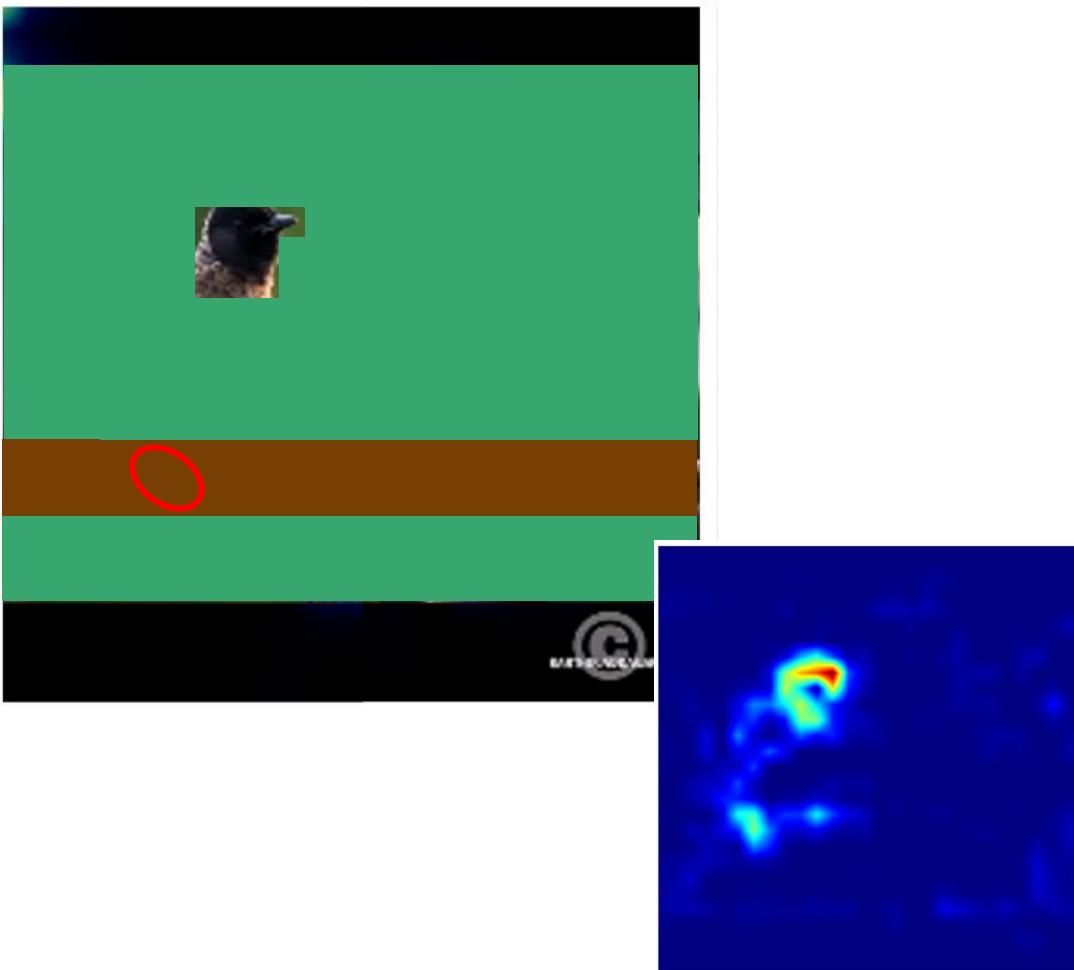
How important are selected features?

- **Insertion:** add important features and see what happens..



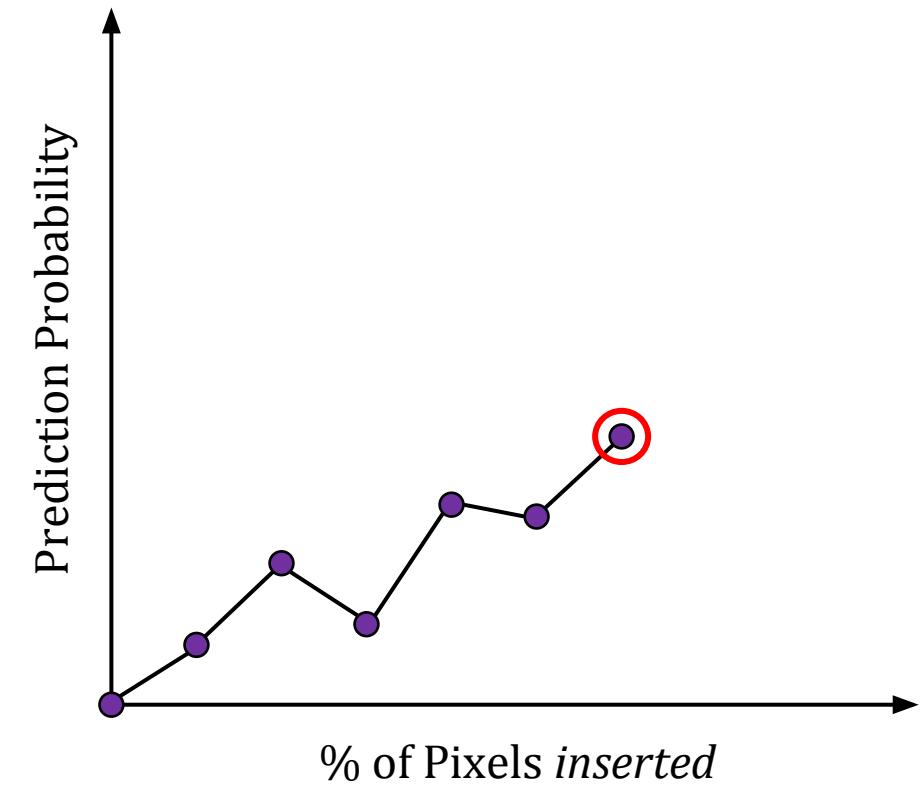
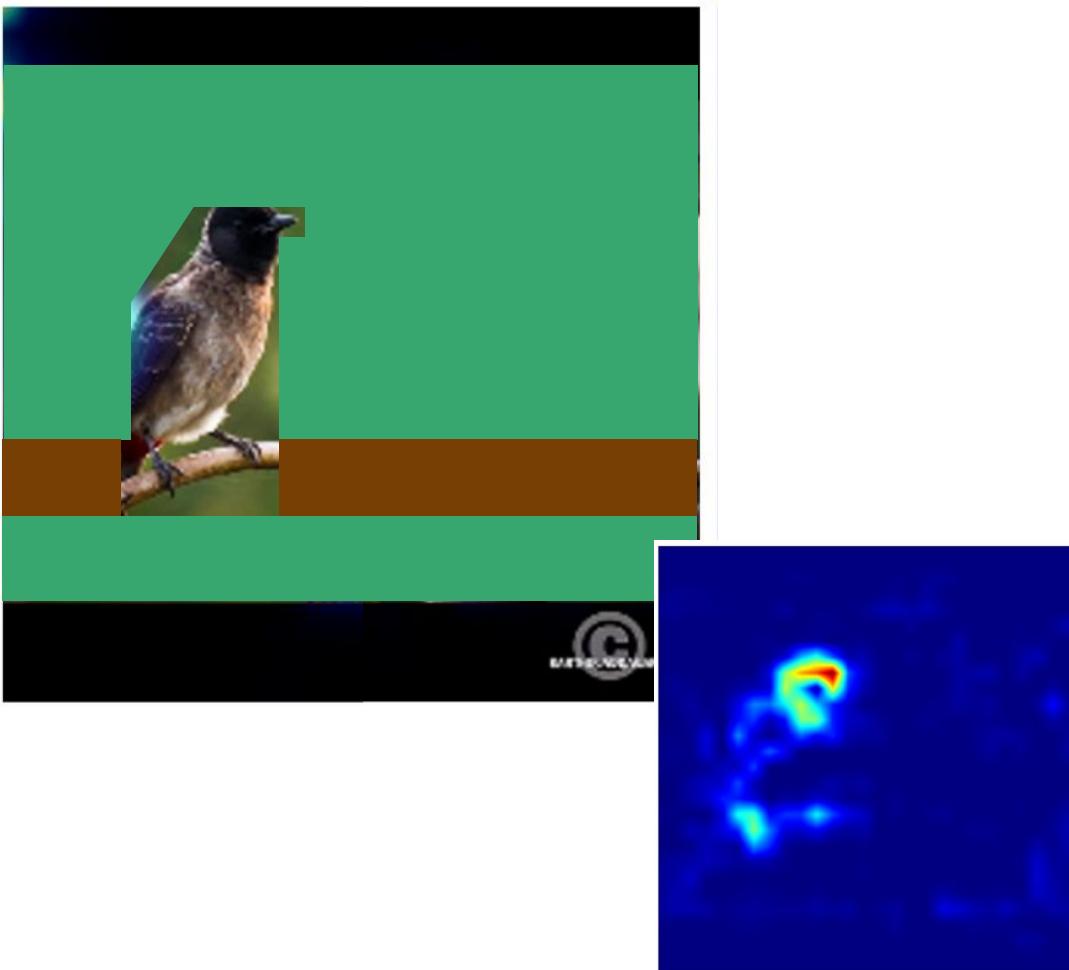
How important are selected features?

- **Insertion:** add important features and see what happens..



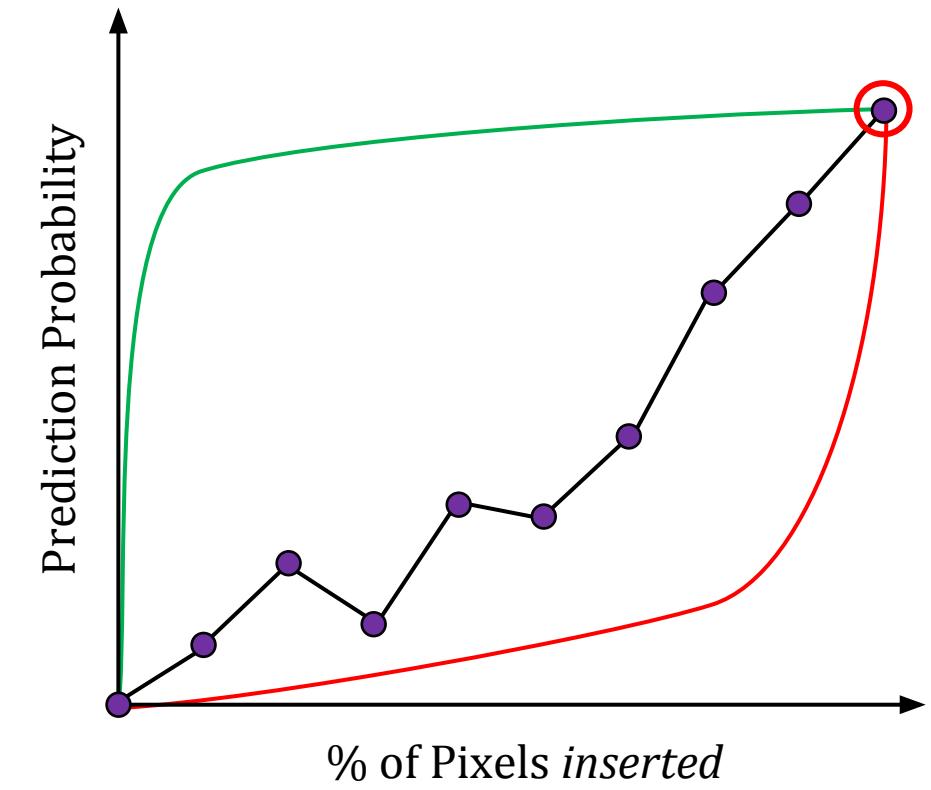
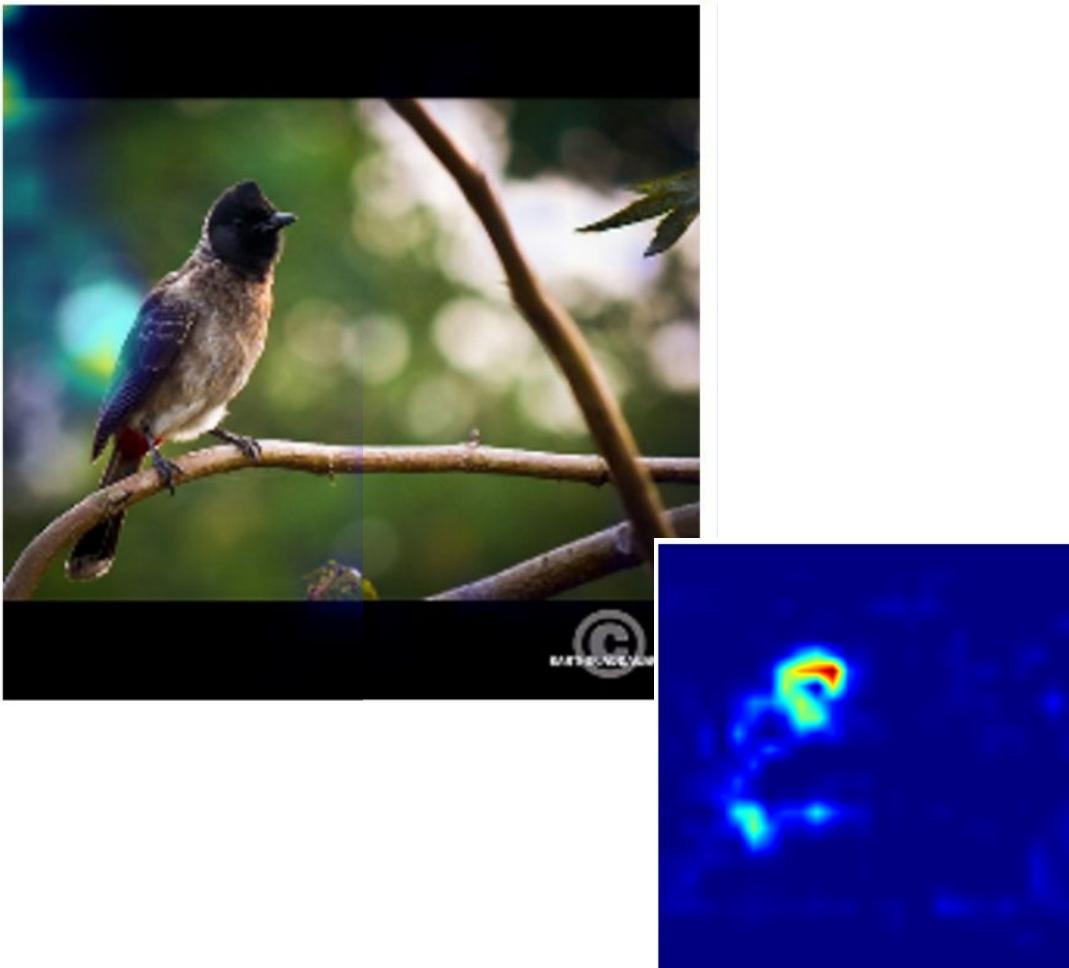
How important are selected features?

- **Insertion:** add important features and see what happens..



How important are selected features?

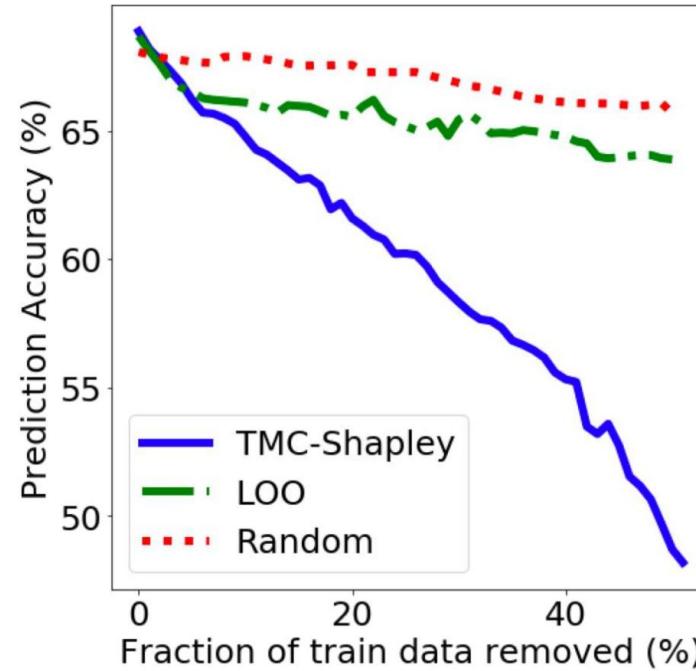
- **Insertion:** add important features and see what happens..



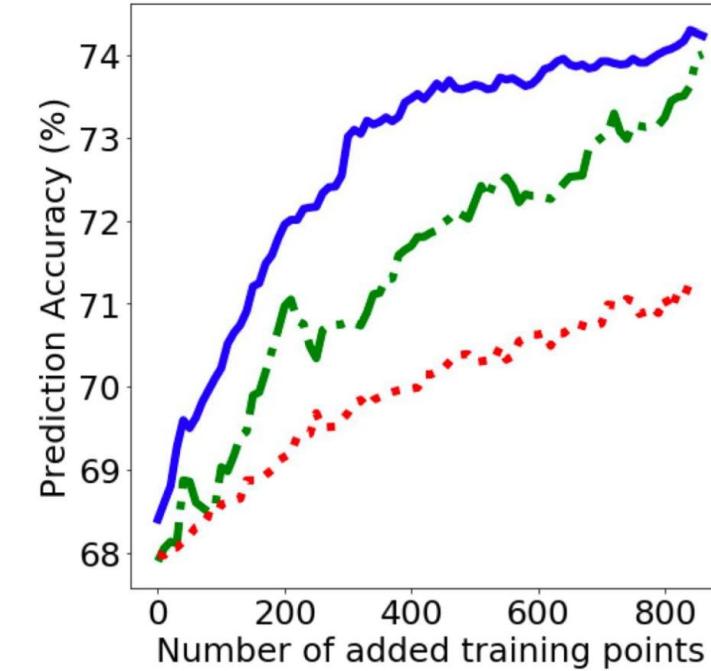
Same Idea: For *Training Data*

Add/remove **influential** training data, see what happens

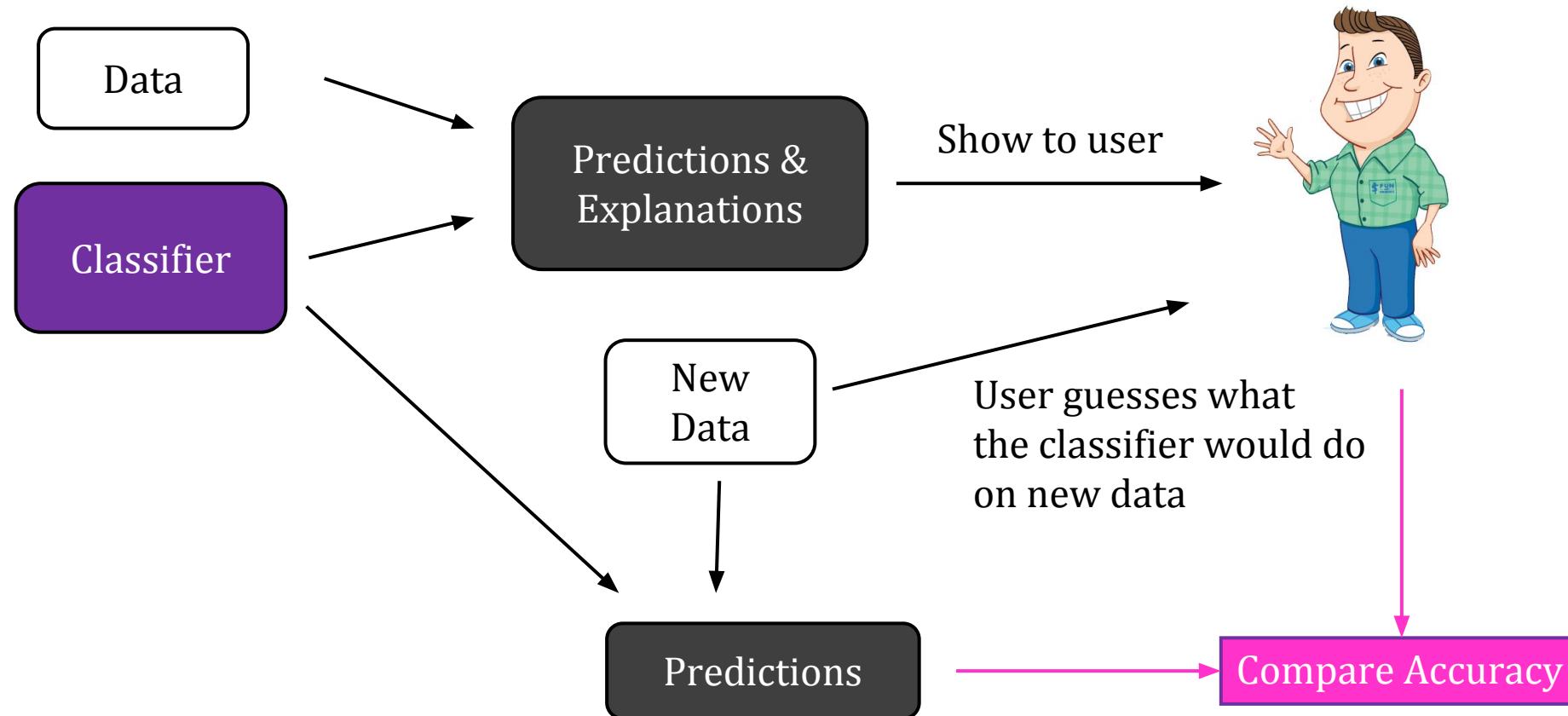
Removing high value data



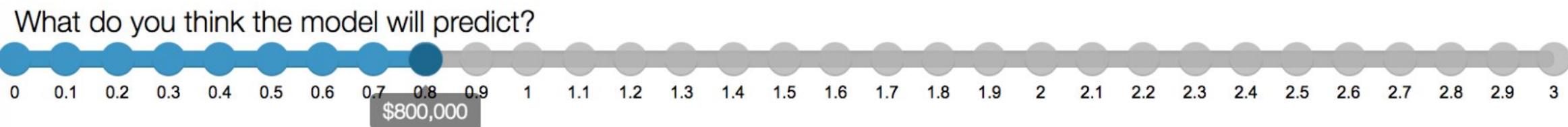
Adding high value data



Predicting Behavior (“Simulation”)



Predicting Behavior (“Simulation”)



How confident are you the model will predict this?

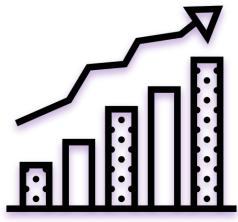
1 2 3 4 5

It's likely the model
will predict
something else

I'm confident the
model will predict
this

(a) Step 1: Participants were asked to guess the model’s prediction and state their confidence.

Evaluating Post hoc Explanations

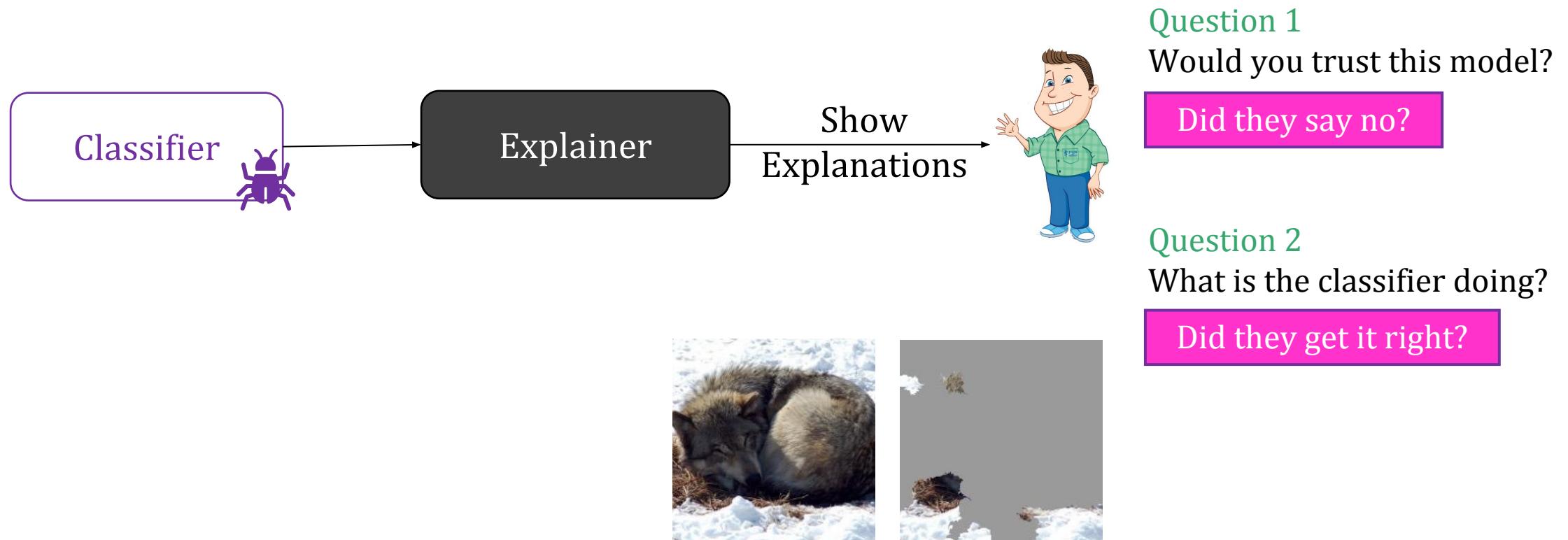


Understand the Behavior

Help make decisions

Useful for Debugging

1. Detecting Problems in Classifiers



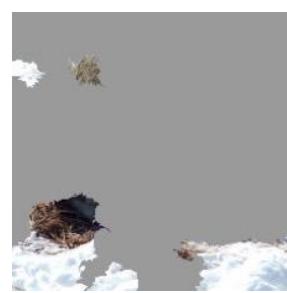
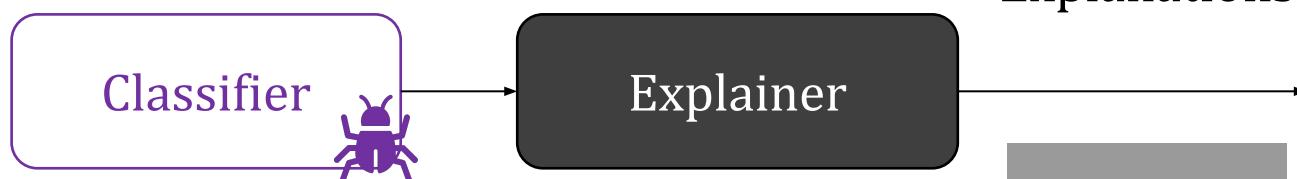
2. Comparing Classifiers



Show
Explanations

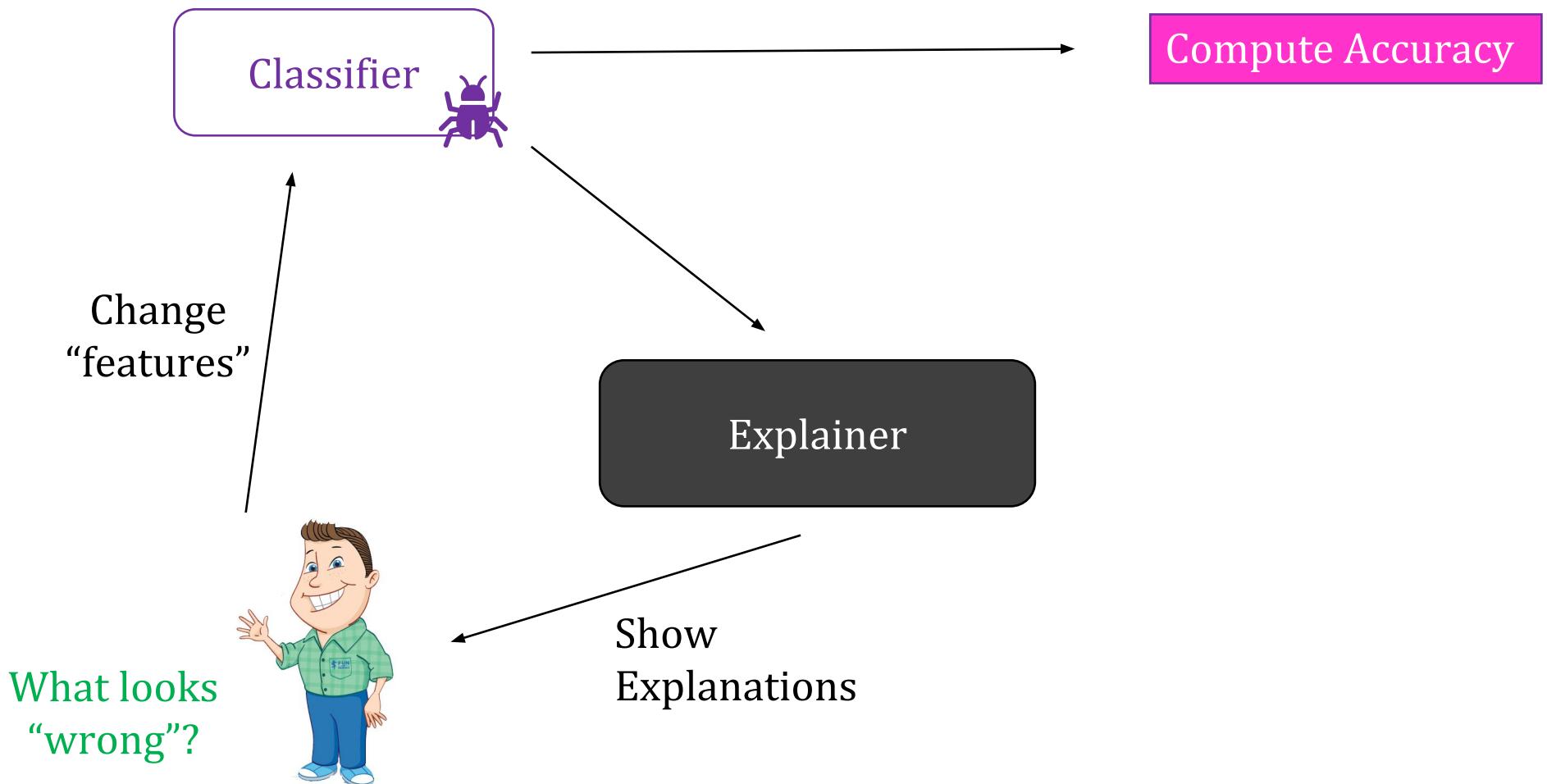


Question
Which algorithm is better?



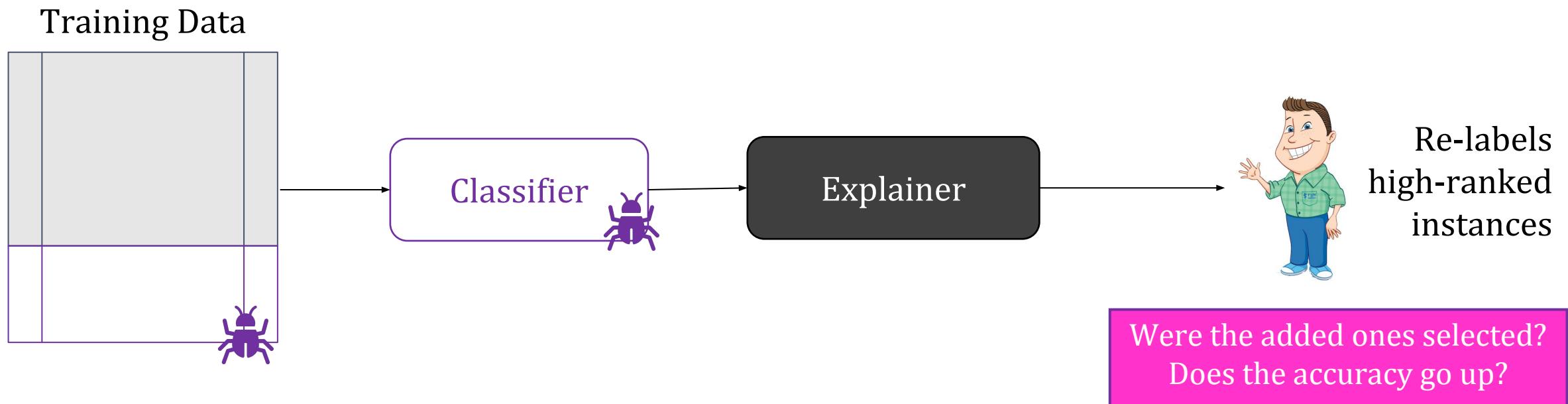
Did they pick the right one?

3. “Fixing” Features of Classifiers

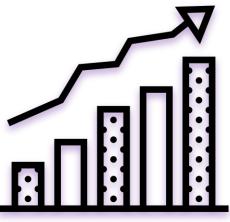


4. Finding Errors in Training Data

- **Prototypical Explanations:** important instances from training data



Evaluating Posthoc Explanations



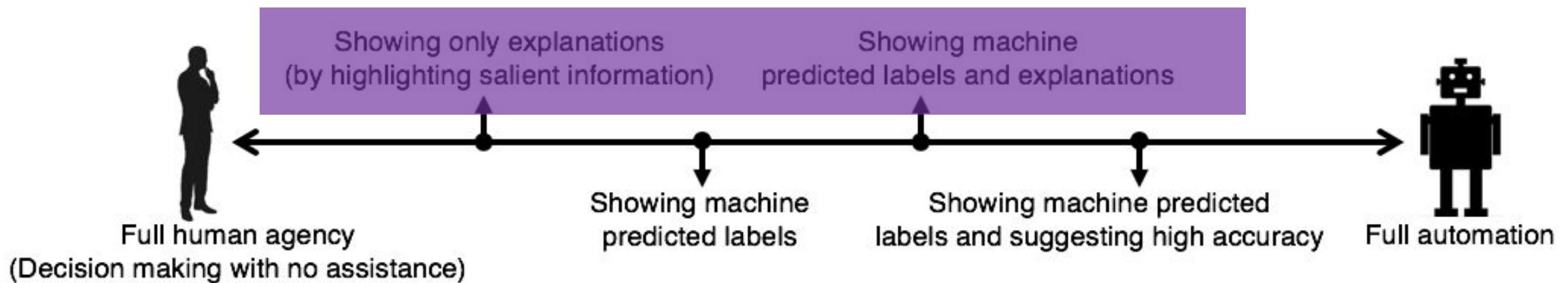
Understand the Behavior

Help make decisions

Useful for Debugging

Human-AI Collaboration

- Are Explanations Useful for Making Decisions?
 - For tasks where the algorithms are not reliable by themselves



Human-AI Collaboration

- Deception Detection: Identify fake reviews online
 - Are Humans better detectors with explanations?

Note: The highlighted words are important words which machine learning classifiers use to decide if a review is genuine or deceptive. The below scale shows level of importance of each word.



I would not stay at this hotel again. The rooms had a fowl odor. It seemed as though the carpets have never been cleaned. The neighborhood was also less than desirable. The housekeepers seemed to be snooping around while they were cleaning the rooms. I will say that the front desk staff was friendly albeit slightly dimwitted.

Genuine

Deceptive

Machine Teaching

Monarch



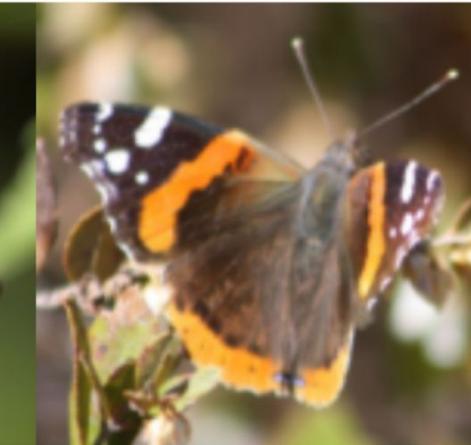
Viceroy



Queen



Red Admiral



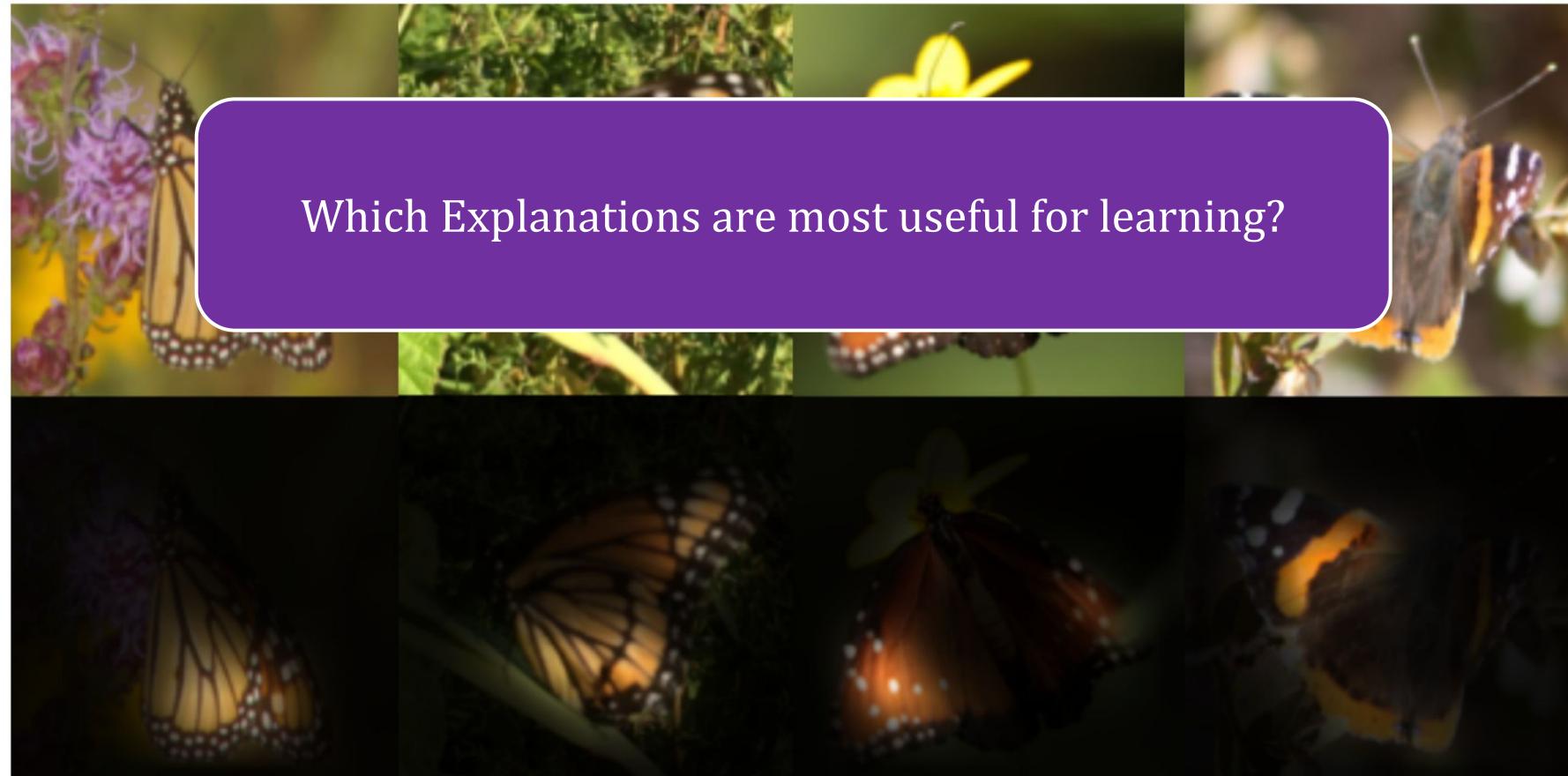
Machine Teaching

Monarch

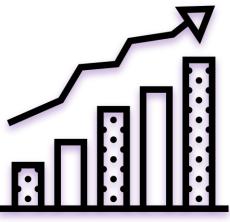
Viceroy

Queen

Red Admiral



Evaluating Posthoc Explanations



Understand the Behavior

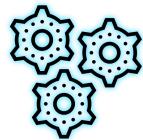
Help make decisions

Useful for Debugging

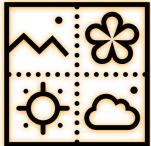
Limitations of Evaluating Explanations

- Evaluation setup is often **very easy/simple** (or **unrealistic**)
 - E.g. “bugs” are obvious artifacts, classifiers are different from each other
 - Instances/perturbations create out-of-domain points
- Sometimes **flawed**
 - E.g. is model explanation same as human explanation?
- Automated **metrics can be *optimized***
- User studies are **not consistent**
 - Affected by choice of: UI, phrasing, visualization, population, incentives, ...
 - ML researchers are not trained for this 😞
- Conclusions are difficult to generalize

Tutorial on Post hoc Explanations



Approaches for Post hoc Explainability



Explanations in Different Modalities



Evaluation of Explanations

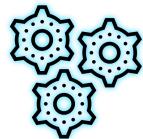


Limits of Post hoc Explainability

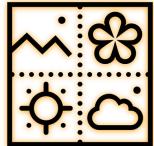


Future of Post hoc Explainability

Tutorial on Post hoc Explanations



Approaches for Post hoc Explainability



Explanations in Different Modalities



Evaluation of Explanations



Limits of Post hoc Explainability



Future of Post hoc Explainability

Limits of Post hoc Explanations



Limitations

- **Faithfulness/Fidelity**
 - Some explanation methods do not '*reflect*' the underlying model.

Limitations

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- **Fragility**
 - Post-hoc explanations can be easily manipulated.

Limitations

- **Faithfulness/Fidelity**
 - Some explanation methods do not '*reflect*' the underlying model.
- **Fragility**
 - Post-hoc explanations can be easily manipulated.
- **Stability**
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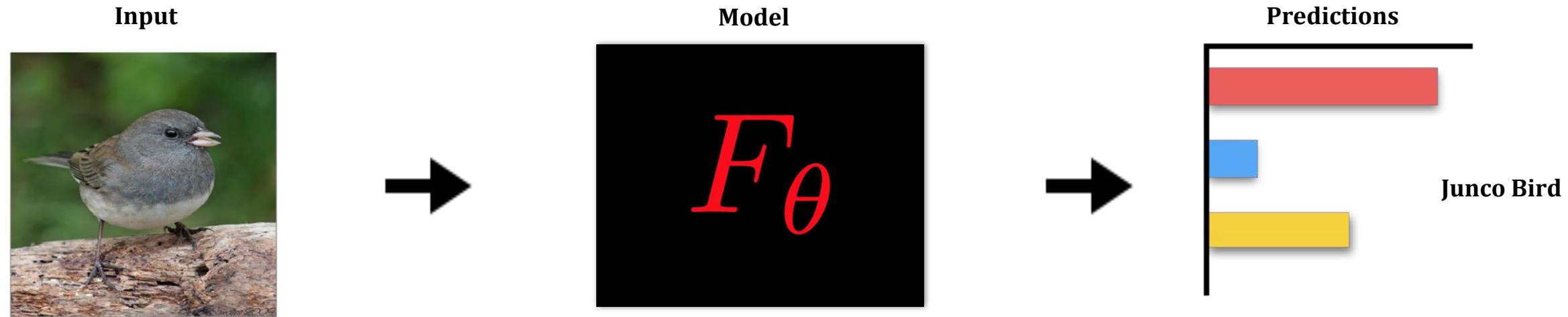
Limitations

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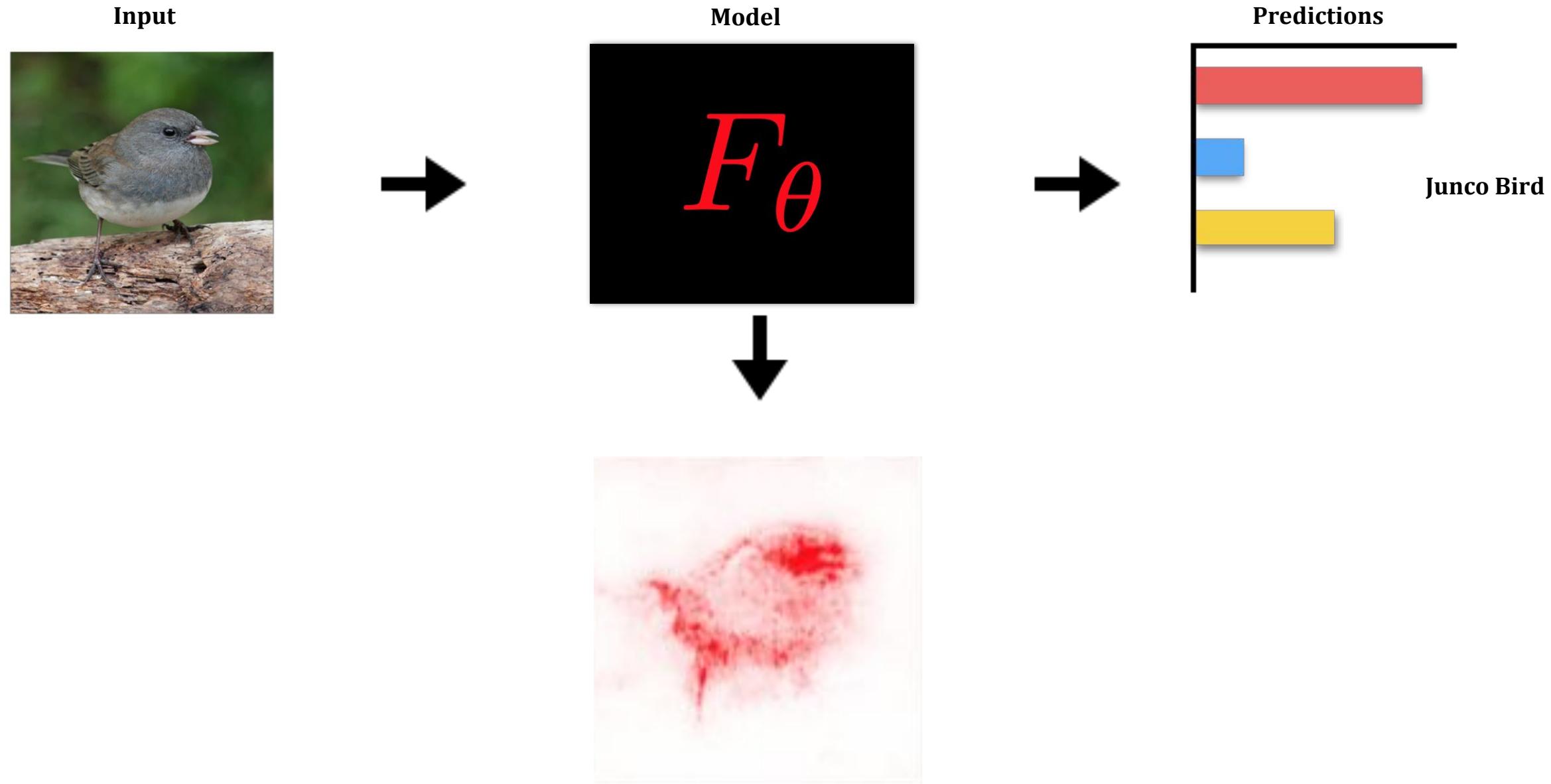
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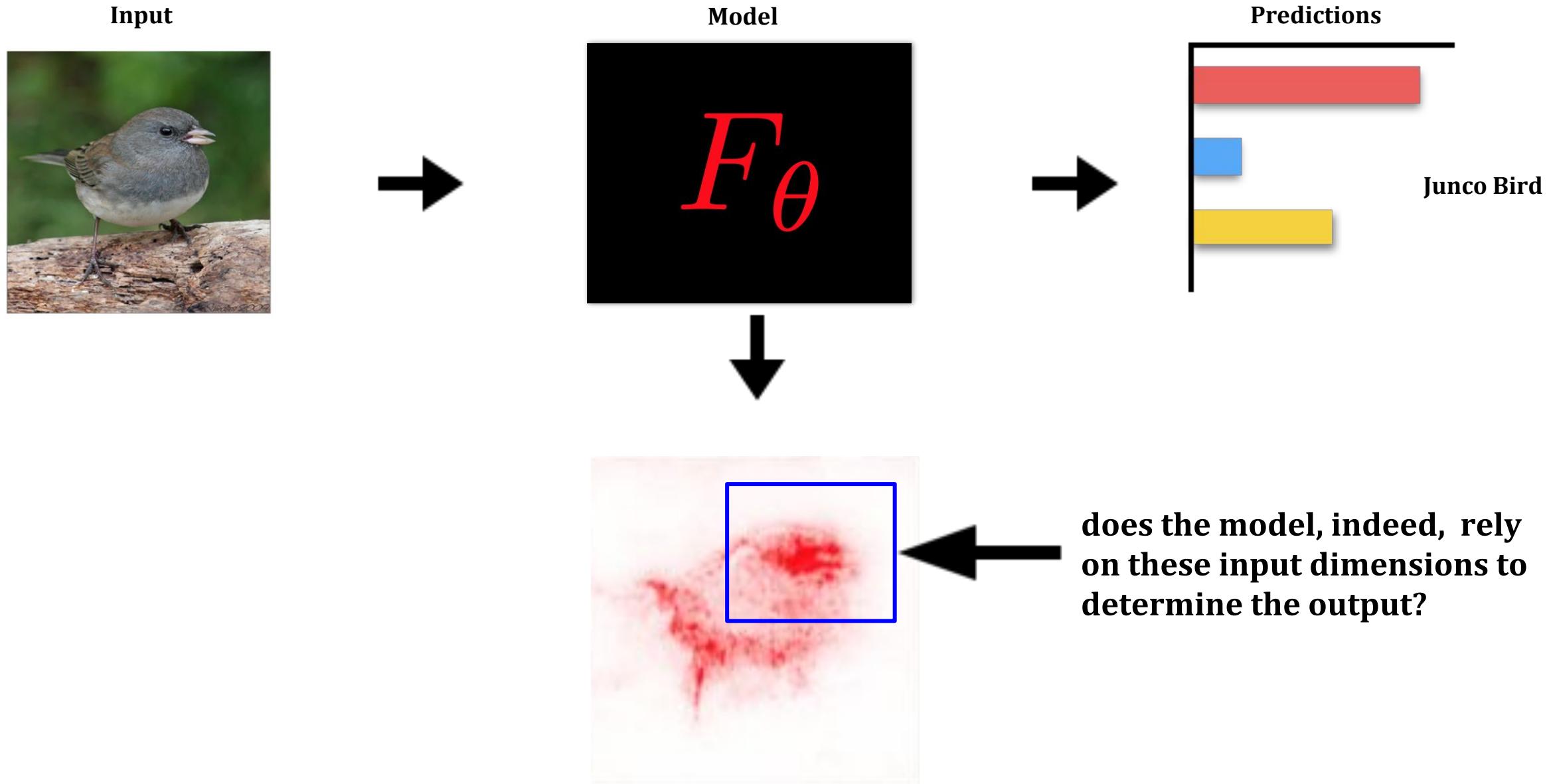
Do Explanations Capture Model-based Discriminative Signals?



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Faithfulness/Fidelity

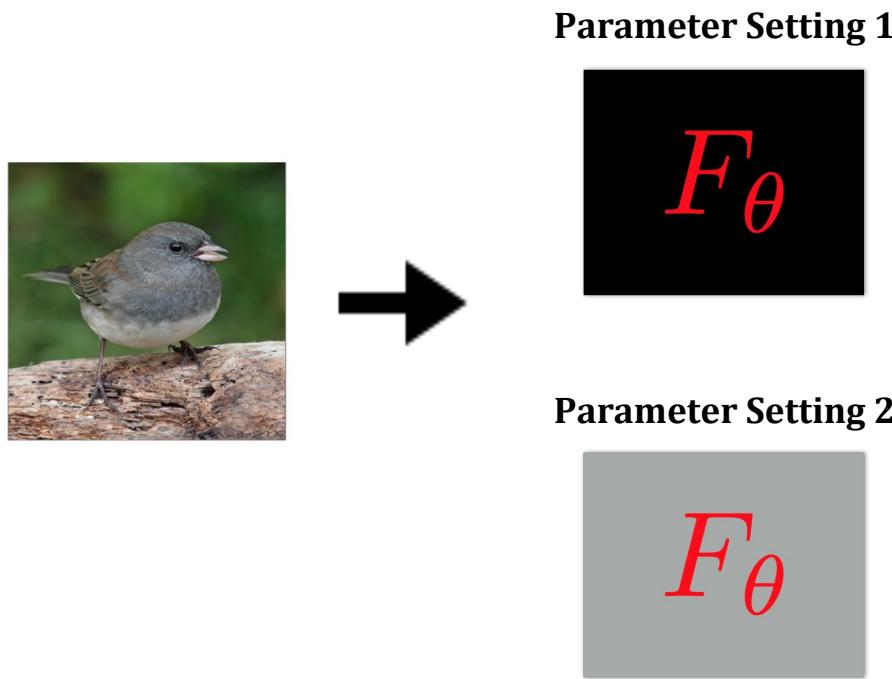
Does the output of an explanation method reflect the underlying '*computation or behavior*' of the black-box model?

Sanity Check for Faithfulness/Fidelity

- **Sensitivity to Model Parameters:** if the parameter settings change, the explanations should change.

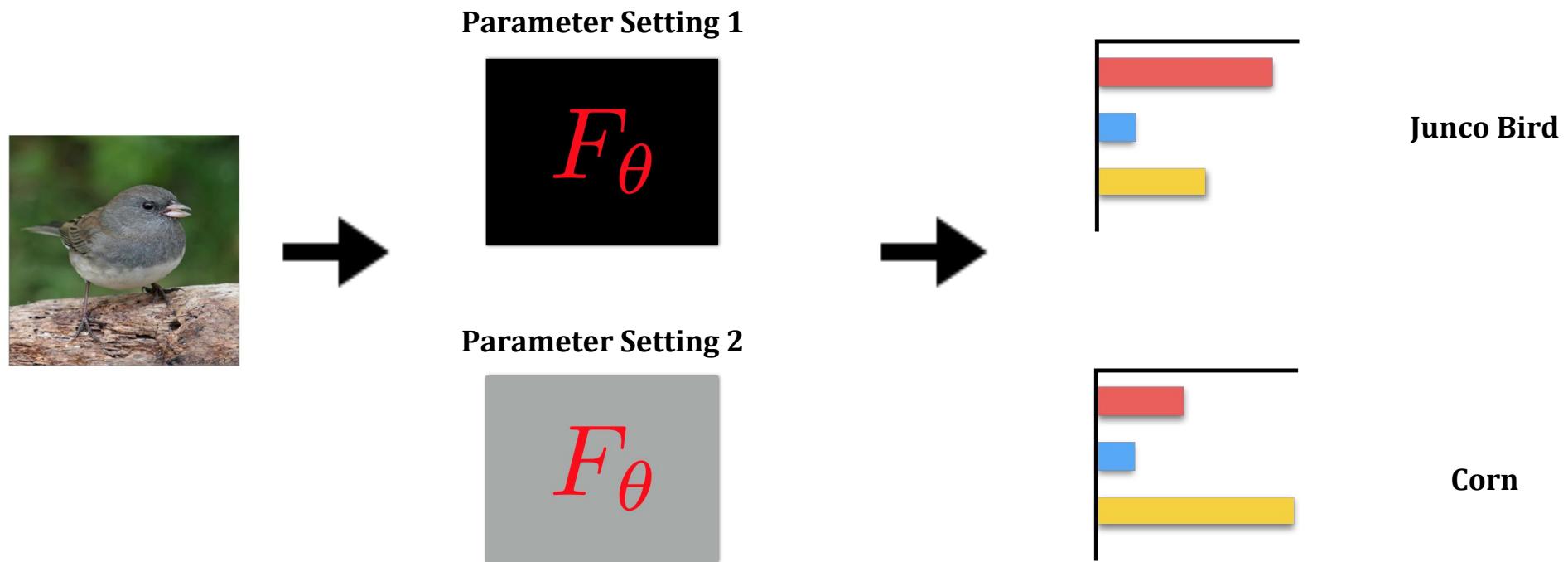
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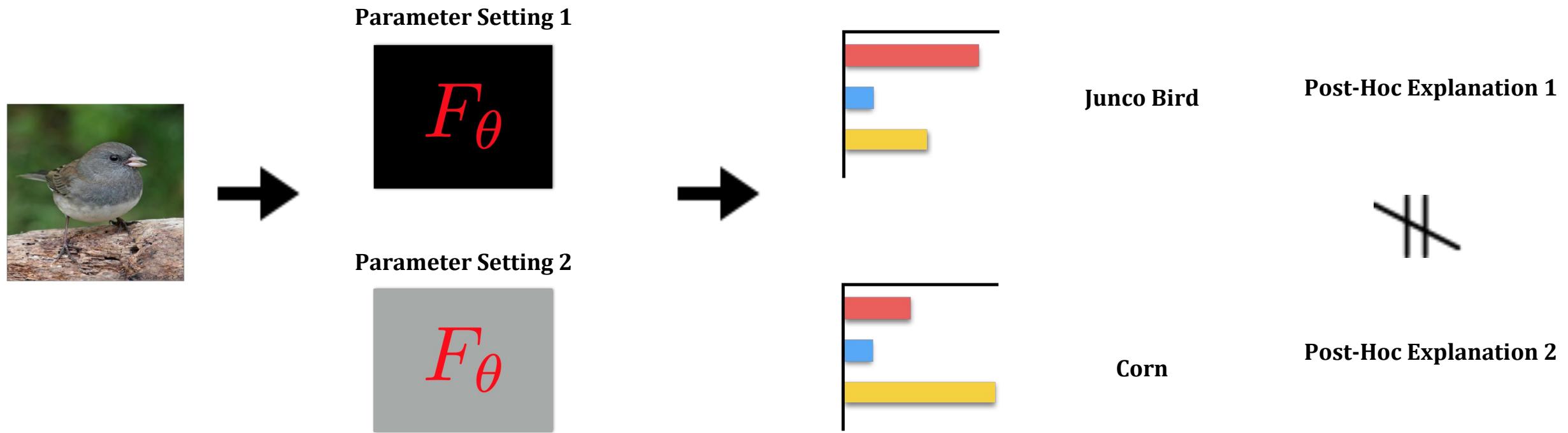
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Sanity Check for Faithfulness/Fidelity

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Cascading Randomization Inception-V3

- **Randomize (re-initialize)** model parameters starting from top layer all the way to the input.



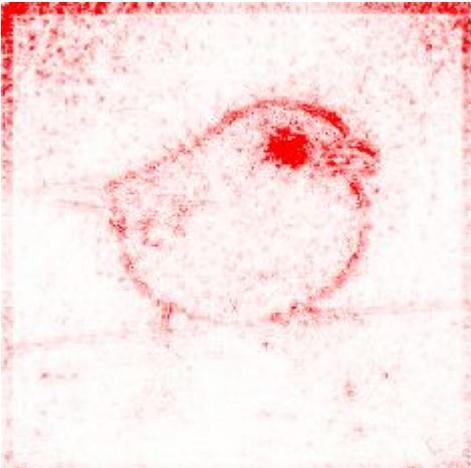
Guided BackProp Explanation Inception-V3 ImageNet

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Normal Model
Explanation



Guided BackProp Explanation Inception-V3 ImageNet

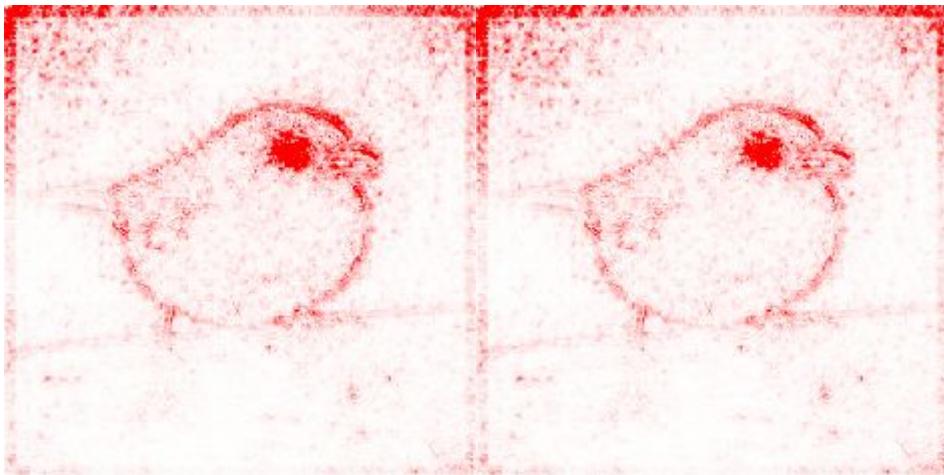
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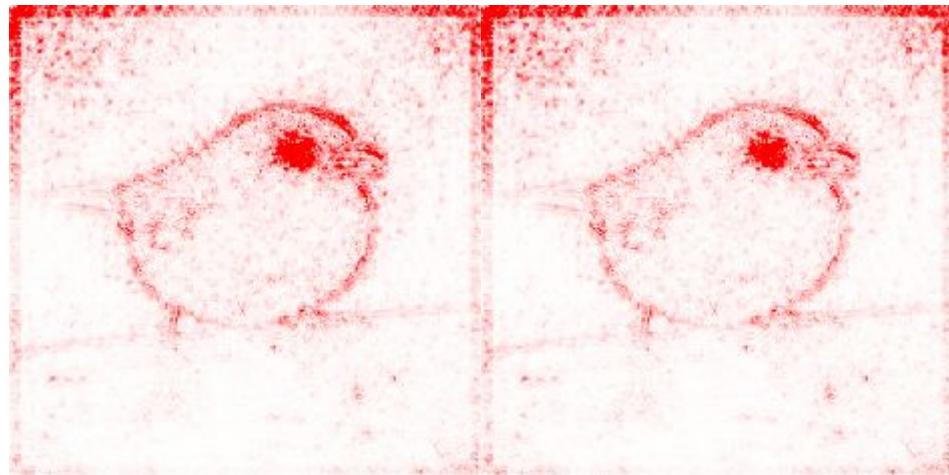


Guided BackProp Explanation Inception-V3 ImageNet

Normal Model
Explanation



Top Layer
Randomized



Cascading Randomization Inception-V3

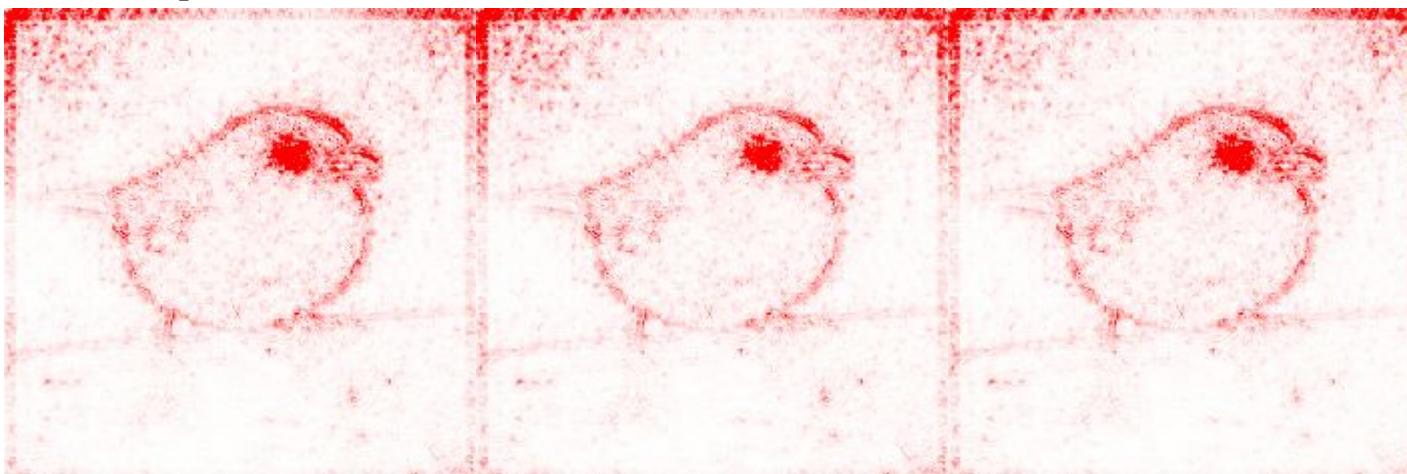
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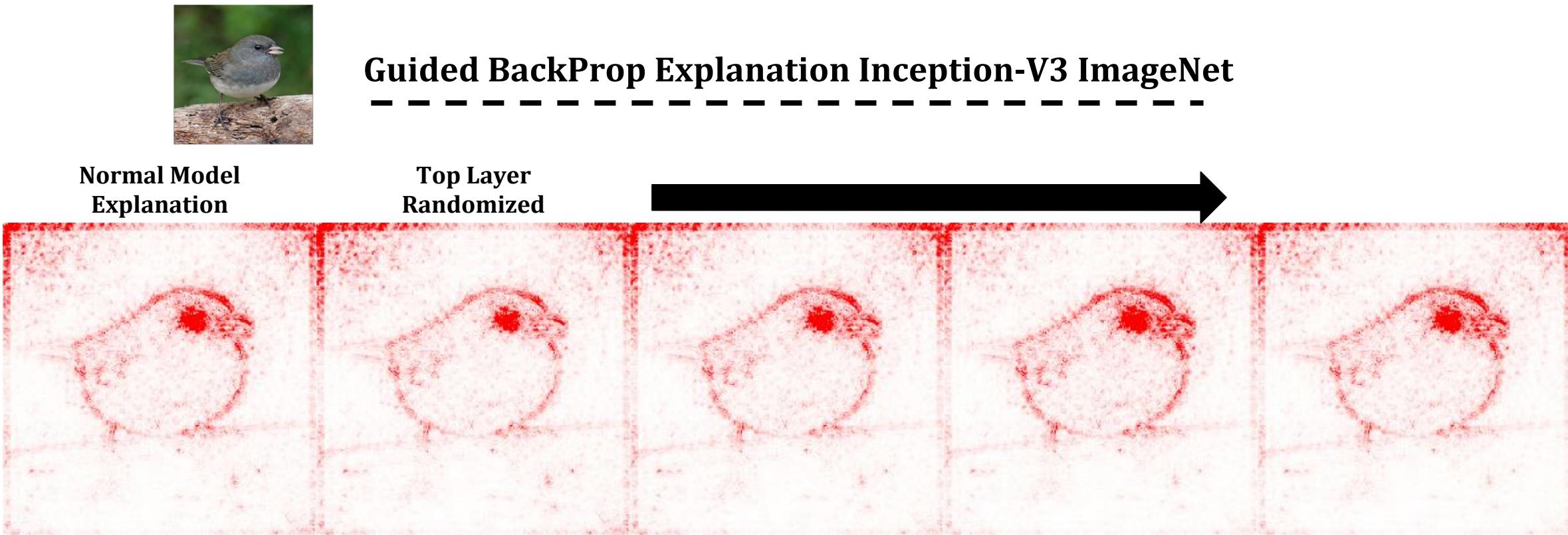
Normal Model
Explanation

Top Layer
Randomized



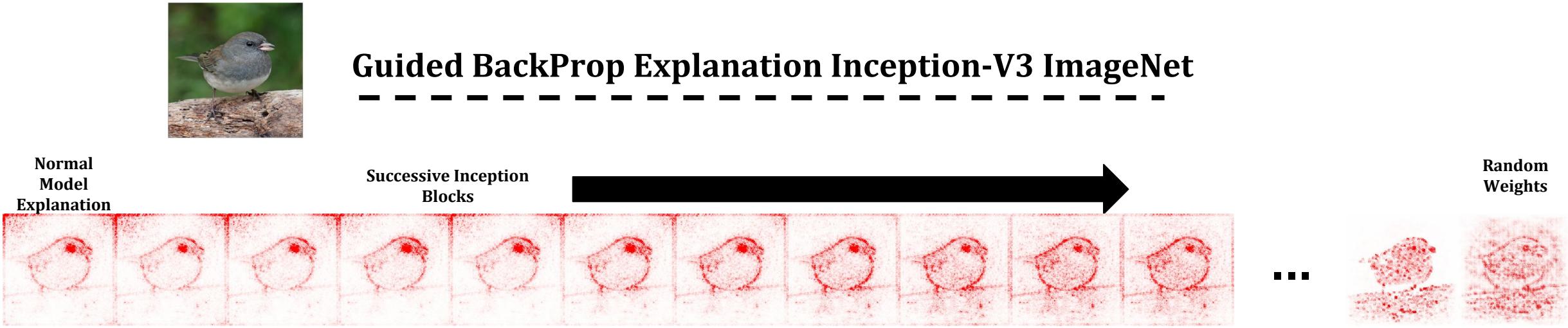
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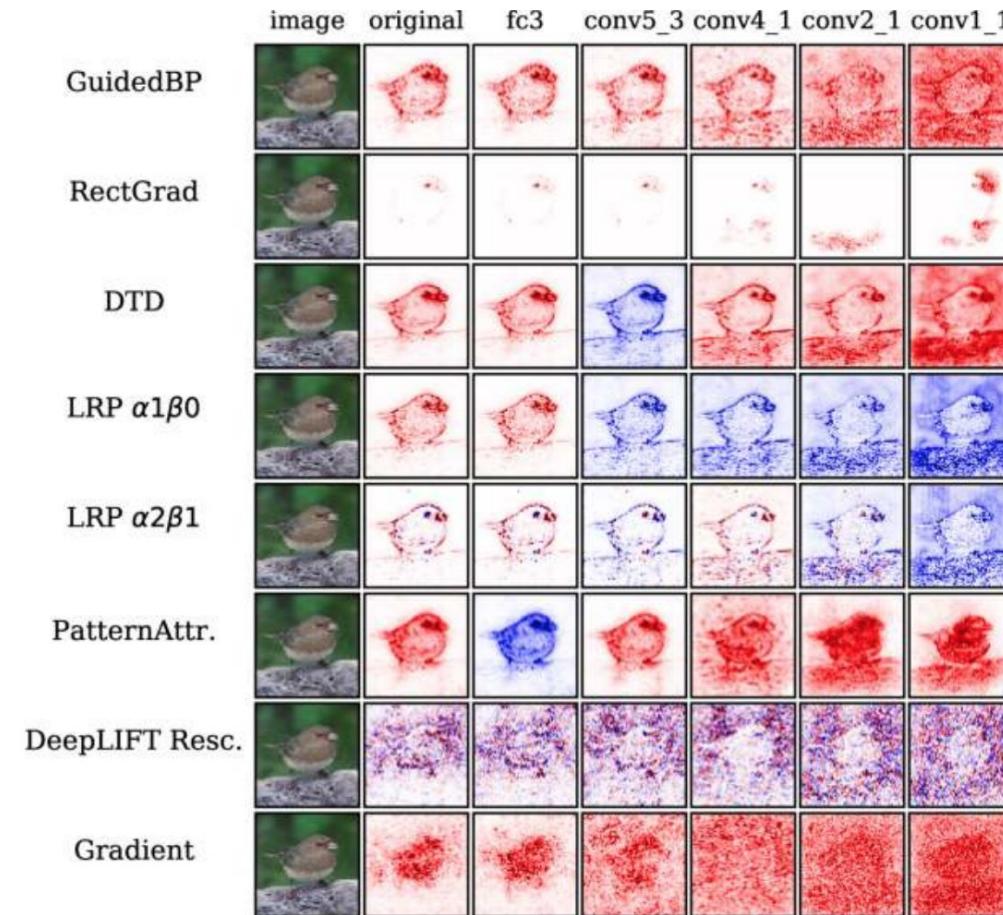
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Guided BackProp is invariant to the higher level weights.

'Modified backprop approaches' are invariant

Method that compute relevance via modified backpropagation and performance positive aggregation along the way are invariant to higher layers.



Source of Invariance

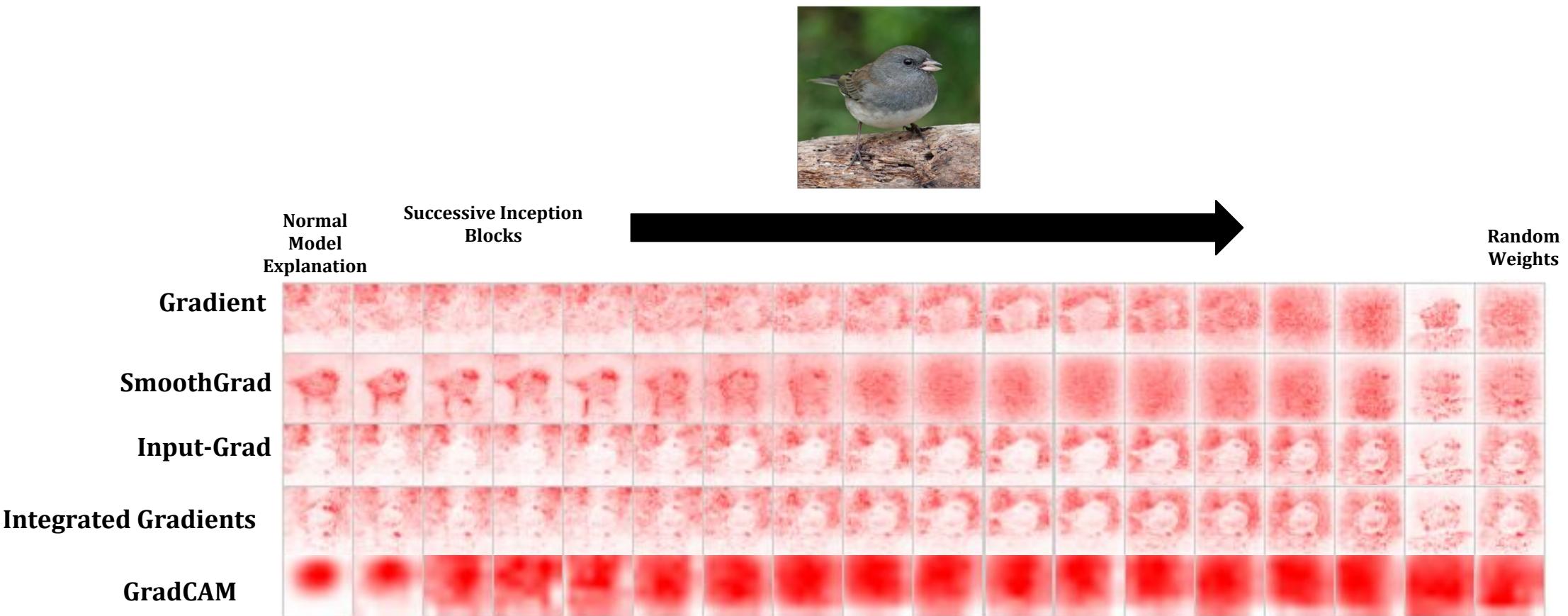
- Guided BackProp and DeConvNet seek to approximately reconstruct the input ([Nie et. al. 2018](#)).
- These modified backprop methods converge to a rank-1 matrix!
This is because the product of a sequence of non-negative matrices (non-orthogonal columns, along with other assumptions) converges to a rank-1 matrix ([*Theorem 1 in Sixt et. al. 2020*](#)).

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- DeConvNet
- Guided BackProp
- Guided GradCAM
- Deep Taylor Decomposition
- Pattern Net and Pattern Attribution (empirically)
- RectGrad

Cascading Randomization Inception-V3



Limitations

- ~~Faithfulness/Fidelity~~

- ~~Some explanation methods do not ‘reflect’ the underlying model.~~

- ~~Fragility~~

- Post-hoc explanations can be easily manipulated.

Post-hoc Explanations are Fragile

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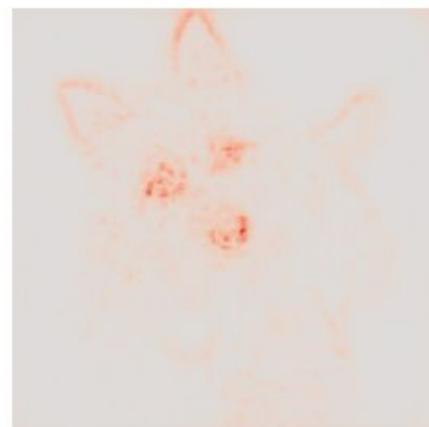
Original Image



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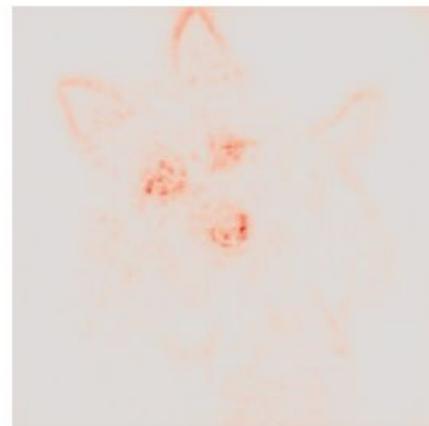
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Manipulated Image



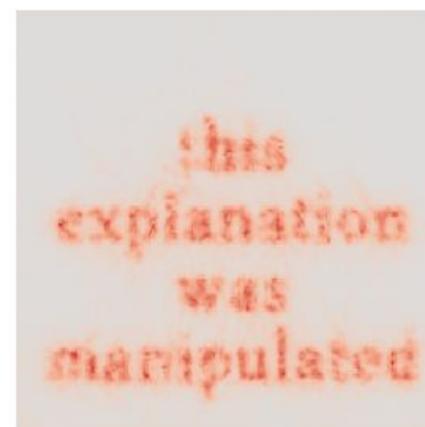
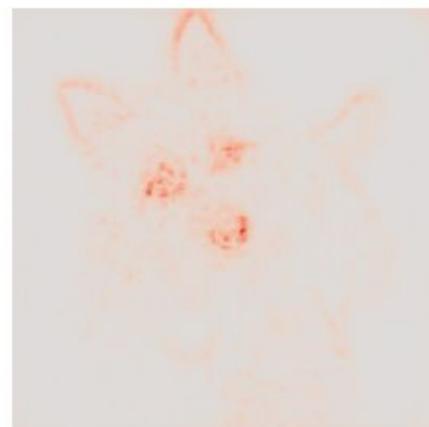
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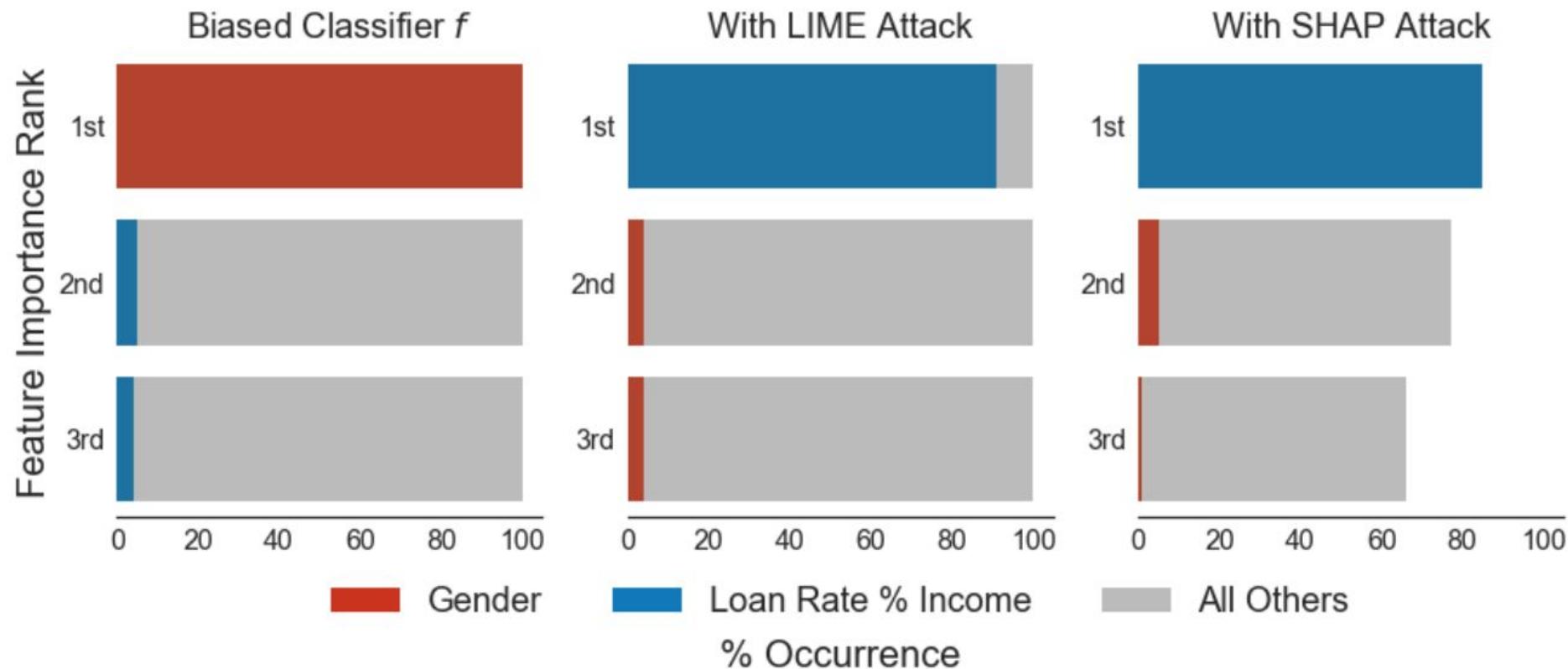


Manipulated Image



Scaffolding Attack on LIME & SHAP

Scaffolding attack used to **hide classifier dependence on gender**.



Adversarial Attack on Explanations

Minimally modify the input with a **small perturbation without changing the model prediction.**

$$\arg \max_{\delta} \mathcal{D}(\mathbf{I}(\mathbf{x}_t; \mathcal{N}), \mathbf{I}(\mathbf{x}_t + \boldsymbol{\delta}; \mathcal{N}))$$

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$$\text{Prediction}(\mathbf{x}_t + \boldsymbol{\delta}; \mathcal{N}) = \text{Prediction}(\mathbf{x}_t; \mathcal{N})$$

Other Attacks

- Shift attack by [Kindermans & Hooker et. al. \(2017\)](#).
- Augmented loss function attack by [Dombrowski et. al. \(2019\)](#).
- Passive and Active fooling loss augmentation attack by [Heo et. al. \(2019\)](#).

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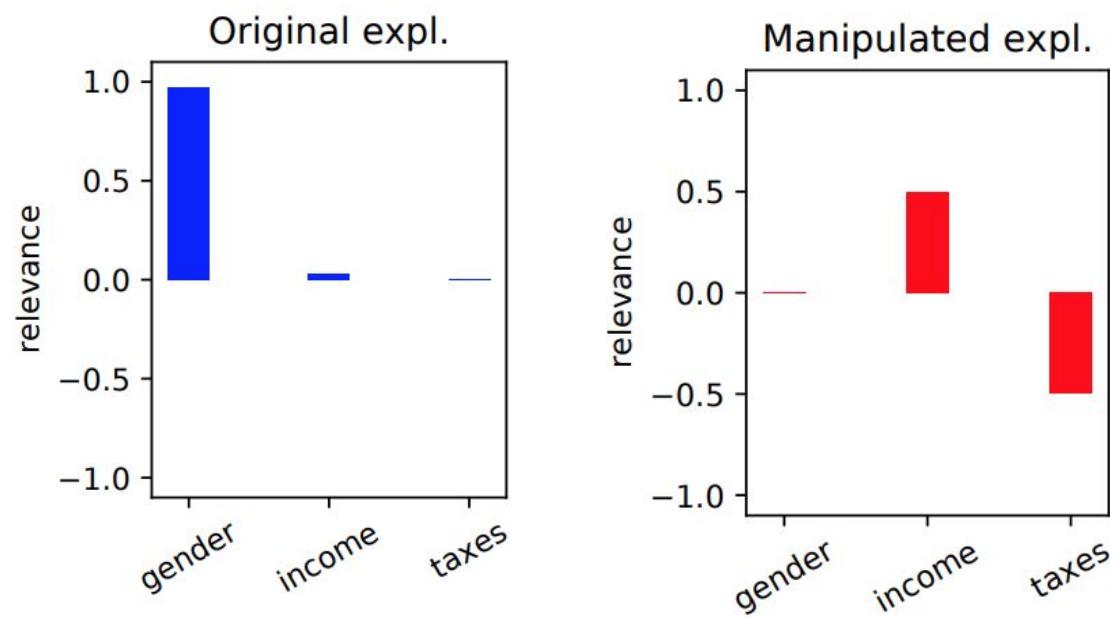
Methods Affected

- LIME
- Gradient
- Input-Gradient
- DeConvNet
- Guided BackProp
- GradCAM
- SHAP
- Integrated Gradients
- LRP
- Deep Taylor Decomposition
- Pattern Attribution
- Training Point Ranking

Defense Against Manipulation

Anders et. al. (2020) propose: 1) Hyperplane method & 2) Autoencoder to defend explanations against manipulation.

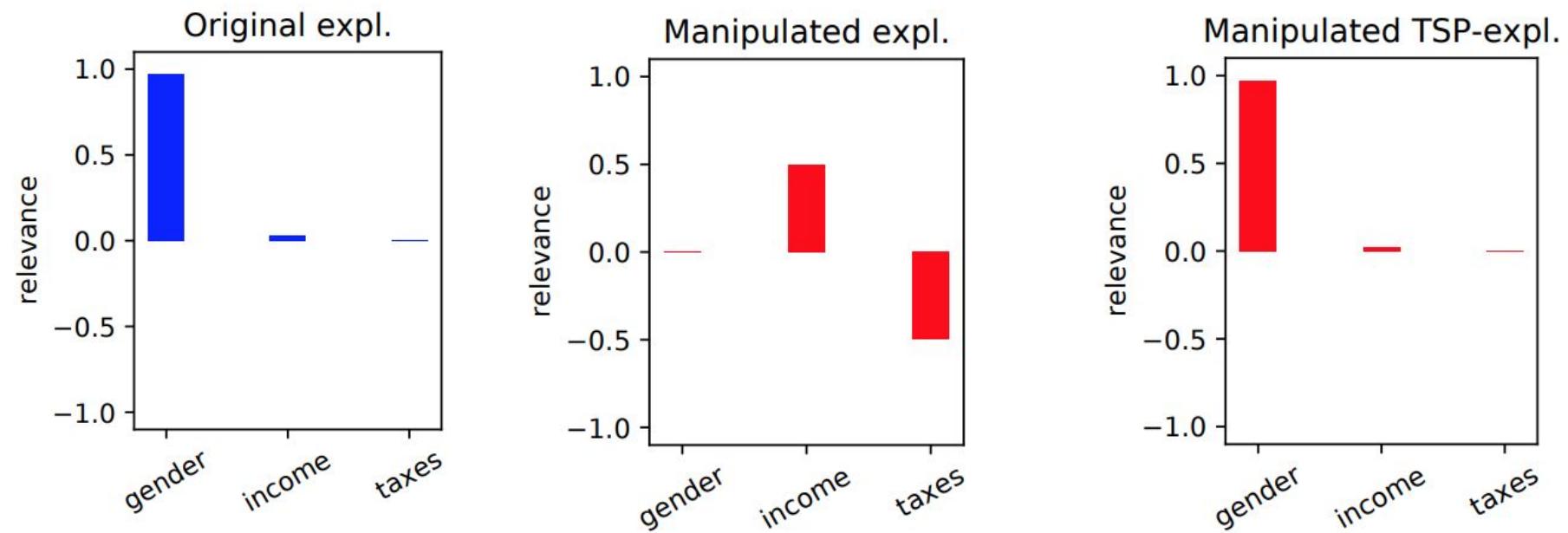
Credit Scoring Example



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Post-hoc explanations can be unstable to small, **non-adversarial**, perturbations to the input.

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‘Local Lipschitz Constant’

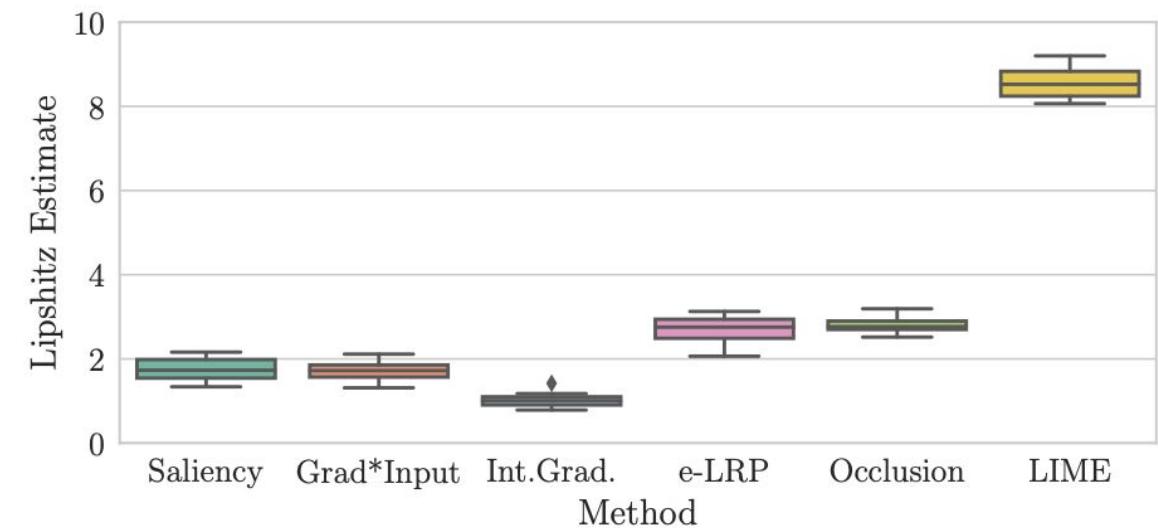
$$\hat{L}(x_i) = \operatorname{argmax}_{x_j \in B_\epsilon(x_i)} \frac{\|f(x_i) - f(x_j)\|_2}{\|x_i - x_j\|_2}$$

Explanation function: LIME, SHAP,
Gradient...etc.

Input

Limitations: Stability

- Perturbation approaches like LIME can be unstable.
- [Yeh et. al. \(2019\)](#) analytically derive bounds on explanations sensitive for certain popular methods and propose stable variants.

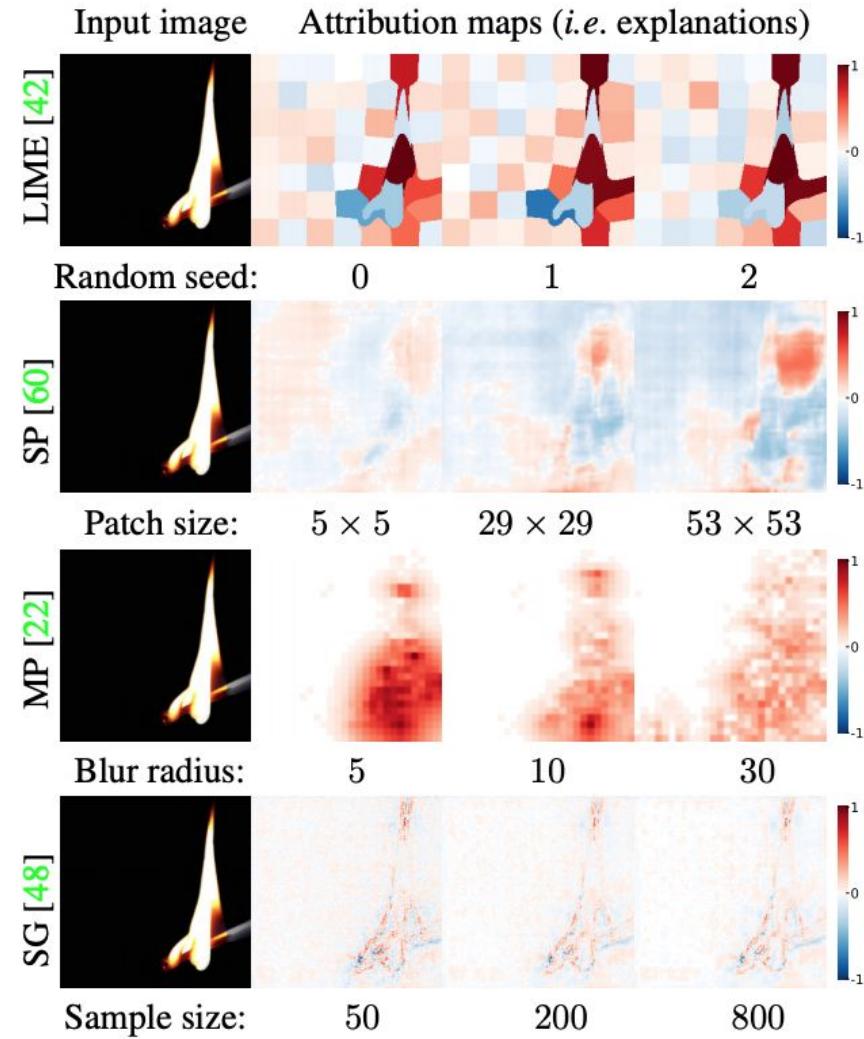


Estimate for 100 tests for an MNIST Model.

[Alvarez et. al. 2018.](#)

Sensitivity to Hyperparameters

Explanations can be highly sensitive to hyperparameters such as **random seed**, number of perturbations, patch size, etc.

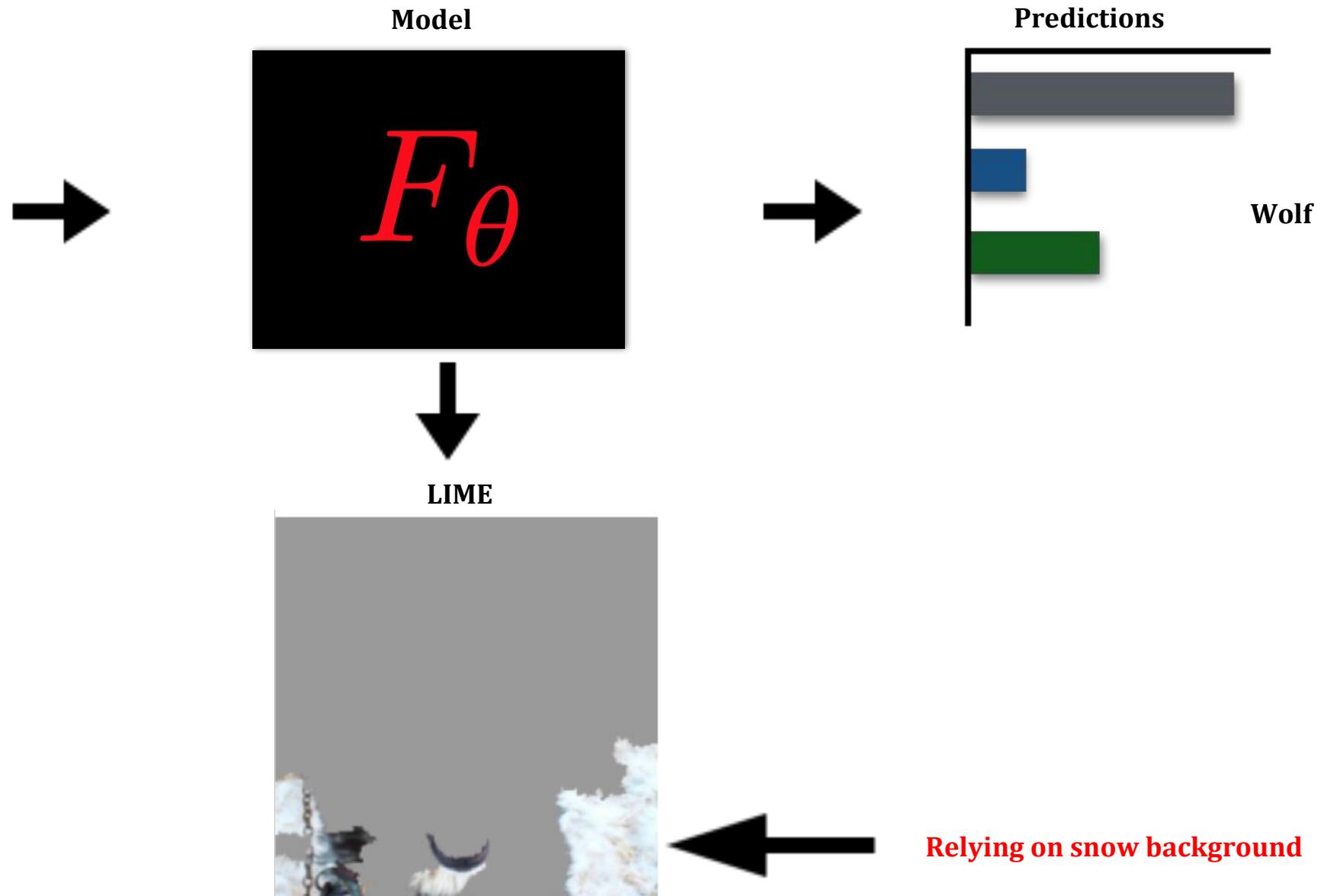
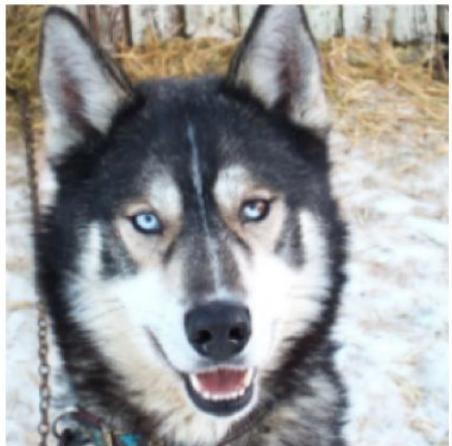


Limitations

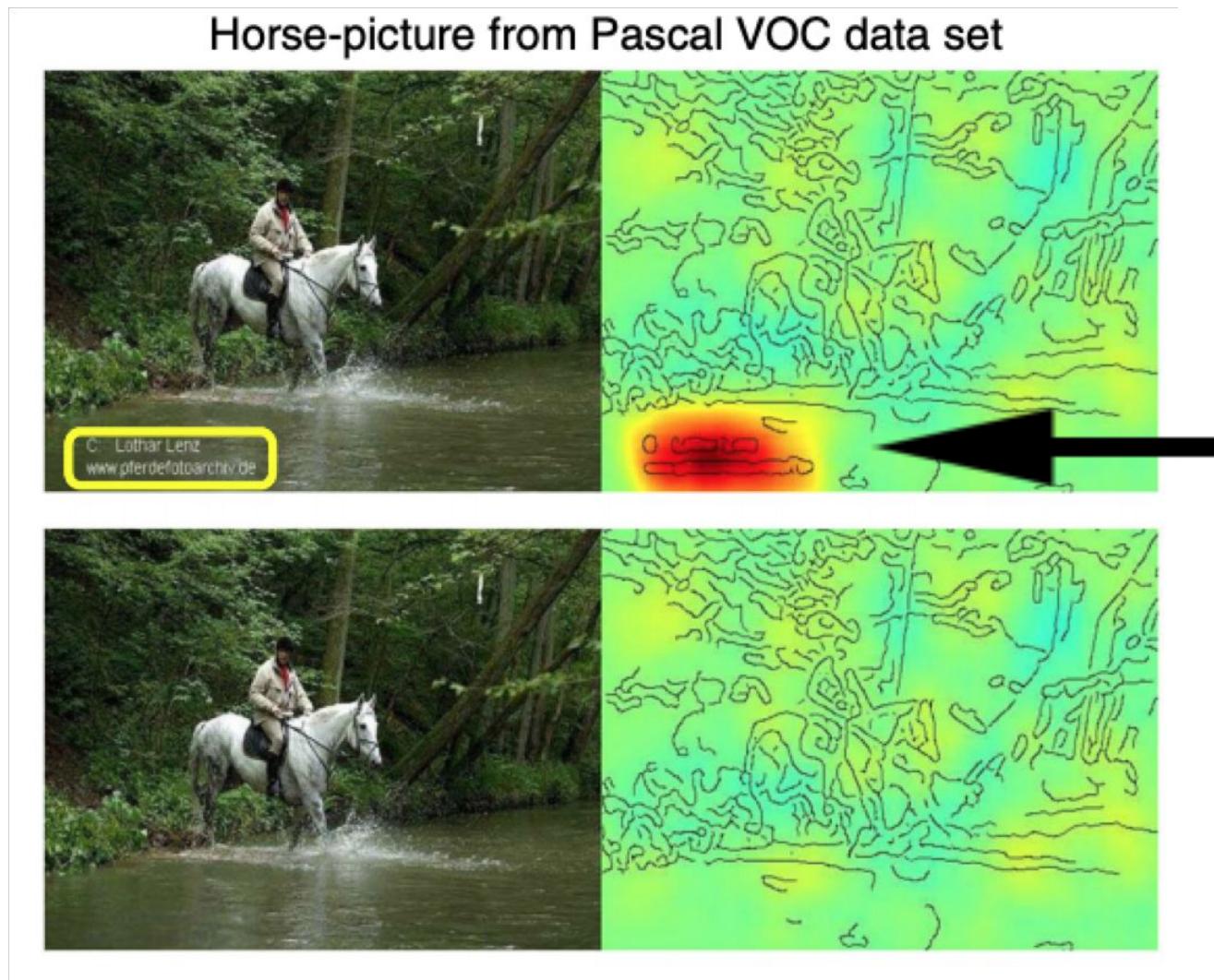
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Model Debugging: Spurious Signals

True Label: Siberian Husky



Model Debugging: Spurious Signals



Relying on Image Captions to find horses.

Explanations as Priors & Model ‘Simulatability’

- Regularizing explanations during training:
 - reduces reliance on **spurious training signals** ([Ross et. al., 2017](#); [Reiger et. al., 2020](#); & [Erion et. al. 2020](#));
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 - improves **robustness to adversarial examples** ([Ross et. al., 2018](#)).
- Explanations help improve ability of **end-users to simulate the model**:
 - tabular LIME improves forward and counterfactual simulatability ([Hase et. al. 2020](#));
 - prototype explanation improves counterfactual simulatability ([Hase et. al. 2020](#)).

Explanations with perfect fidelity can still mislead

In a bail adjudication task, **misleading** high-fidelity explanations improve end-user (domain experts) trust.

True Classifier relies on race

If Race ≠ African American:
If Prior-Felony = Yes and Crime-Status = Active, then Risky
If Prior-Convictions = 0, then Not Risky

If Race = African American:
If Pays-rent = No and Gender = Male, then Risky
If Lives-with-Partner = No and College = No, then Risky
If Age ≥35 and Has-Kids = Yes, then Not Risky
If Wages ≥70K, then Not Risky

Default: Not Risky

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High fidelity ‘misleading’ explanation

If Current-Offense = Felony:
If Prior-FTA = Yes and Prior-Arrests ≥ 1, then Risky
If Crime-Status = Active and Owns-House = No and Has-Kids = No, then Risky
If Prior-Convictions = 0 and College = Yes and Owns-House = Yes, then Not Risky

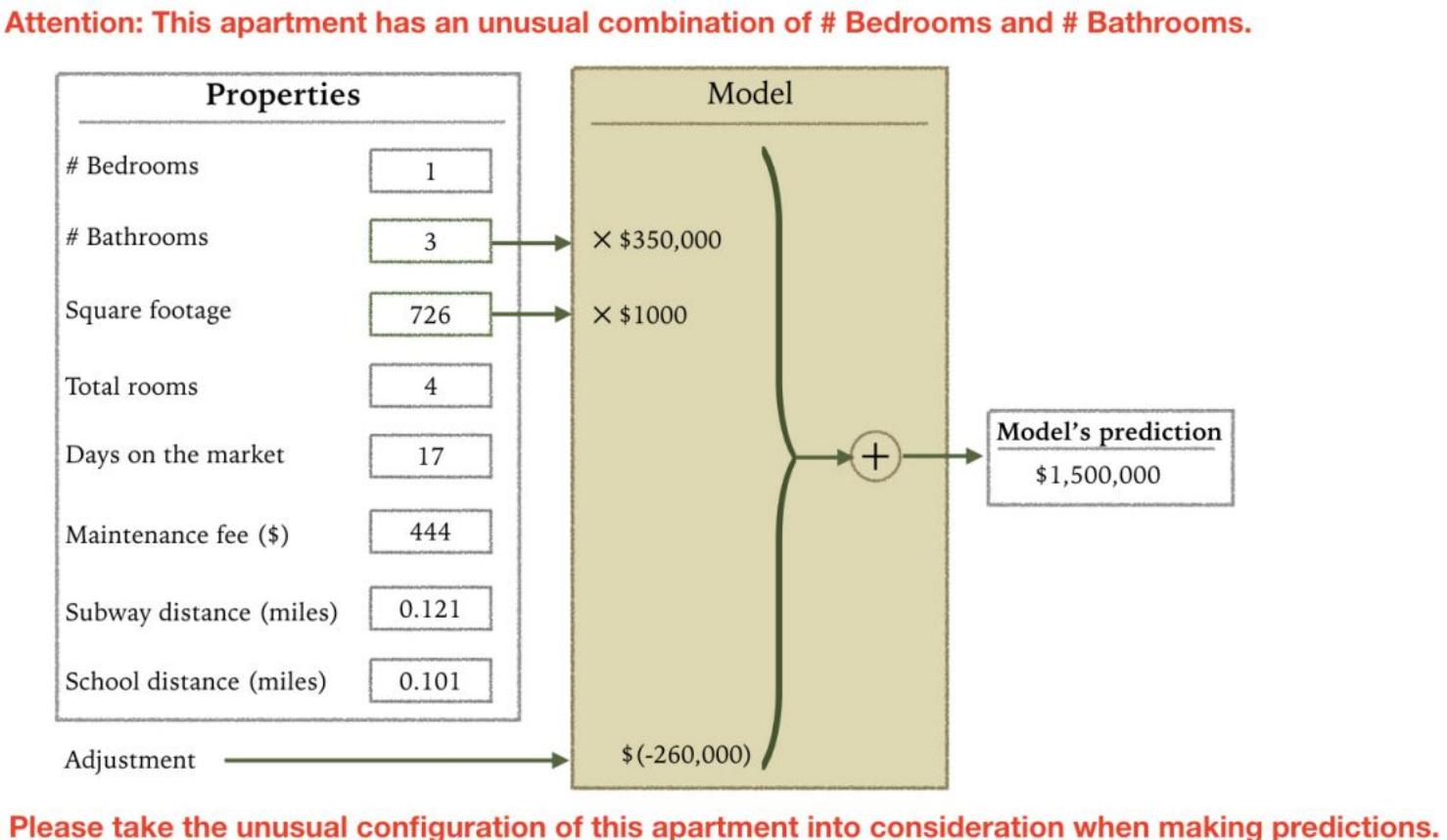
If Current-Offense = Misdemeanor and Prior-Arrests > 1:
If Prior-Jail-Incarcerations = Yes, then Risky
If Has-Kids = Yes and Married = Yes and Owns-House = Yes, then Not Risky
If Lives-with-Partner = Yes and College = Yes and Pays-Rent = Yes, then Not Risky

If Current-Offense = Misdemeanor and Prior-Arrests ≤ 1:
If Has-Kids = No and Owns-House = No and Prior-Jail-Incarcerations = Yes, then Risky
If Age ≥ 50 and Has-Kids = Yes and Prior-FTA = No, then Not Risky

Default: Not Risky

Difficulty using explanations for debugging

In a housing price prediction task, Amazon mechanical turkers are unable to use linear model coefficients to diagnose model mistakes.



Difficulty using explanations for debugging

In a dog breeds classification task, users familiar with machine learning **rely on labels, instead of saliency maps**, for diagnosing model errors.

Using the output and explanation of the dog classification model below, do you think this specific model is ready to be sold to customers?



Algorithm Explanation



Algorithm Explanation



Algorithm Explanation

DEFINITELY NOT	PROMPTLY	UNSURE/MAYBE	PROMPTLY	DEFINITELY
<input type="radio"/>				

What were your motivation for your response above?

On some or all of the images, the dog breed was wrong.

The dog breeds were correct.

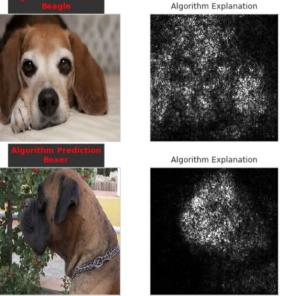
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Other, please specify

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Algorithm Prediction
Beagle

Algorithm Explanation

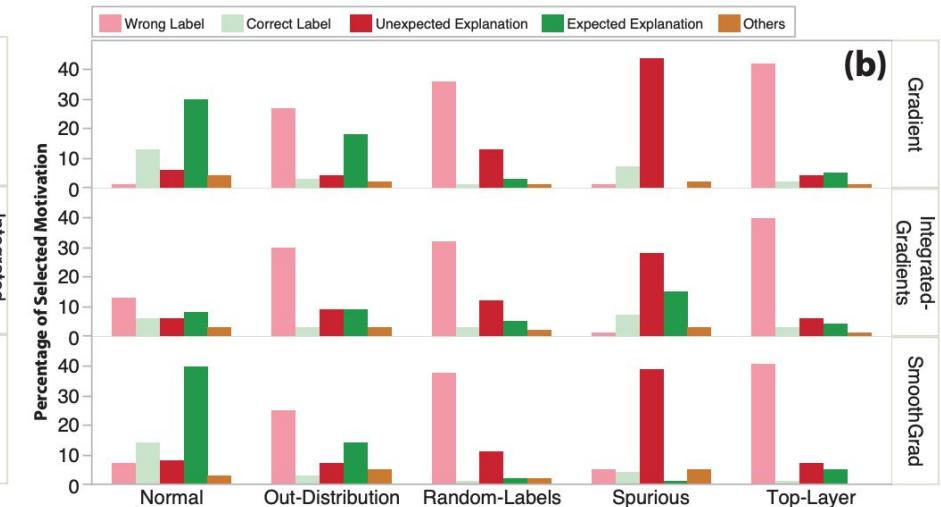
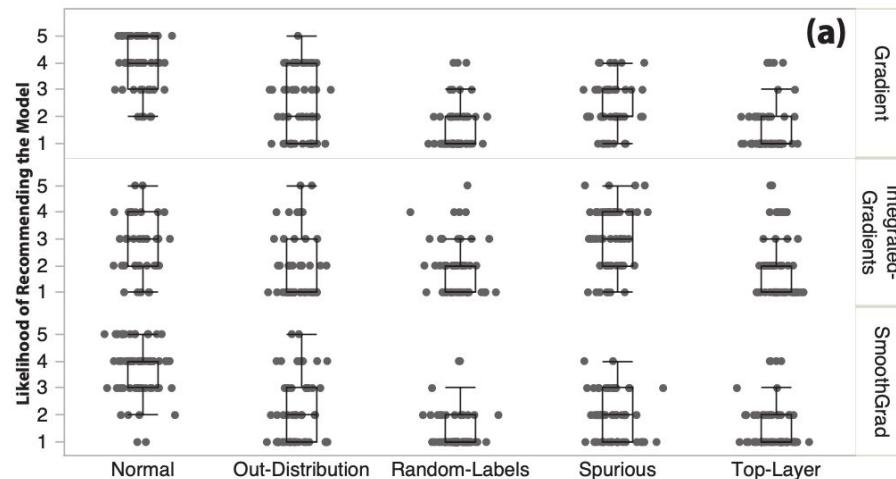
Algorithm Prediction
Boxer

Algorithm Explanation

DEFINITELY NOT PROBABLY NOT UNSURE/MAYBE PROBABLY DEFINITELY

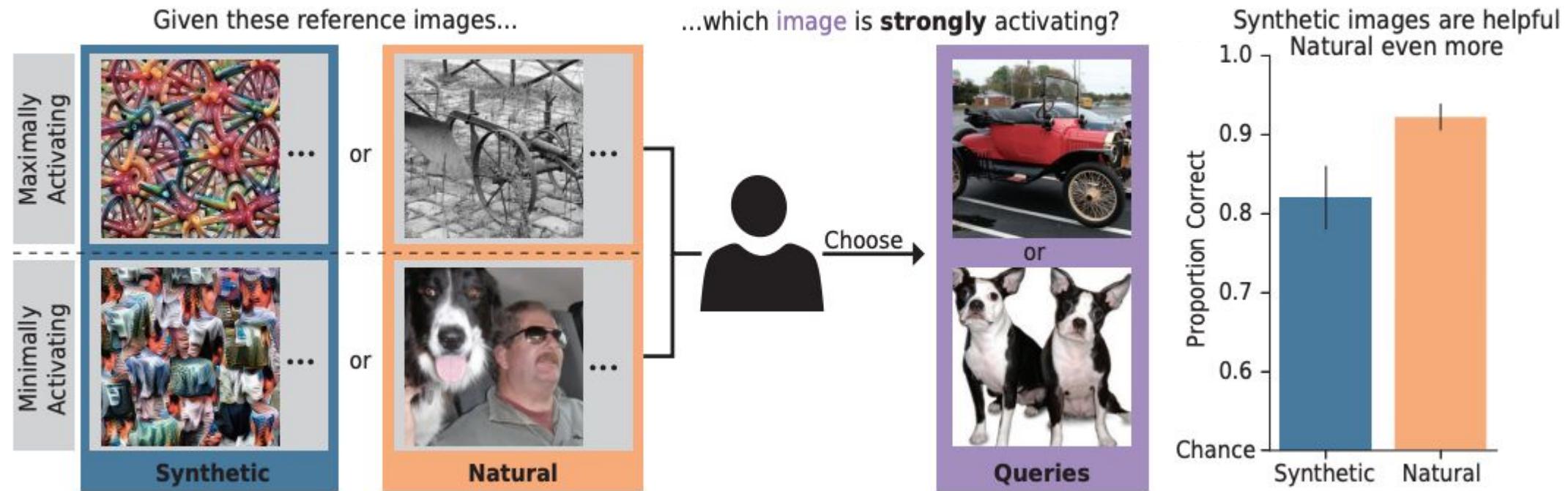
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- Other, please specify



Natural images more helpful than feature visualization

Users found natural images more helpful than feature visualization in deciding whether an image strongly activated a neuron.



Conflicting Evidence on Utility of Explanations

- **Mixed evidence:**
 - simulation and benchmark studies show that explanations are useful for debugging;
 - however, recent user studies show limited utility in practice.

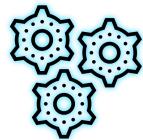
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 - however, recent user studies show limited utility in practice.
- Rigorous **user studies** and **pilots with end-users** can continue to help provide feedback to researchers on what to address (see: [Alqaraawi et. al. 2020](#), [Bhatt et. al. 2020](#) & [Kaur et. al. 2020](#)).

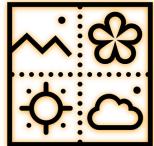
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Tutorial on Post hoc Explanations



Approaches for Post hoc Explainability



Explanations in Different Modalities



Evaluation of Explanations

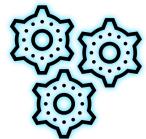


Limits of Post hoc Explainability

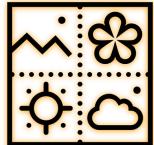


Future of Post hoc Explainability

Tutorial on Post hoc Explanations



Approaches for Post hoc Explainability



Explanations in **Different Modalities**



Evaluation of Explanations



Limits of Post hoc Explainability



Future of Post hoc Explainability

Future of Post hoc Explainability

Emerging Topics in Explainability Research



Future of Post hoc Explainability

Towards Better Post hoc Explanations

Methods for More Reliable
Post hoc Explanations

Theoretical Analysis of
Post hoc Explanation Methods

Rigorous Evaluation of the Utility of
Post hoc Explanations

Other Emerging Directions

Post hoc Explainability
Beyond Classification

Intersections with Differential Privacy

Intersections with Fairness

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Methods for More Reliable Post hoc Explanations

Post hoc explanations have several limitations:
not faithful to the underlying model, unstable, fragile

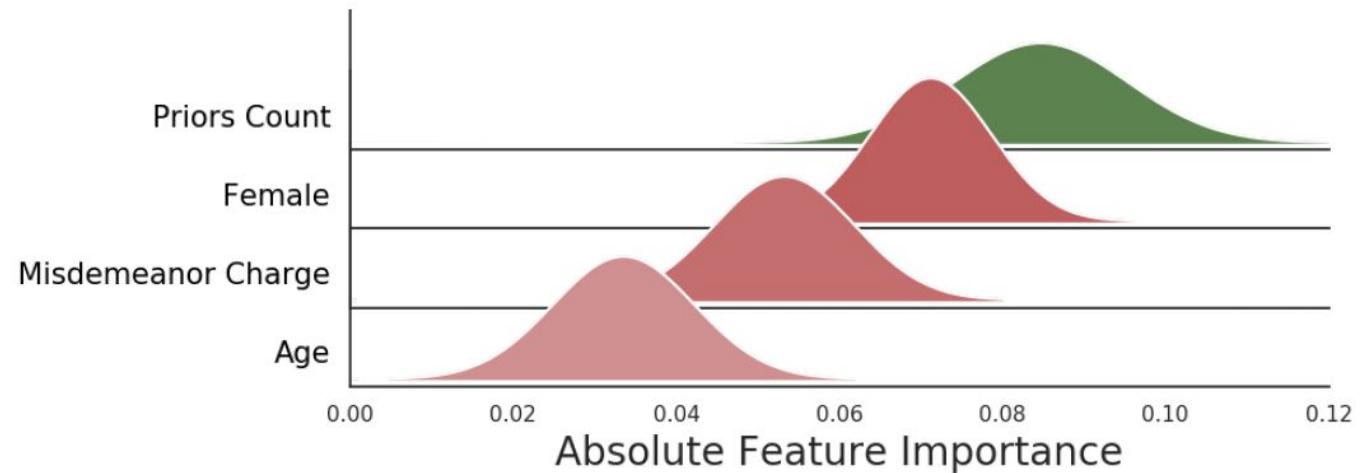
- Modeling **uncertainty** in post hoc explanations [Guo et. al. 2018, Slack et. al. 2020]
- Generating post hoc explanations that are **stable** as well as **robust to distribution shifts** [Chalasani et. al., 2020, Lakkaraju et. al. 2020]
- Generating **causal explanations** that are faithful to the underlying model [Goyal et. al., 2020]

Modeling Uncertainty in Post hoc Explanations

Model Agnostic

*Bayesian versions of LIME/SHAP
with closed form solutions*

*Generate post hoc explanations with
user specified confidence levels*



I need an explanation where true
feature importance lies within ± 0.5
of estimated values with 95%
confidence



Stable and Robust Post hoc Explanations

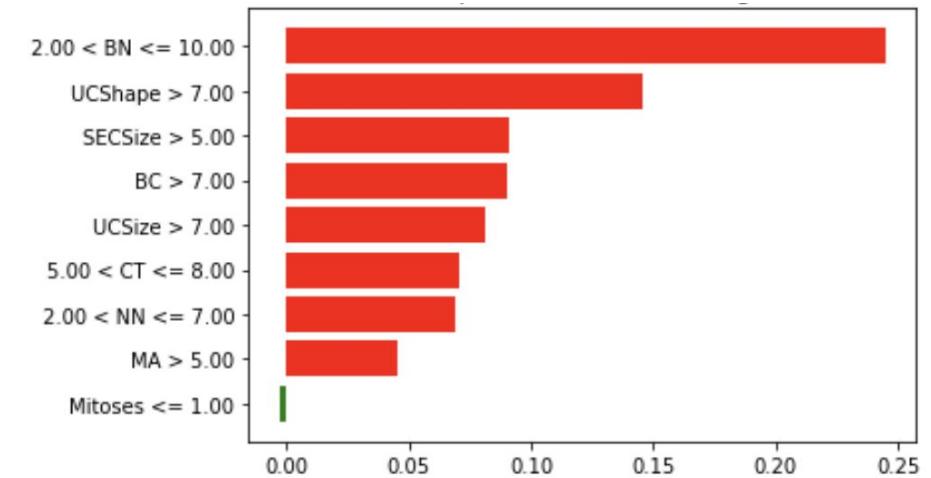
- Leverages **minimax objective** and **adversarial training** to generate explanations that are stable and robust to distribution shifts

$$\hat{E} = \arg \min_{E \in \mathcal{E}} \max_{\delta \in \Delta} \mathbb{E}_{p_\delta(x)} [\ell(E(x), B^*(x))]$$

worst-case over
distribution shifts

mismatch between explanation
and black box predictions

- Generic framework -- can be instantiated to generate ***model agnostic local/global explanations*** of various types (e.g., feature importances, rules)



If $X_1 < 7.0$ and $X_2 < 2.0$, then Benign

If $X_2 \geq 5.0$, then Malignant

If $X_6 \geq 9.0$, then Malignant

If $X_1 \geq 7.0$, then Malignant

If $X_4 \geq 4.0$, then Malignant

Default Rule (Benign)

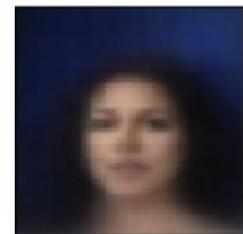
Faithful Causal Explanations

Identifying vulnerabilities in existing post hoc explanation methods and proposing approaches to address these vulnerabilities is a critical research direction going forward!

causal effects



$p(\text{woman}) = 0.94$



$p(\text{woman}) = 0.92$

$$\text{EncDec-CaCE}_j = 0.94 - 0.92 = 0.02$$

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Towards Better Post hoc Explanations

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Theoretical Analysis of
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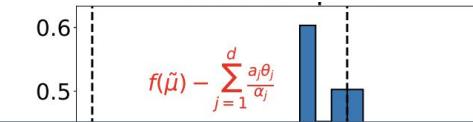
Post hoc Explainability
Beyond Classification

Intersections with Differential Privacy

Intersections with Fairness

Theoretical Analysis of Post hoc Explanation Methods

- Theoretical analysis of LIME



- Theoretical analysis shedding light on the fidelity, stability, and fragility of post hoc explanation methods can be extremely valuable to the progress of the field!
- The coefficients obtained are proportional to the gradient of the function to be explained
 - Local error of surrogate model is bounded away from zero with high probability

Future of Post hoc Explainability

Towards Better Post hoc Explanations

Methods for More Reliable
Post hoc Explanations

Theoretical Analysis of
Post hoc Explanation Methods

Rigorous Evaluation of the Utility of
Post hoc Explanations

Other Emerging Directions

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Rigorous Evaluation of the Utility of Post hoc Explanations

- Domain experts and end users seem to be over trusting explanations & the underlying models based on explanations
 - Law school students trusted underlying model 9.8 times more when shown a misleading explanation which “white-washes” the model
 - Data scientists over trusted explanations without even comprehending them -- *“Participants trusted the tools because of their visualizations and their public availability”*

Responses from Data Scientists Using Explainability Tools (GAM and SHAP)

“I didn’t fully grasp what SHAP values were. This is a pretty popular tool and I get the log-odds concept in general. I figure they were showing SHAP values for a reason. Maybe it’s easier to judge relationships using log-odds instead of predicted value. Anyway, so it made sense I suppose.” (P6, SHAP)

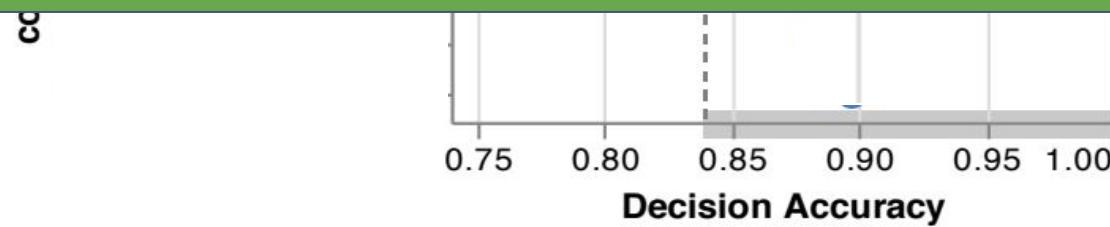
“[The tool] assigns a value that is important to know, but it’s showing that in a way that makes you misinterpret that value. Now I want to go back and check all my answers”... [later] “Okay, so, it’s not showing me a whole lot more than what I can infer on my own. Now I’m thinking... is this an ‘interpretability tool’?” (P4, SHAP)

“Age 38 seems to have the highest positive influence on income based on the plot. Not sure why, but the explanation clearly shows it... makes sense.” (P9, GAMs)

“[The tool] shows visualizations of ML models, which is not something anything else I have worked with has done. It’s very transparent, and that makes me trust it more” (P9, GAMs).

Are Explanations Helping Humans in Real World Tasks?

- Evaluating the effect of explanations on human-AI collaboration
- Rigorous user studies and evaluations to ascertain the utility of different post hoc explanation methods in various contexts is extremely critical for the progress of the field!



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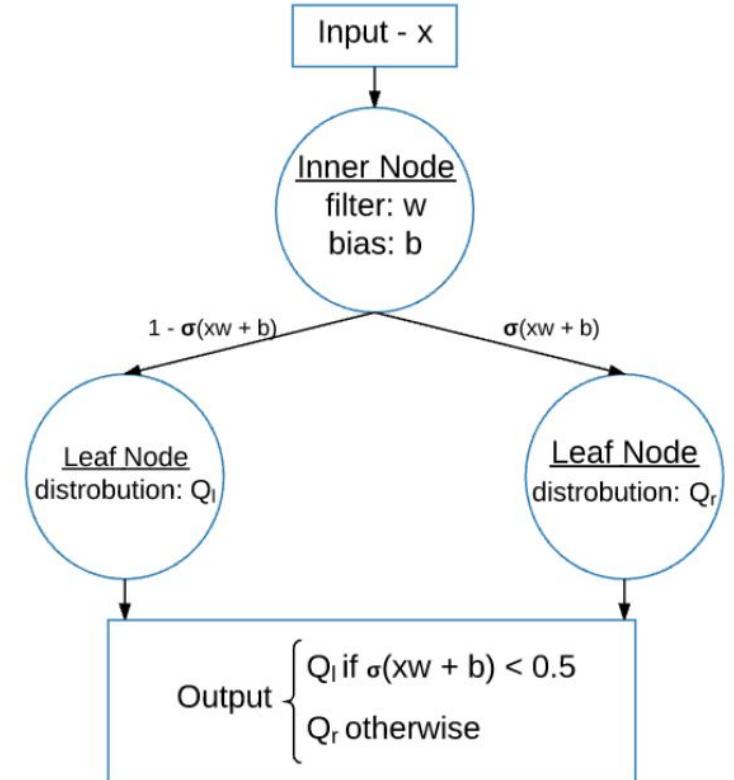
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Beyond Classification: Explainability for RL

- Model distillation using soft decision trees to understand RL policies
 - Map states to actions
- Summarize agent behavior by identifying important states in a policy
 - A state is important if different actions lead to substantially different outcomes



Beyond Classification: Explainability for RL

- Causal explanations of the behavior of model free RL agents
- Generate explanations of agent behaviour based on counterfactual analysis of the causal model

Explaining the actions of a StarCraft II agent

Question

Why not *build_barracks* (A_b)?

Explanation

Because it is more desirable to do action *build_supply_depot* (A_s) to have more Supply Depots (S) as the goal is to have more Destroyed Units (D_u) and Destroyed buildings (D_b).

Beyond Classification: Explainability for GNNs

Takes a trained CNN and its predictions and returns an explanation in the form of a graph.

Lots of real world applications call for models/algorithms that go beyond classification. Exciting opportunities to explore explainability in these settings!



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Intersections with Differential Privacy

- Need for more theoretical, methodological, and empirical research exploring this intersection!

learning them

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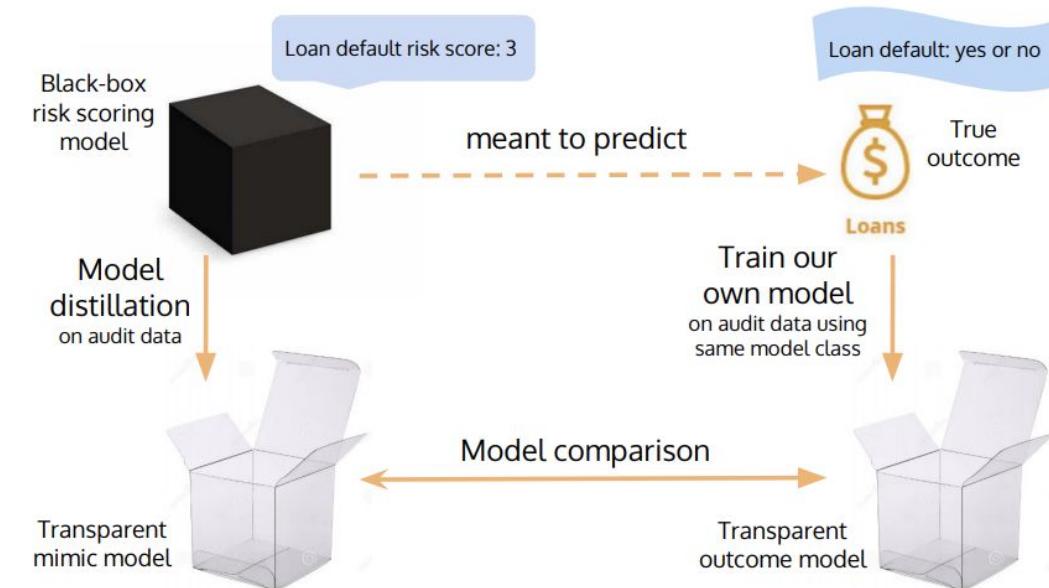
Intersections with Differential Privacy

Intersections with Fairness



Intersections with Fairness

Distill and Compare: Compare the transparent/distilled down versions of risk scoring model and true outcome model to detect biases in risk scoring models.



Intersections with Fairness

- It is commonly hypothesized that post hoc explanations can help with detecting model biases.
 - Need for more rigorous theoretical and empirical studies to quantitatively evaluate this hypothesis
- Can post hoc explanations help detect unfairness?
 - How do they complement existing statistical notions of unfairness?

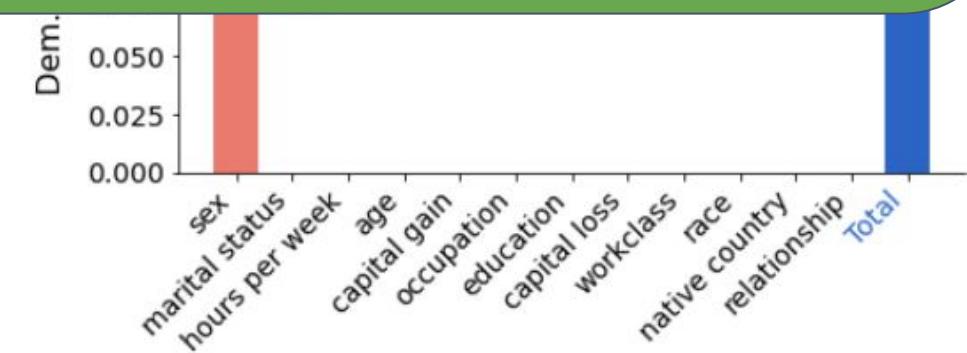
Intersections with Fairness

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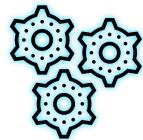
The connections between explainability and fairness need to be explored more thoroughly both through rigorous analysis and user studies.

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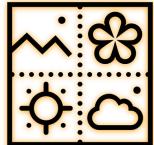
functions which ‘explain’ the unfairness



Tutorial on Post hoc Explanations



Approaches for Post hoc Explainability



Explanations in **Different Modalities**



Evaluation of Explanations



Limits of Post hoc Explainability



Future of Post hoc Explainability

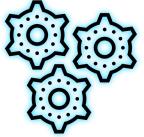


In Conclusion

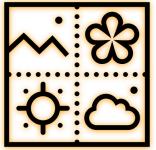
Summary of Tutorial



Motivation for Explainability



Approaches for Post hoc Explainability



Explanations in Different Modalities



Evaluation of Explanations



Limits of Post hoc Explainability



Future of Post hoc Explainability

Parting Thoughts...

When introducing a new explanation method:

- Who are the target end users that the method will help?
- A clear statement about what capability and/or insight the method aims to provide to its end users
- Careful analysis and exposition of the limitations and vulnerabilities of the proposed method
- Rigorous user studies (preferably with actual end users) to evaluate if the method is achieving the desired effect
- Use quantitative metrics (and not anecdotal evidence) to make claims about explainability³⁰⁷

Thank You!



Hima Lakkaraju
Harvard University



Julius Adebayo
MIT



Sameer Singh
UC Irvine

Slides and Video: explainml-tutorial.github.io