Explainable AI

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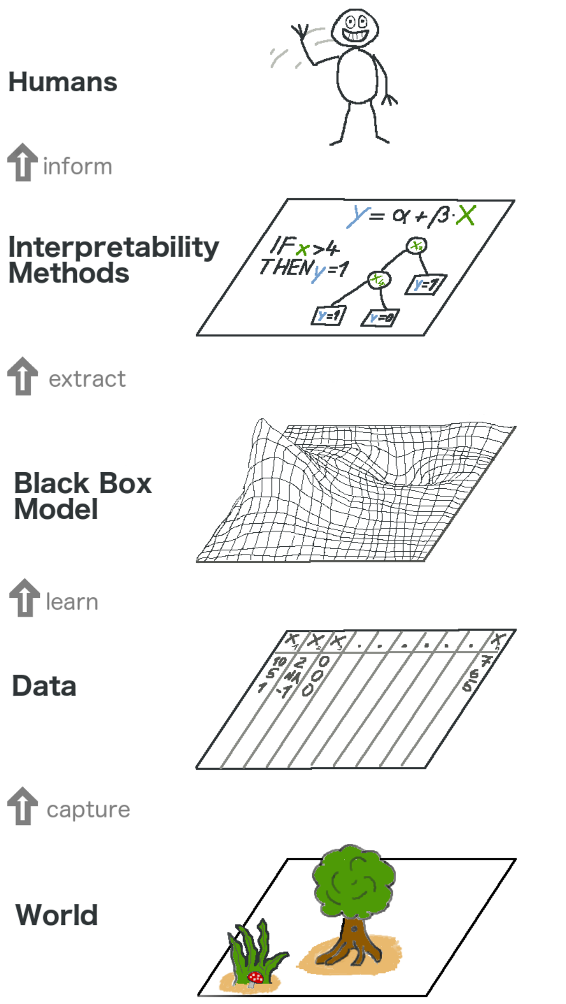
A recap of the bigger picture

- It’s great that interpretable machine learning fuses the work of statisticians and machine learning specialists.
  - Traditionally, statisticians deal with the Data layer, such as planning clinical trials or designing surveys. They skip the Black Box Model layer and go right to the Interpretability Methods layer
  - Machine learning specialists also deal with the Data layer, such as collecting labeled samples of skin cancer images or crawling Wikipedia. Then they train a black box machine learning model. The Interpretability Methods layer is skipped and humans directly deal with the black box model predictions



Humans

inform

Interpretability Methods

extract

Black Box Model

learn

Data

capture

World

https://christophm.github.io/interpretable-ml-book/agnostic.html

Why interpretable model?

- The importance of interpretability
  - Reliability - A self-driving car automatically detects cyclists based on a deep learning system. You want to be 100% sure that the abstraction the system has learned is error-free, because running over cyclists is quite bad
  - Fairness - A model says a bank shouldn't loan someone money, and the bank is legally required to explain the basis for each loan rejection
  - Causality - A healthcare provider wants to identify what factors are driving each patient's risk of disease so they can directly address those factors with targeted health interventions
  - Trust - The process of integrating machines and algorithms into our daily lives requires interpretability to increase social acceptance
- Models can only be *debugged and audited* when they can be interpreted
  - You can then informing feature engineering, directing future data collection or informing human decision-making, etc

What types of insights are possible

- Many people say machine learning models are "black boxes", in the sense that they can make good predictions but you can't understand the logic behind those predictions
    - This statement is true in the sense that some data scientists don't know how to extract insights from models yet
- However, there are techniques to extract the following insights
    - How does the learning algorithm create the model?
    - How does the trained model make predictions?
    - What features in the data did the model think are most important? How does each feature affect the model's predictions in a big-picture sense?
    - For any single prediction from a model, how did each feature in the data affect that particular prediction?

What is a good explanation for human?

1. Explanations are contrastive - The best explanation is the one that highlights the greatest difference between the object of interest and the reference object

- A complete explanation of the physician's question why the drug does not work might include: The patient has had the disease for 10 years, 11 genes are over-expressed, the patients body is very quick in breaking the drug down into ineffective chemicals, …
    - A contrastive explanation might be much simpler: In contrast to the responding patient, the non-responding patient has a certain combination of genes that make the drug less effective
- Creating contrastive explanations is application-dependent because it requires a point of reference for comparison. The solution for the automated creation of contrastive explanations might also involve finding *prototypes* or archetypes in the data

2. Explanations are selected - People do not expect explanations that cover the actual and complete list of causes of an event

- Make the explanation very short, give only 1 to 3 reasons, even if the world is complex

What is a good explanation for human?

3. Explanations focus on the abnormal - If one of the input features for a prediction was abnormal in any sense (like a rare category of a categorical feature) and influenced the prediction, it should be included in an explanation

- An abnormal feature in our house price prediction example might be that a rather expensive house has two balconies

4. Good explanations are consistent with prior beliefs of the explainee - Humans tend to ignore information that is inconsistent with their prior beliefs

5. Good explanations are general and probable - A cause that can explain many events is very general and could be considered a good explanation

1. Interpretable Models (intrinsically interpretable models)

- Use models that are intrinsically interpretable if possible
  - A model with monotonicity constraints ensures that the relationship between a feature and the target outcome always goes in the same direction over the entire range of the feature
    - Monotonicity is useful for the interpretation of a model because it makes it easier to understand a relationship

Algorithm	Linear	Monotone	Interaction	Task
Linear regression	Yes	Yes	No	regr
Logistic regression	No	Yes	No	class
Decision trees	No	Some	Yes	class, regr
RuleFit	Yes	No	Yes	class, regr
Naive Bayes	No	Yes	No	class
k-nearest neighbors	No	No	No	class, regr

Interpretable Models - Decision Rules

- Decision rules follow a general structure: IF the conditions are met THEN make a certain prediction
  - New in machine learning is that the decision rules are learned through an algorithm
- The baseline OneR algorithm selects the one that carries the most information about the outcome of interest and creates decision rules from this feature
  1. Discretize the continuous features by choosing appropriate intervals
  2. For each feature:
     1. Create a cross table between the feature values and the (categorical) outcome
     2. For each value of the feature, create a rule which predicts the most frequent class of the instances that have this particular feature value
     3. Calculate the total error of the rules for the feature
  3. Select the feature with the smallest total error

Location	Size	Pets	Price
good	small	yes	high
good	big	no	high
good	big	no	high
bad	medium	no	medium
good	medium	only cats	medium
good	small	only cats	medium
bad	medium	yes	medium
bad	small	yes	low
bad	medium	yes	low
bad	small	no	low

	Price=low	Price=medium	Price=high
Location=bad	3	2	0
Location=good	0	2	3

$\frac{4}{10}$

	Price=low	Price=medium	Price=high
Size=big	0	0	2
Size=medium	1	3	0
Size=small	2	1	1

$\frac{3}{10}$

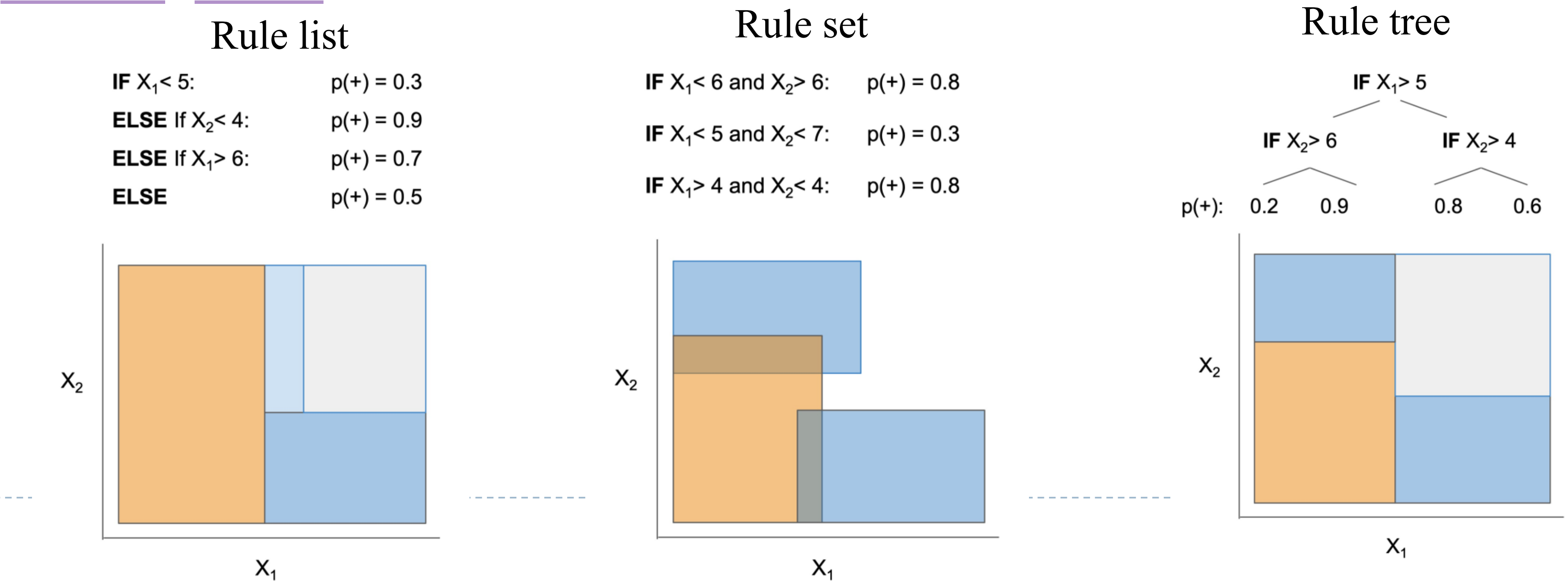
	Price=low	Price=medium	Price=high
Pets=no	1	1	2
Pets=only cats	0	2	0
Pets=yes	2	1	1

$\frac{4}{10}$

IF Size=small THEN Price=low
ELSE IF Size=medium THEN Price=medium
ELSE IF Size=big THEN Price=high

Interpretable Models - Decision Rules

- OneR prefers features with many possible levels like decision tree
  - Imagine a dataset that contains only noise and no signal. Some features have more levels than others. The features with more levels can now more easily overfit. A feature that has a separate level for each instance from the data would perfectly predict the entire dataset
- There are many other popular alternatives: sequential covering, Bayesian rule lists, Rulefit, FIGS



Rule list

IF $X_1 < 5$: p(+) = 0.3

ELSE If $X_2 < 4$: p(+) = 0.9

ELSE If $X_1 > 6$: p(+) = 0.7

ELSE p(+) = 0.5

Rule set

IF $X_1 < 6$ and $X_2 > 6$: p(+) = 0.8

IF $X_1 < 5$ and $X_2 < 7$: p(+) = 0.3

IF $X_1 > 4$ and $X_2 < 4$: p(+) = 0.8

Rule tree

2. Model-Agnostic Methods (post hoc interpretation methods)

- The great advantage of model-agnostic interpretation methods over model-specific ones is their flexibility
  - **Model flexibility**: The interpretation method can work with any machine learning model, such as random forests and deep neural networks
  - **Explanation flexibility**: You are not limited to a form of explanation. In some cases it might be useful to have a linear formula, in other cases a graphic with feature importance
  - **Representation flexibility**: The explanation system should be able to use different feature representations as the model being explained. For a text classifier uses word embedding vectors, it might be preferable to use the presence of individual words for the explanation
- Model-agnostic interpretation methods can be further distinguished into local and global methods
  - Global methods describe how features *affect the prediction on average*. In contrast, local methods aim to *explain individual predictions*

Global Methods - Partial dependence plots (PDP)

- While feature importance shows what variables most affect predictions, partial dependence plots show *how a feature affects predictions*
- This is useful to answer questions like:
  - Controlling for all other house features, what impact do longitude and latitude have on home prices? Are predicted health differences between two groups due to differences in their diets, or due to some other factor?
- If you are familiar with linear or logistic regression models, partial dependence plots can be interpreted similarly to the coefficients in those models
  - Though, partial dependence plots on **sophisticated models** can capture more complex patterns than coefficients from simple models
  - Like permutation importance, partial dependence plots are calculated after a *model has been fitted*

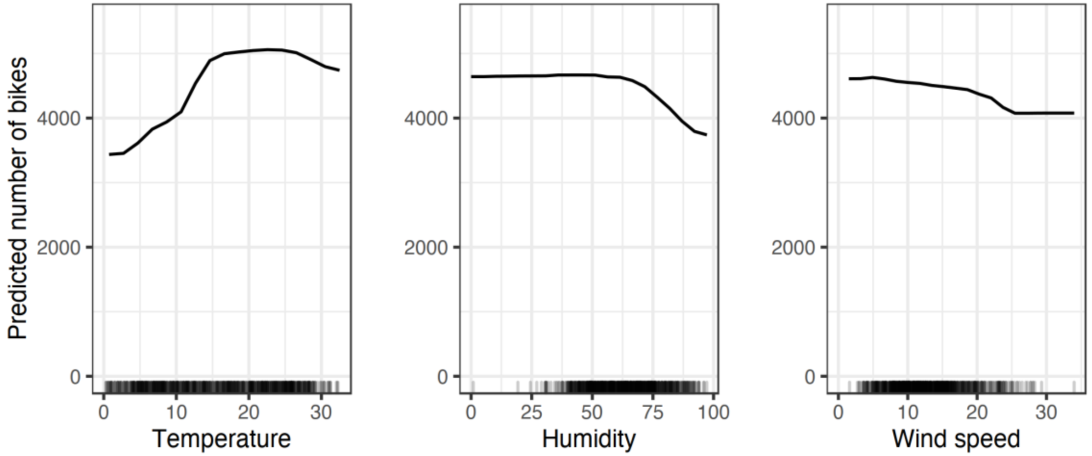
Partial dependence plots (PDP)

- The partial dependence function for regression is defined as

$$\hat{f}_S(x_S) = E_{X_C}\left[\hat{f}(x_S, X_C)\right] = \int \hat{f}(x_S, X_C)p(x_C)dx_C = \frac{1}{n}\sum_{i=1}^{n} \hat{f}\left(x_S, X_C^{(i)}\right)$$

The x_S are the features for which the partial dependence function should be plotted and X_C are the other features used in the model $\hat{f}$, which are here treated as random variables

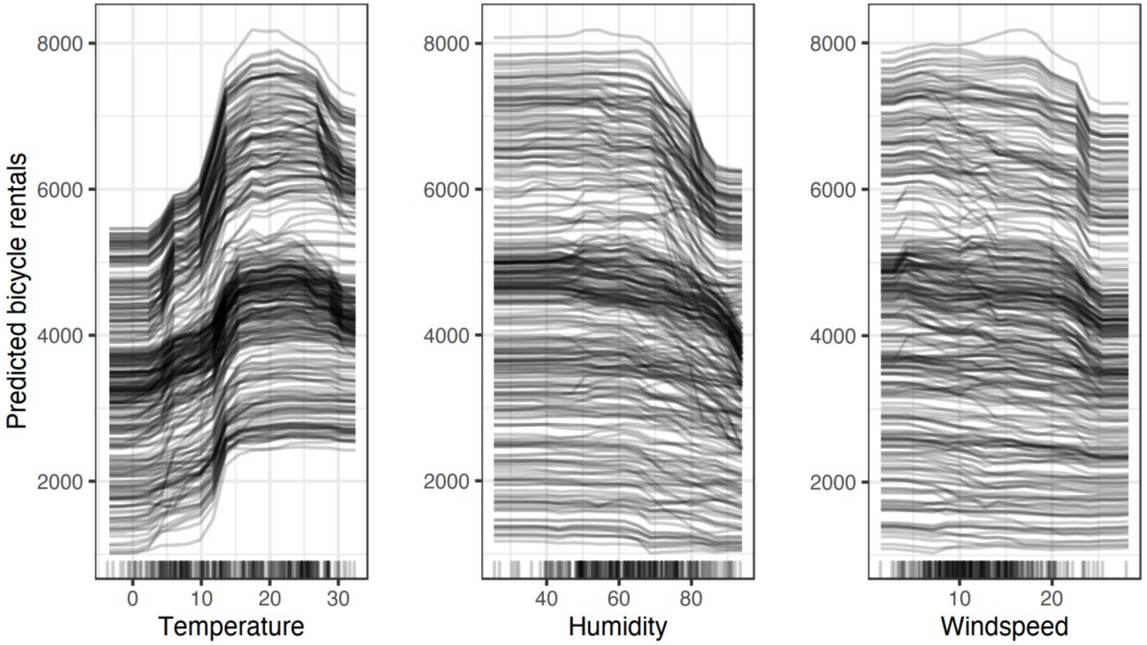
- It works by marginalizing the model output over the distribution of the features in set C, so that the function shows the relationship between the S we are interested in and the predicted outcome. Computing this integral for various values of x_S produces a PDP plot



- It is assumed that the feature(s) for which the partial dependence is computed are not correlated with other features

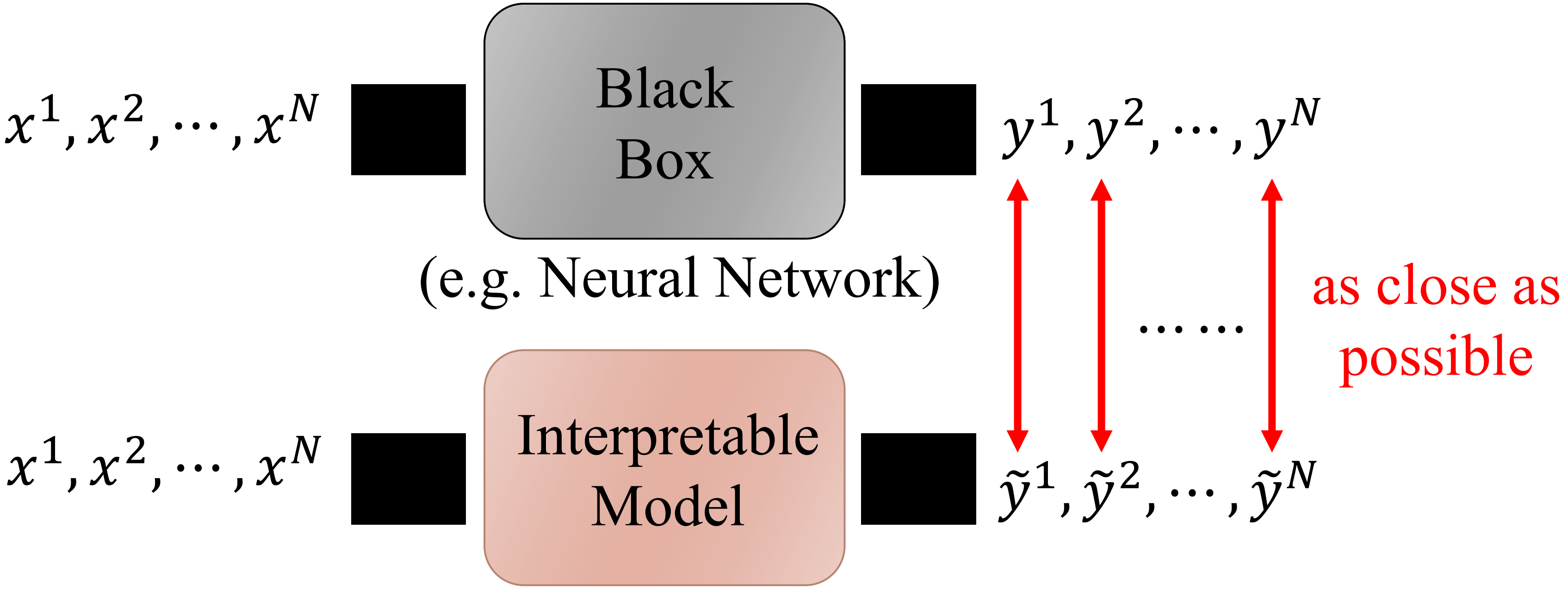
3. Local Methods - Individual conditional expectation (ICE) plot

- Similar to a PDP, an individual conditional expectation (ICE) plot shows the dependence between the target function and an input feature of interest
  - Unlike a PDP, which shows the average effect of the input feature, an ICE plot visualizes the dependence of the prediction *on a feature for each sample* separately with one line per sample. A PDP is the average of the lines of an ICE plot
  - In ICE plots, for each instance in $\{(x_S, X_C^{(i)})\}_{i=1}^{N}$ the curve $\hat{f}_S^{(i)}$ is plotted against x_S
  - Unlike PDP, ICE curves can uncover heterogeneous relationships



Local Methods - Local Surrogate (LIME)

- Using an interpretable model to mimic the behavior of an uninterpretable model

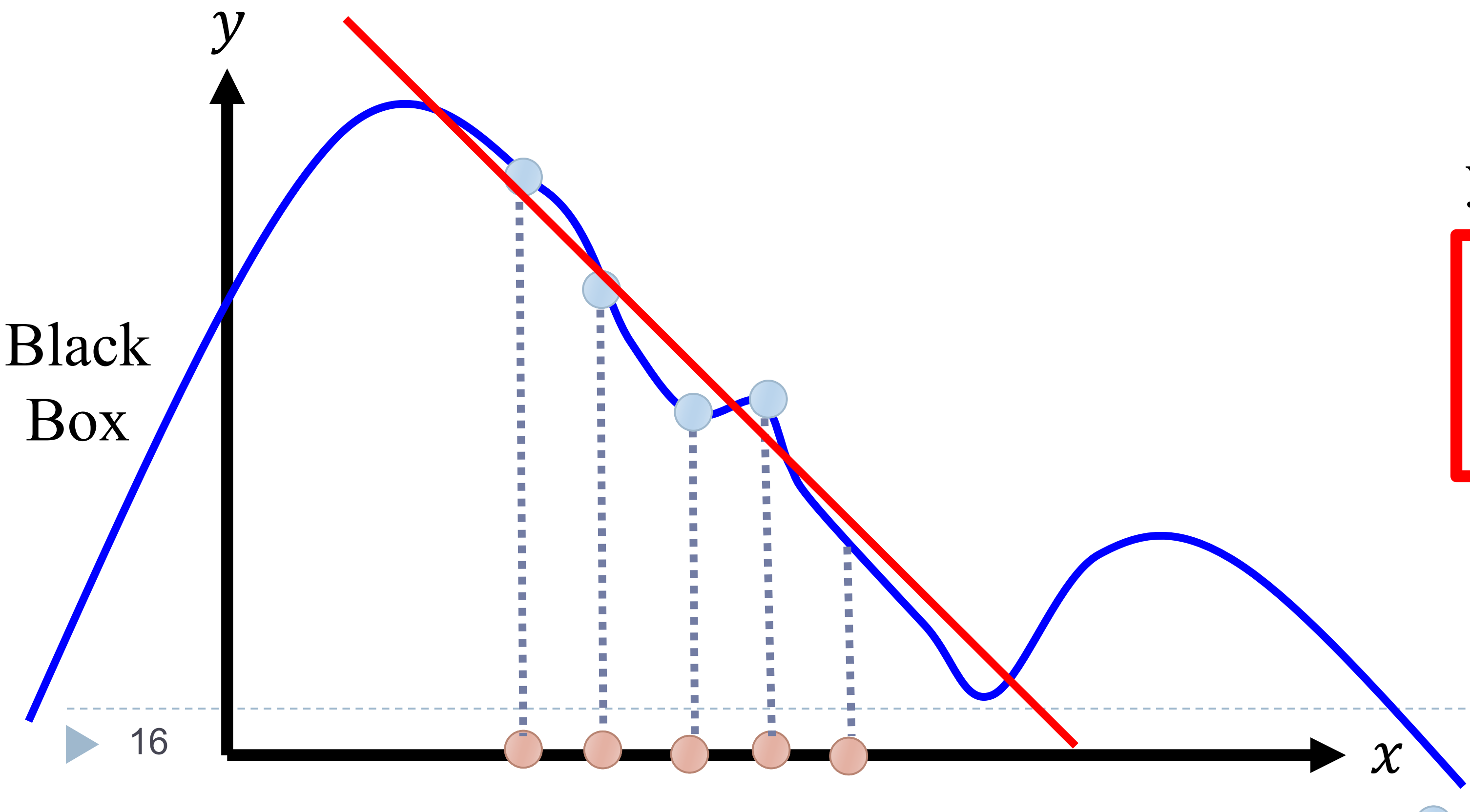


Problem: Interpretable model cannot mimic complex one…

However, it can mimic a local region!

Local Interpretable Model-Agnostic Explanations (LIME)

- For text and images, the solution is to turn single words or super-pixels on or off. In the case of tabular data, LIME creates new samples by perturbing each feature individually, drawing from a normal distribution with mean and standard deviation taken from the feature



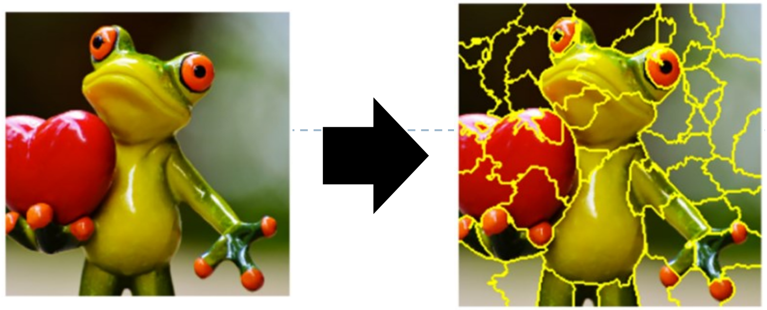
1. Given a data point you want to explain

2. Sample at the nearby points by perturb dataset to get the black box predictions for these new points

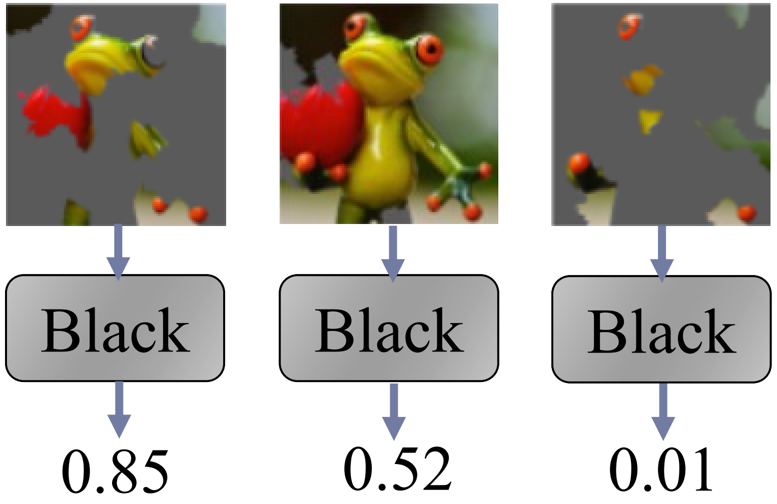
3. Fit with interpretable model on the weighted samples

4. Interpret the linear model

LIME — Image data



1. Given a data point you want to explain
2. Sample at the nearby
   - Each image is represented as a set of superpixels (segments)

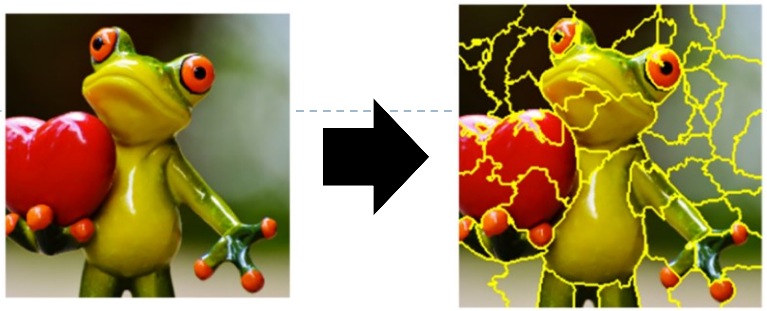


Randomly delete some segments.

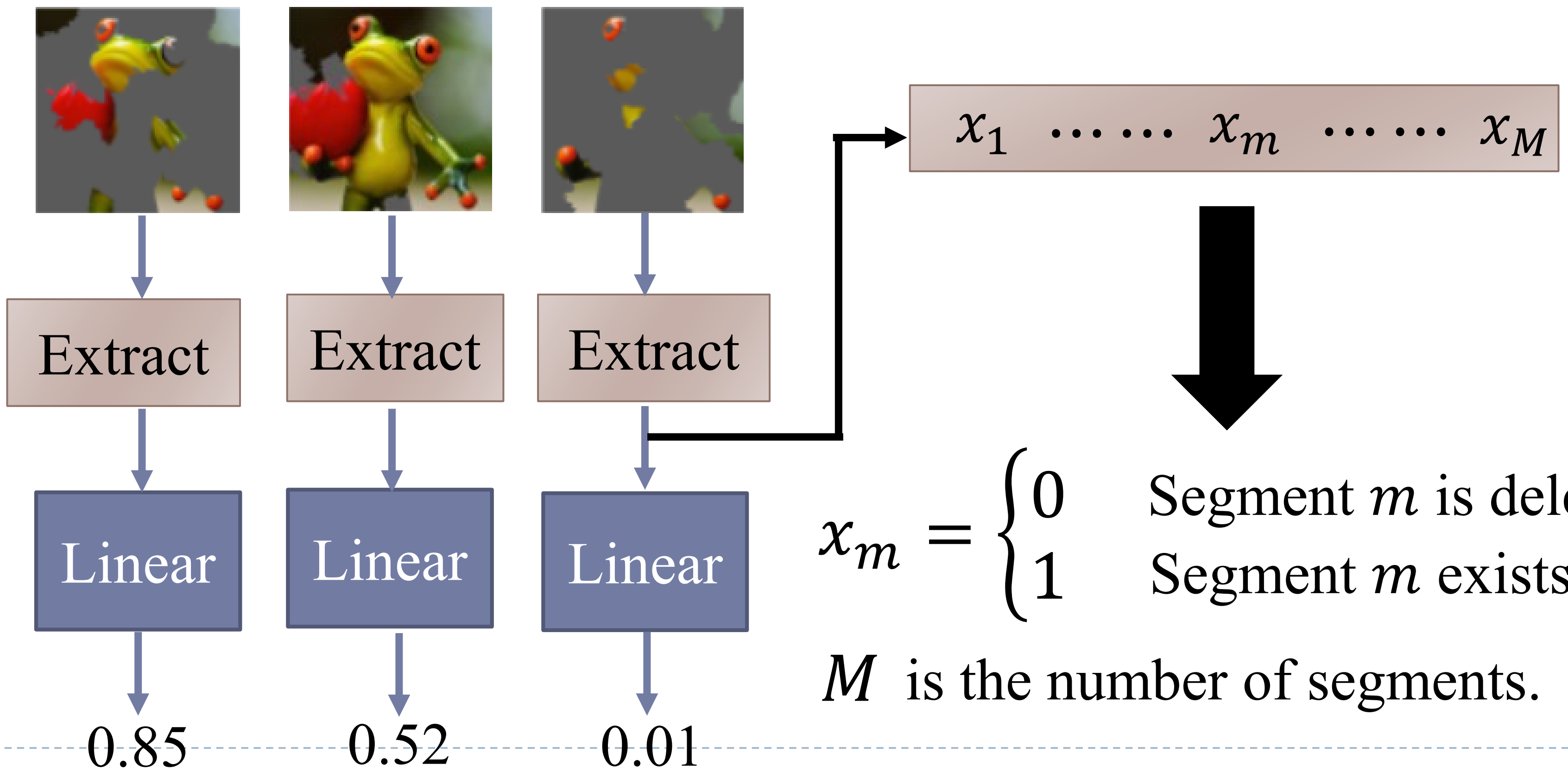
Compute the probability of "frog" by black box

https://medium.com/@kstseng/lime-local-interpretable-model-agnostic-explanation-%E6%8A%80%E8%A1%93%E4%BB%8B%E7%B4%B9-a67b6c34c3f8

LIME — Image data



3. Fit with linear (or interpretable) model



Extract

Extract

Extract

Linear

Linear

Linear

0.85

0.52

0.01

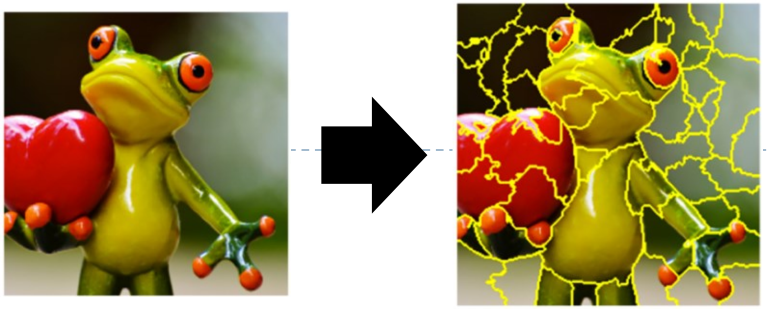
$x_1 \quad \cdots\cdots \quad x_m \quad \cdots\cdots \quad x_M$

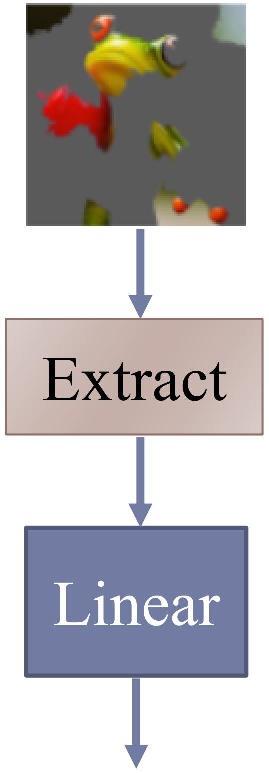
$$x_m = \begin{cases} 0 & \text{Segment } m \text{ is deleted.} \\ 1 & \text{Segment } m \text{ exists.} \end{cases}$$

M is the number of segments.

LIME — Image data

4. Interpret the model you learned





Extract

Linear

0.85

$$y = w_1 x_1 + \cdots + w_m x_m + \cdots + w_M x_M$$

$$x_m = \begin{cases} 0 & \text{Segment } m \text{ is deleted.} \\ 1 & \text{Segment } m \text{ exists.} \end{cases}$$

M is the number of segments.

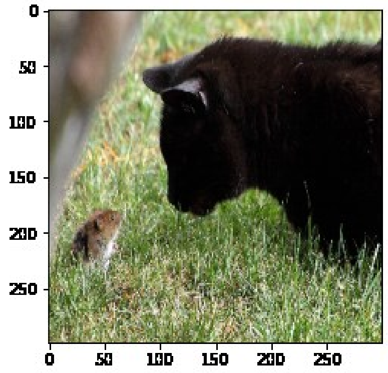
If $w_m \approx 0$ → segment m is not related to “frog”

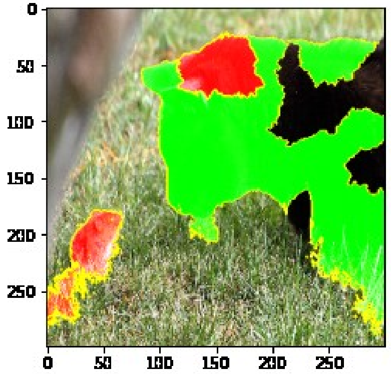
If w_m is positive

→ segment m indicates the image is “frog”

If w_m is negative

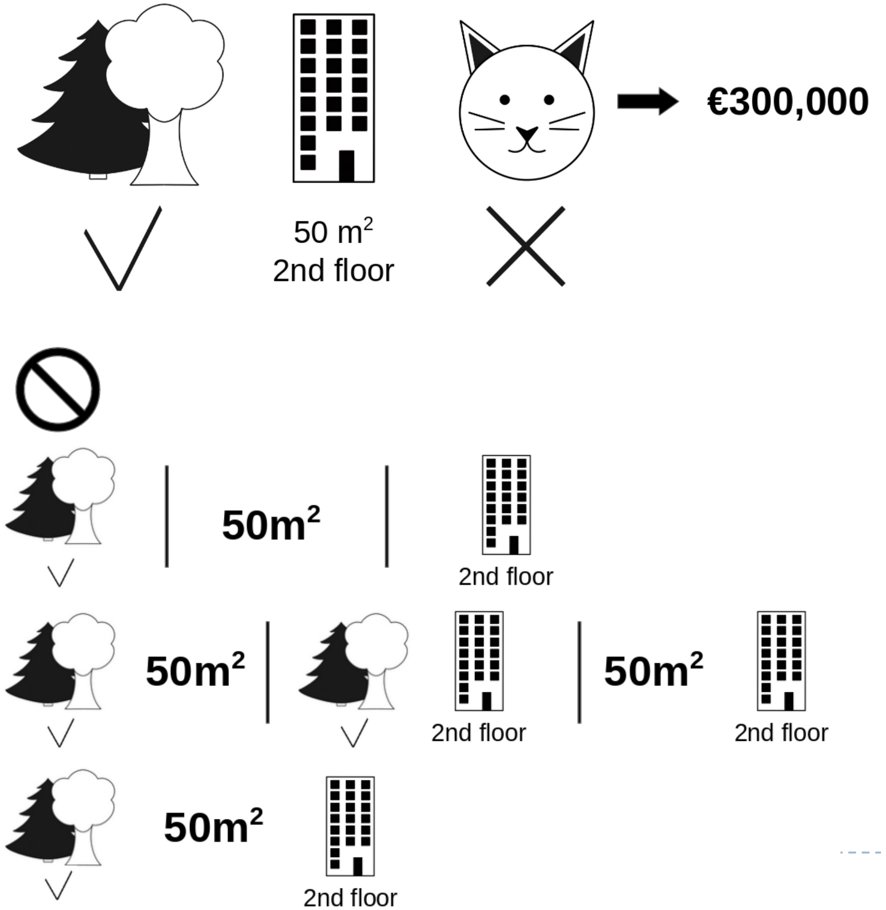
→ segment m indicates the image is not “frog”





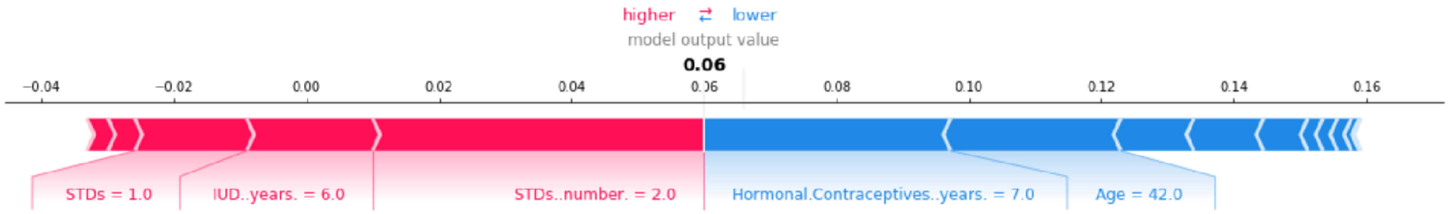
Local Methods - SHAP (SHapley Additive exPlanations)

- A prediction can be explained by assuming that each feature value of the instance is a “player” in a game where the prediction is the payout
  - *Shapley values* breakdown a prediction to show the impact of each feature
    - The figure shows all coalitions of feature values that are needed to determine the Shapley value for cat-banned
  - For each of these coalitions we compute the predicted apartment price with and without the feature value cat-banned and take the difference to get the marginal contribution.
    - The Shapley value is the (weighted) average of marginal contributions
    - We replace the feature values of features that are not in a coalition with random values

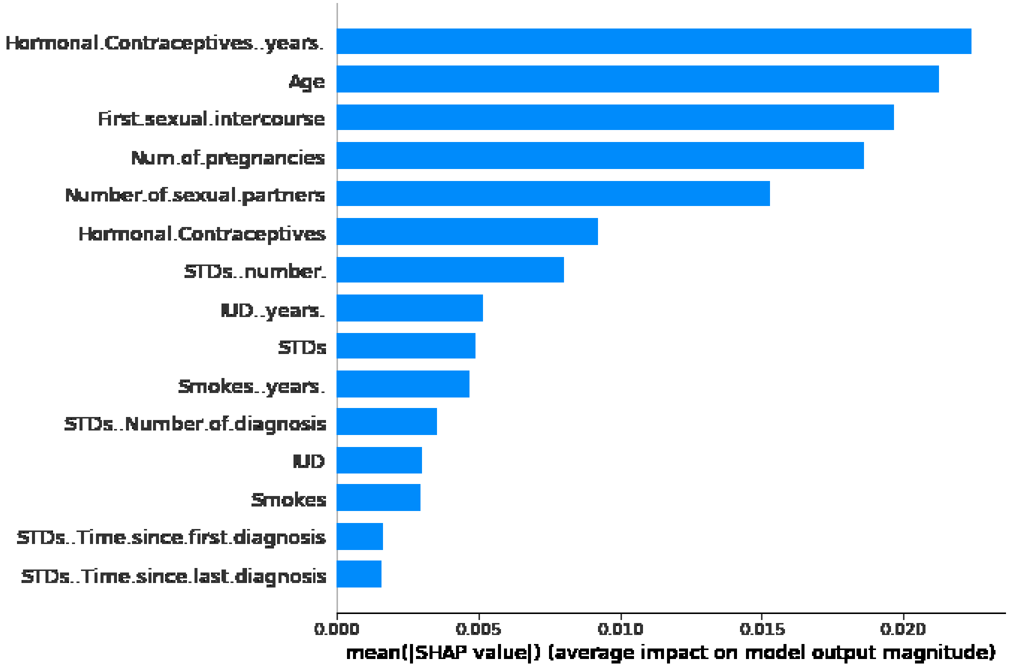


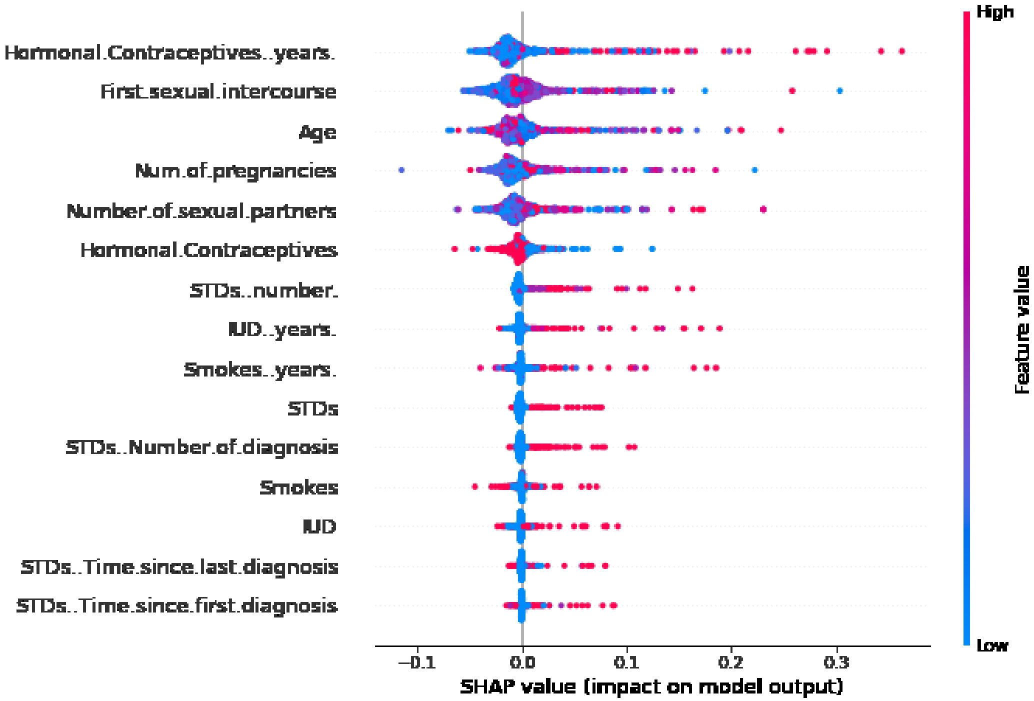
Local Methods - SHAP (SHapley Additive exPlanations)

- SHAP assign an estimated Shapley value to *individual predictions for each feature*
  - SHAP proposed KernelSHAP, an alternative, kernel-based estimation approach for Shapley values inspired by local surrogate models. In addition, TreeSHAP, an efficient estimation approach for tree-based models is also proposed. The force plot, we predicted 0.06, whereas the base value is 0.066
    - Each feature value is a force that either increases or decreases the prediction. The prediction starts from the baseline. The baseline for Shapley values is the average of all predictions. In the plot, each Shapley value is an arrow that pushes to increase (positive value) or decrease (negative value) the prediction. STD stands for sexually transmitted disease



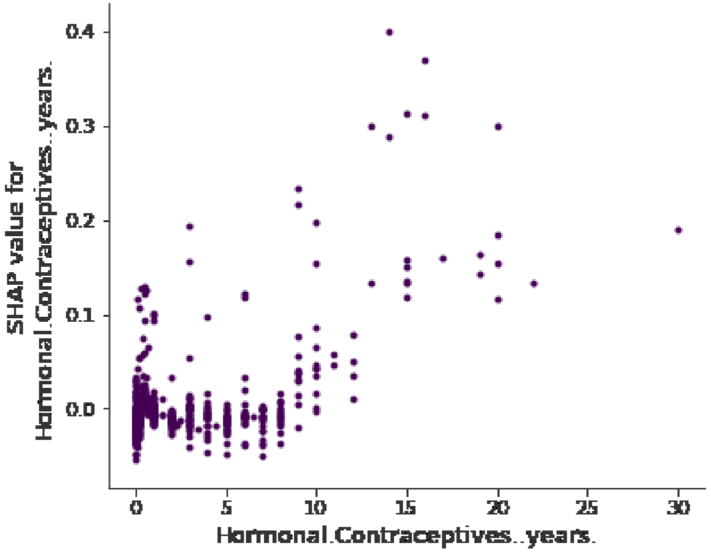
- Permutation importance doesn't tell you how each features matter
  - If a feature has medium permutation importance, that could mean it has a large effect for a few predictions, but no effect in general, or a medium effect for all predictions
- SHAP summary plots give us a view of feature importance and what is driving it
  - Each point on the summary plot is a Shapley value for a feature and an instance
  - The features are ordered according to their importance

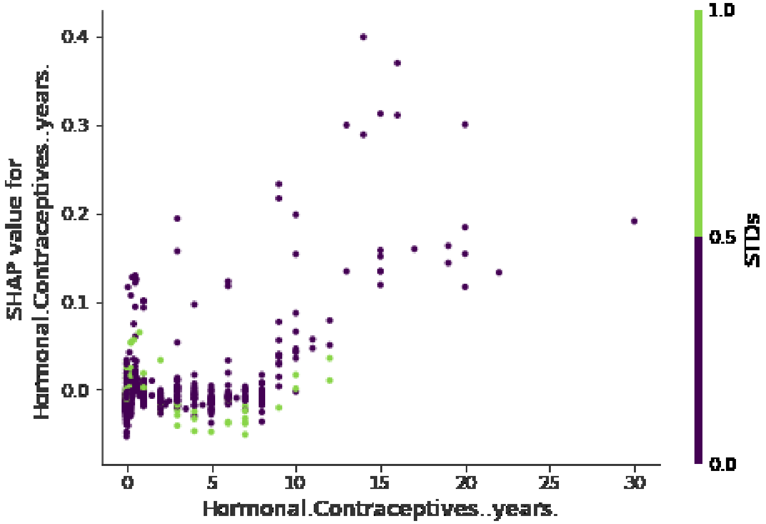




Local Methods - SHAP (SHapley Additive exPlanations)

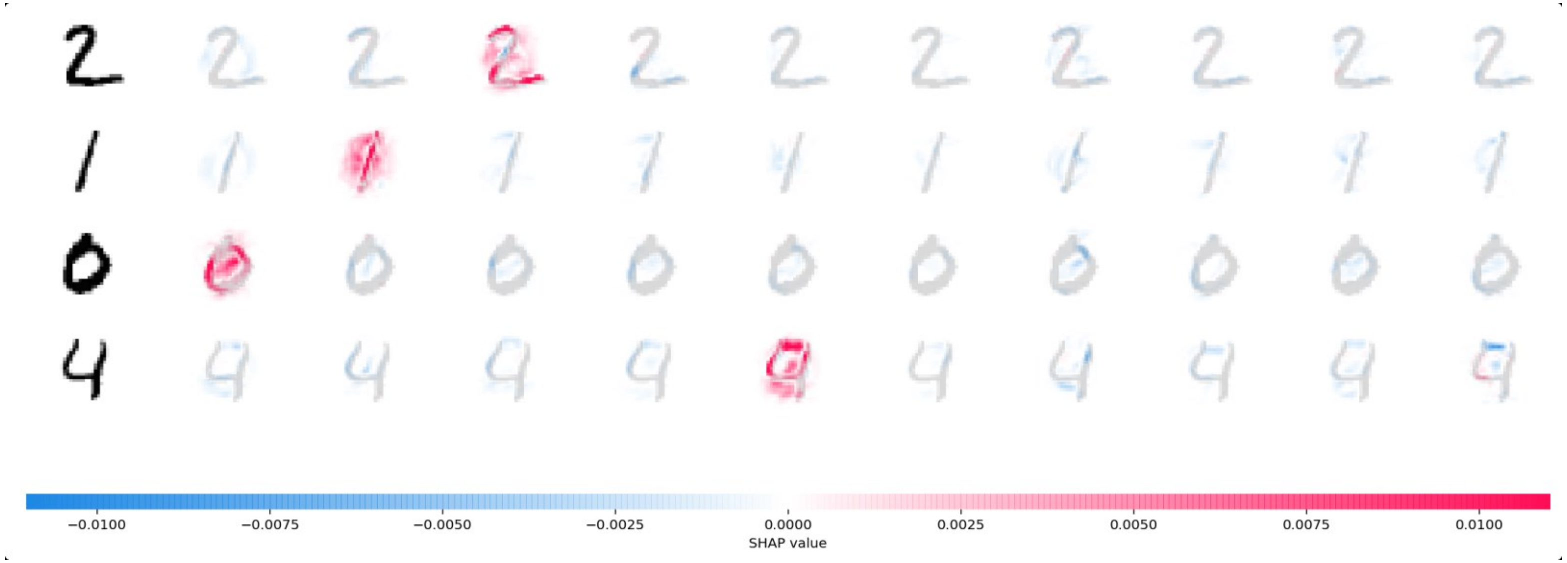
- We've previously used Partial Dependence. But what is the distribution of effects? Is the effect of having a certain value pretty constant, or does it vary a lot depending on the values of other features
  - SHAP dependence contribution plots provide a similar insight to PDP's
  - Each dot represents a row of the data. The horizontal location is the actual value from the dataset, and the vertical location shows what having that value did to the prediction

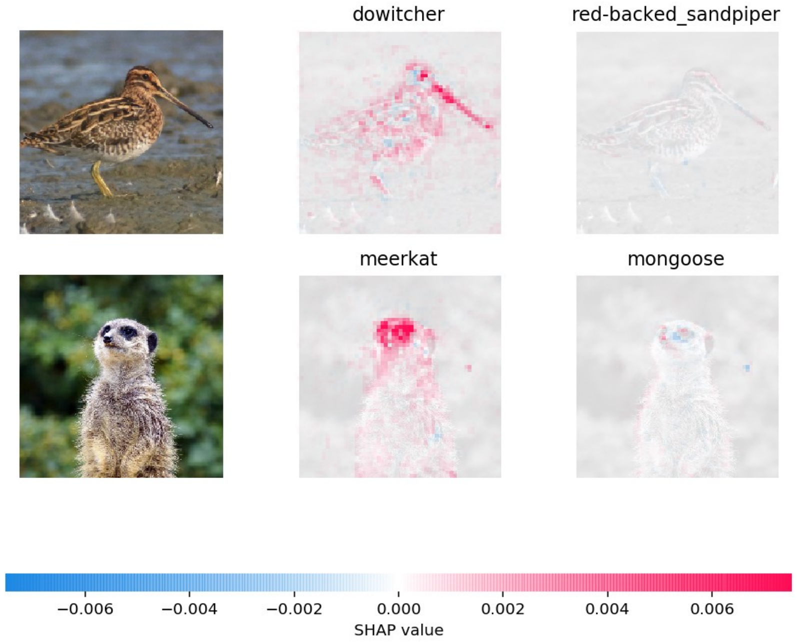




Local Methods - SHAP (SHapley Additive exPlanations)

- Extended to deep learning models
  - Deep SHAP (DeepLift) is a high-speed approximation algorithm for *Shapley* values
  - GradientShap combines ideas from Integrated Gradients, SHAP, and SmoothGrad into a single expected value equation. This allows an entire dataset to be used as the background distribution and allows local smoothing



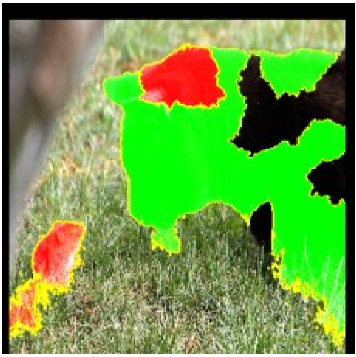


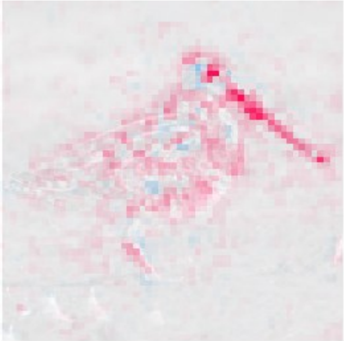
4. Neural Network Interpretation

- It’s often said that deep learning models are “black boxes”: they learn representations that are difficult to extract and present in a human-readable form. Although this is partially true for certain types of deep learning models, it’s definitely not true for convnets
  - The representations learned by convnets are highly amenable to visualization, in large part because they’re representations of visual concepts. Since 2013, a wide array of techniques has been developed for visualizing and interpreting these representations
    - Neural networks learn features and concepts in their hidden layers and we need special tools to uncover them
    - The gradient can be utilized to implement interpretation methods that are more computationally efficient than model-agnostic methods that look at the model “from the outside”

Neural Network Interpretation

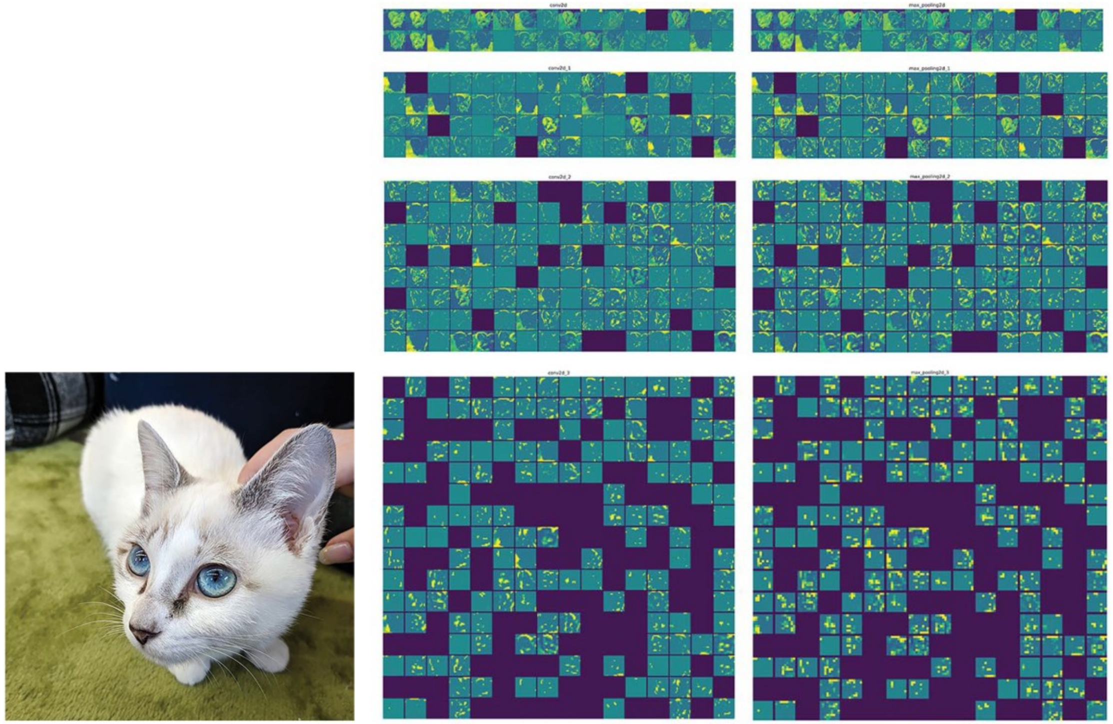
- **Visualizing intermediate convnet outputs** (intermediate activations) - Useful for understanding how successive convnet layers transform their input, and for getting a first idea of the meaning of individual convnet filters
- **Visualizing convnet filters** - Useful for understanding precisely what visual pattern or concept each filter in a convnet is receptive to
- **Visualizing heatmaps of class activation in an image** - Useful for understanding which parts of an image were identified as belonging to a given class, thus allowing you to localize objects in images





Visualizing intermediate activations

- There are a few things to note here:
  - The first layer acts as a collection of various *edge detectors*. At that stage, the activations retain almost all of the information present in the initial picture
  - As you go deeper, the activations become increasingly abstract and less visually interpretable. They begin to encode higher-level concepts such as “cat ear” and “cat eye.”
  - The sparsity of the activations increases with the depth of the layer: in the first layer, almost all filters are activated by the input image, but in the following layers, more and more filters are blank. This means the *pattern encoded by the filter isn’t found* in the input image

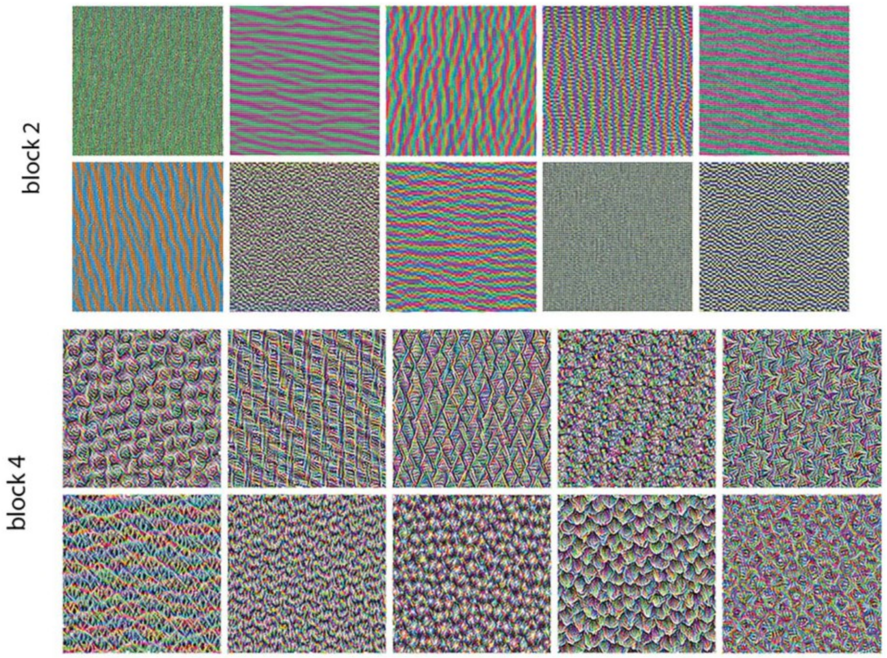


Visualizing intermediate activations

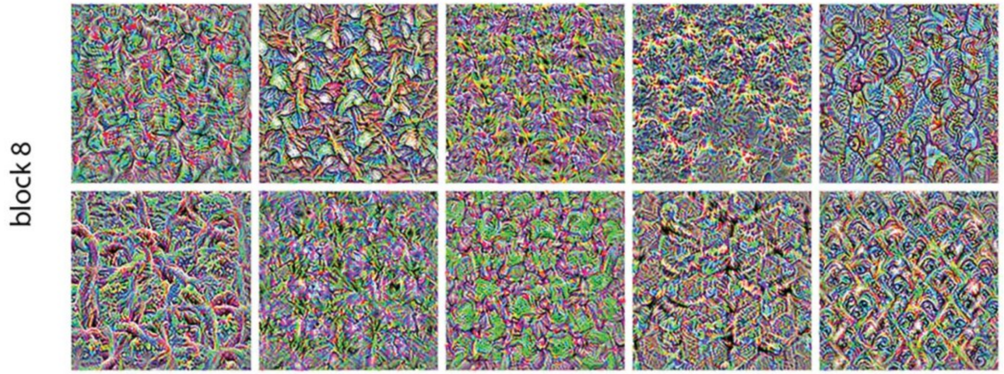
- Visualizing intermediate activations consists of displaying the values returned by various convolution and pooling layers in a model, given a certain input
  - We have just evidenced an important universal characteristic of the representations learned by DNNs
    - The features extracted by a layer become increasingly abstract with the depth of the layer
    - The activations of higher layers carry less and less information about the specific input being seen, and more and more information about the target
  - A DNN effectively acts as an information distillation pipeline, with raw data going in (in this case, RGB pictures) and being repeatedly transformed so that irrelevant information is filtered out (for example, the specific visual appearance of the image), and useful information is magnified and refined (for example, the class of the image)

Visualizing convnet filters

- Another easy way to inspect the filters learned by convnets is to display the visual pattern that each filter is meant to respond to
  - This can be done with *gradient ascent in input space*: applying gradient ascent to the value of the input image of a convnet so as to maximize the response of a specific filter, starting from a blank input image. The resulting input image will be one that the chosen filter is maximally responsive to



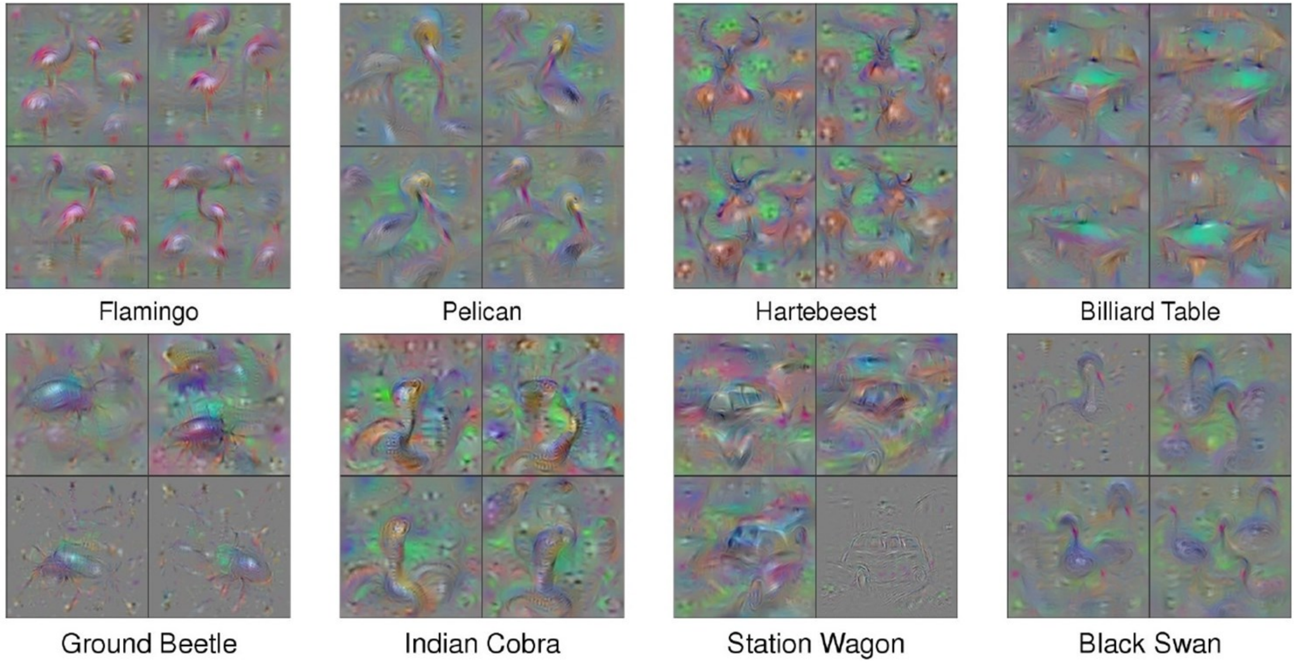
$$img^* = arg\max_{img} \sum_{x,y} h_{n,x,y,z}(img)$$



Visualizing convnet filters

- These filter visualizations tell you a lot about how convnet layers see the world
  - The filters from the first layers in the model encode simple directional edges and colors (or colored edges, in some cases). The filters from layers a bit further up the stack, such as in block4, encode simple textures made from combinations of edges and colors
  - The filters in higher layers begin to resemble textures found in natural images: feathers, eyes, leaves, and so on
  - You could also perform $img^* = arg\max_{img} y_i$ to ask the network what a class looks like
    - This may require some constraints

https://arxiv.org/abs/1506.06579



Flamingo

Pelican

Hartebeest

Billiard Table

Ground Beetle

Indian Cobra

Station Wagon

Black Swan

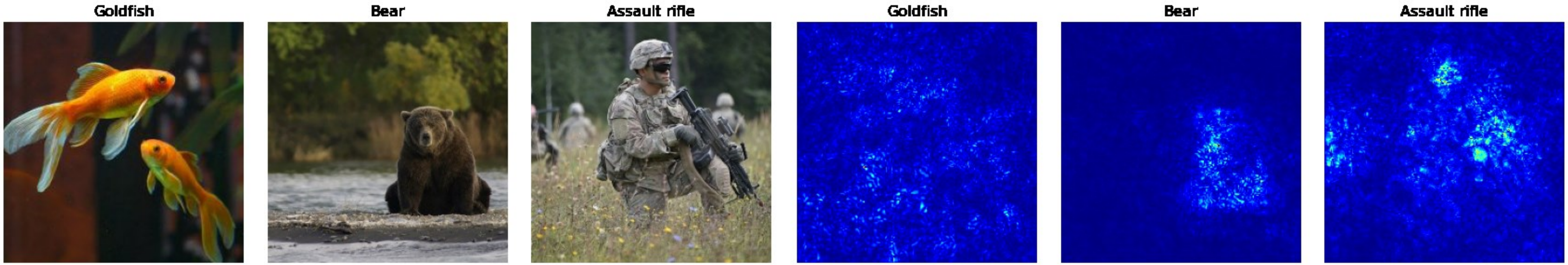
Visualizing heatmaps of class activation

- We'll introduce one last visualization technique—one that is useful for understanding which parts of a given image led a convnet to its final decision
  - This general category of techniques is called class activation map (CAM) or saliency maps visualization, and it consists of producing heatmaps of class activation over input images.
  - Occlusion- or perturbation-based: Methods like SHAP and LIME manipulate parts of the image to generate explanations (model-agnostic)
  - Gradient-based: Many methods compute the gradient of the prediction (or classification score) with respect to the input features. The gradient-based methods (of which there are many) mostly differ in how the gradient is computed

Visualizing heatmaps of class activation

- The idea of Vanilla Gradient, introduced by Simonyan et al. in 2013
  1. Perform a forward pass of the image of interest
  2. Compute the gradient of class score of interest with respect to the input pixels:

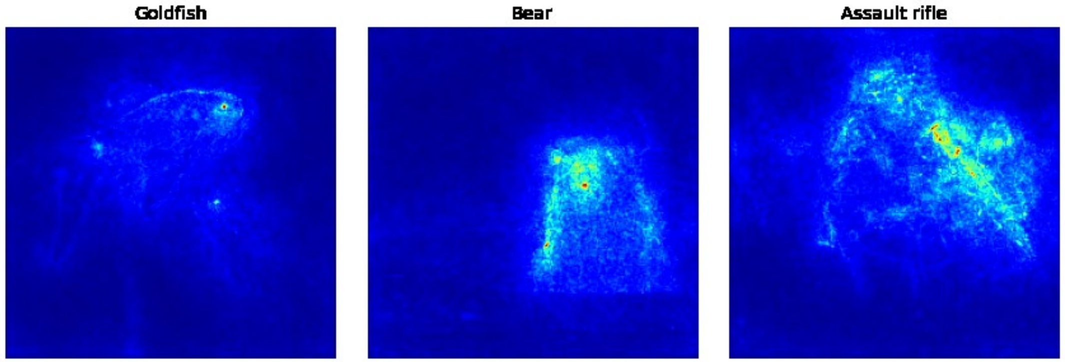
     $E_{grad}(I_0) = \frac{\partial y_c}{\partial I}|_{I=I_0}$ which means we approximate $y_c(I) \approx E_{grad}(I)^T I + b$
  3. Visualize the gradients. You can either show the absolute values or highlight negative and positive contributions separately
- Vanilla Gradient has a saturation problem

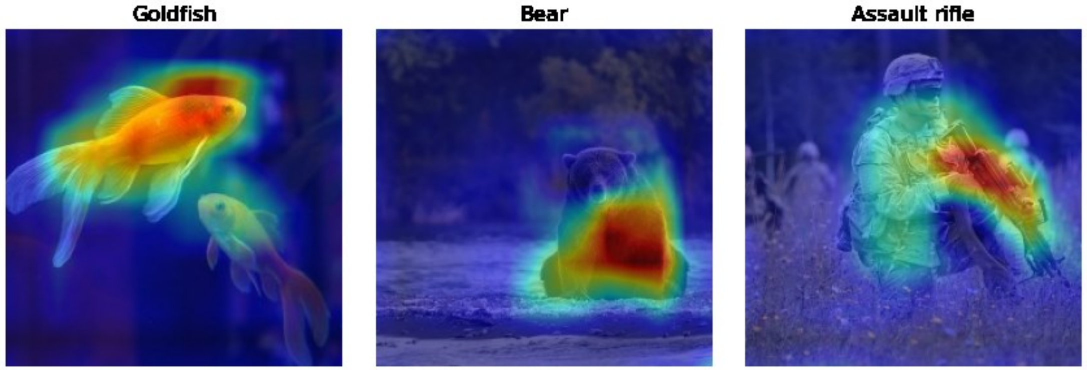


Visualizing heatmaps of class activation

- Other alternatives
  - SmoothGrad, Integrated Gradients, Grad-CAM, Grad-CAM++, ScoreCAM, etc.

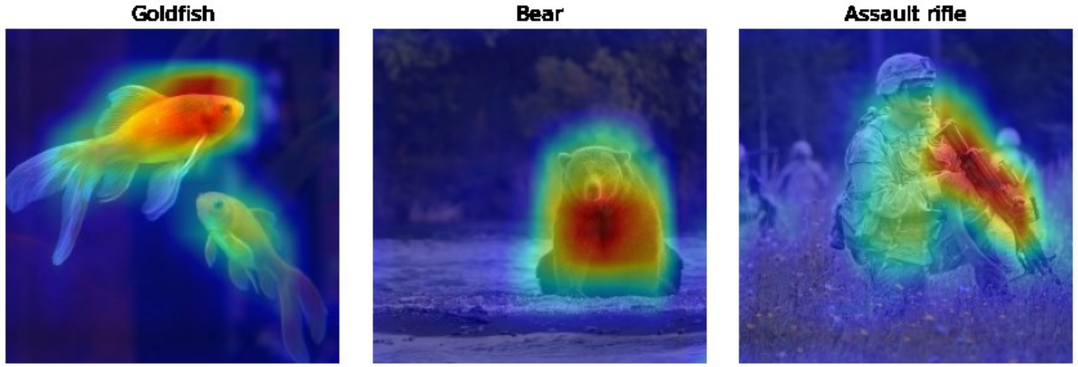
SmoothGrad

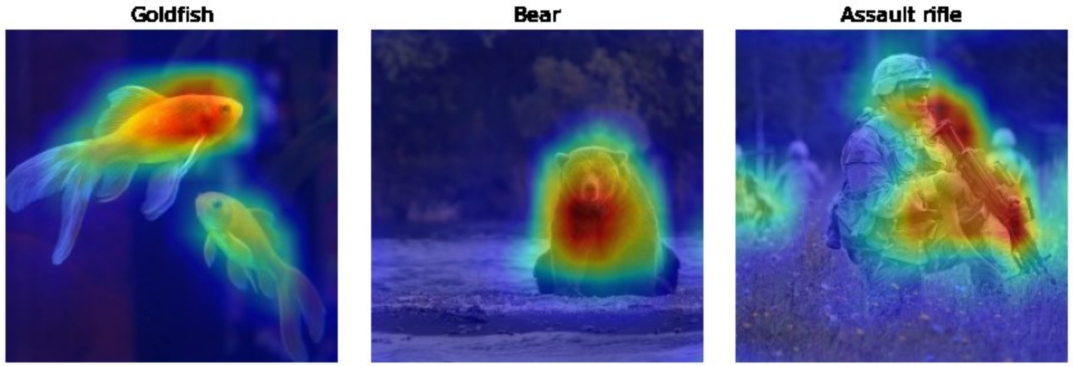




Grad-CAM

Grad-CAM++





ScoreCAM

Conclusion

- We need an interpretable models!
  - Loan issuers are required by law to explain their models
  - Medical diagnosis model is responsible for human life. Can it be a black box?
  - If a model is used at the court, we must make sure the model behaves in a nondiscriminatory manner
  - If a self-driving car suddenly acts abnormally, we need to explain why
- Make people (your customers, your boss, yourself) comfortable
  - Don’t be afraid about black box model. We do not completely know how brains work! But we trust the decision of humans!
- Several methods you can choose from
  - https://csinva.io/notes/cheat_sheets/interp.pdf

References

[1] https://christophm.github.io/interpretable-ml-book/

[2] Deep learning with Python, 2nd Edition Chapter 9

[3] https://www.kaggle.com/learn/machine-learning-explainability

[4] https://speech.ee.ntu.edu.tw/~hylee/ml/ml2021-course-data/xai_v4.pptx

Appendix

Resources

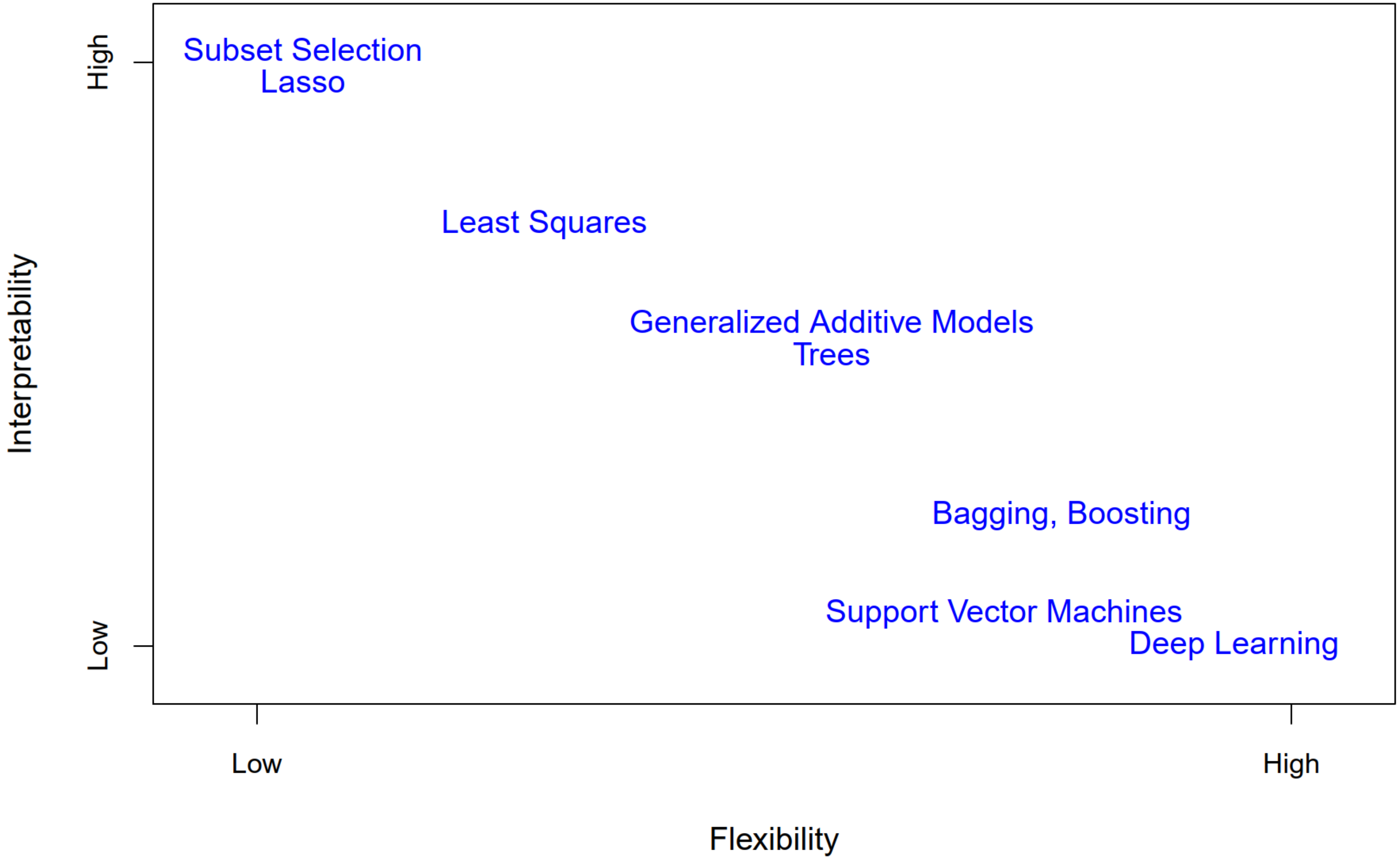
- Lectures or books
  - https://christophm.github.io/interpretable-ml-book/
  - https://github.com/kdd-lab/XAI-Survey
  - https://github.com/jphall663/awesome-machine-learning-interpretability
  - https://github.com/wangyongjie-ntu/Awesome-explainable-AI
  - Local Model-Agnostic Methods - Counterfactual Explanations
  - Global Model-Agnostic Methods - Prototypes and Criticisms
  - Speech - https://speech.ee.ntu.edu.tw/~hylee/ml/ml2021-course-data/xai_v4.pptx
- Tree base visualization
  - https://github.com/parrt/dtreeviz
- Prototype and Counterfactual
  - https://github.com/Trusted-AI/AIX360
  - https://github.com/SeldonIO/alibi

Resources

- Casual
  - https://github.com/uber/causalml
- Decision Rules
  - https://github.com/csinva/imodels
- Local methods
  - https://github.com/slundberg/shap
  - https://github.com/marcotcr/lime
- Unify framework
  - https://github.com/interpretml/interpret
- Network visualization
  - https://github.com/keisen/tf-keras-vis
  - https://github.com/PAIR-code/saliency
  - https://github.com/sicara/tf-explain
  - https://github.com/pytorch/captum (Also contains LIME and SHAP)

Some trade-offs when selecting models

- Prediction accuracy versus interpretability
  - Linear models are easy to interpret; thin-plate splines are not.
  - Parsimony versus black-box
    - We often prefer a simpler model involving fewer variables over a black-box predictor involving them all.
  - Good fit versus over-fit or under-fit
    - How do we know when the fit is just right?


Subset Selection
Lasso
Least Squares
Generalized Additive Models
Trees
Bagging, Boosting
Support Vector Machines
Deep Learning
Interpretability
High
Low
Flexibility
Low
High

Example-Based Explanations

- Example-based explanation methods select particular instances to explain the behavior of models or to explain the underlying data distribution
  - The difference to model-agnostic methods is that the example-based methods explain a model by selecting instances of the dataset and not by creating summaries of features (such as feature importance or partial dependence)
  - Example-based methods work well if the feature values of an instance carry more context, meaning the data has a structure, like images or texts do
- For instance
  - A physician sees a patient with an unusual cough and a mild fever. The symptoms remind her of another patient she had years ago with similar ones. She suspects that the patient could have the same disease and she takes a blood sample to test for this specific disease
  - A data scientist works on a new project for one of his clients: Analysis of the risk factors that lead to the failure of production machines for keyboards. The data scientist remembers a similar project he worked on and reuses parts of the code from the old project

Example-Based Explanations

- These stories illustrate how we humans think in examples or analogies. The blueprint of example-based explanations is
  - Thing B is similar to thing A and A caused Y, so I predict that B will cause Y as well
  - Implicitly, decision trees and KNN works like a example-based method
- The following interpretation methods are all example-based:
  - **Prototypes** are a selection of representative instances from the data and criticisms are instances that are not well represented by those prototypes
  - **Counterfactual explanations** tell us how an instance has to change to significantly change its prediction. By creating counterfactual instances, we learn about how the model makes its predictions and can explain individual predictions
  - **Influential instances** are the training data points that were the most influential for the parameters of a prediction model or the predictions themselves. Analyzing influential instances helps to find problems with the data and debug the model