Explainable AI (XAI)

CS 3244 Machine Learning

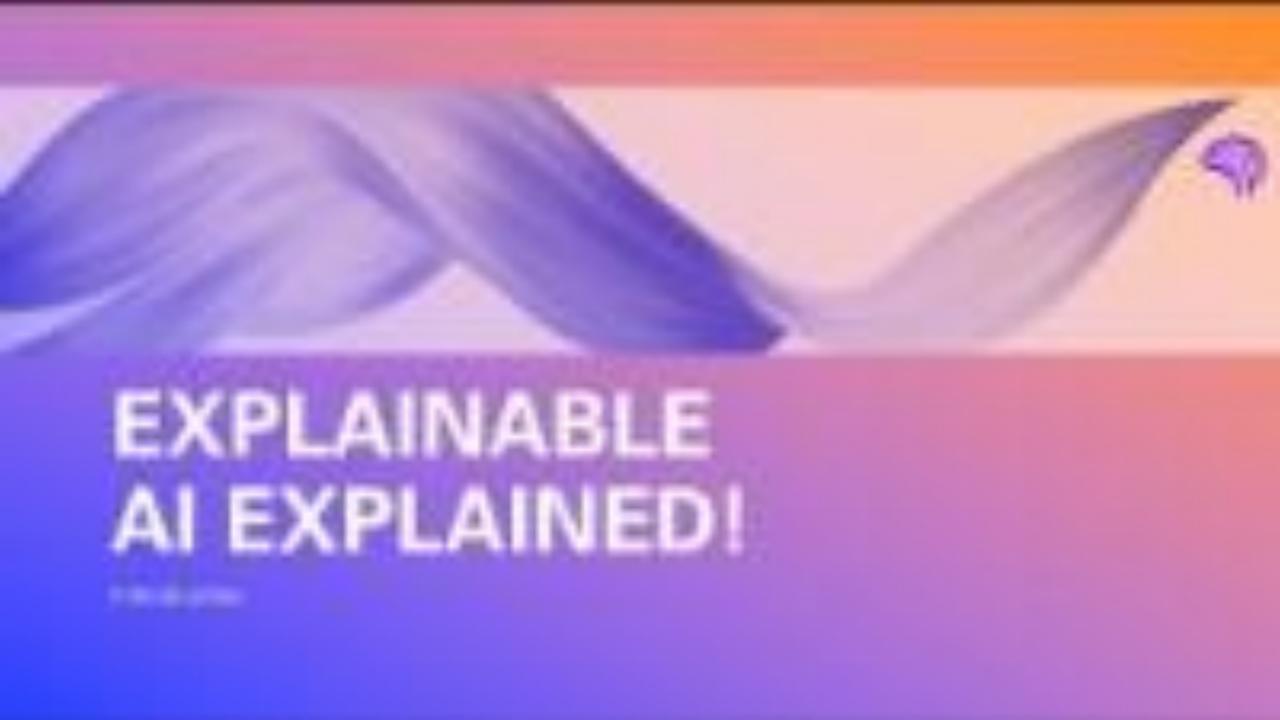


Week 11A: Learning Outcomes

- 1. Describe multiple methods to interpret feature importance
- Appropriately interpret feature attributions from each type of explanation
- 3. Describe how LIME explanations are generated
- 4. Describe how Grad-CAM explanations are generated

Week 11A: Lecture Outline

- 1. Introduction
 - 1. Motivation for Explainable AI (XAI)
 - 2. Explaining Why: Feature Importance
- 2. Explanation techniques
 - 1. Glassbox Models (Linear Regression, Logistic Regression)
 - 2. Model-Agnostic Explanations (LIME)
 - 3. Model-Specific Explanations (Grad-CAM)
- 3. Human-centered XAI (not in exam)



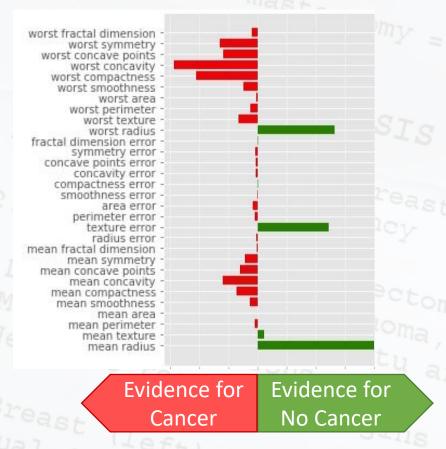
Case 1: Does patient have cancer?

Feature	Value	
worst area	1315.00	
mean radius	16.13	
worst radius	20.96	
area error	54.18	
worst perimeter	136.80	
worst texture	31.48	
mean perimeter	108.10	
smoothness error	0.01	
mean area	798.80	
mean concave points	0.10	

Prediction: Cancer

Further reading: https://coderzcolumn.com/tutorials/machine-learning/how-to-use-lime-to-understand-sklearn-models-predictions

Why??



Explanation: Feature Attributions

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Case 2: Is this skin cancer?



Prediction: Skin Cancer

Why??



Explanation: Highlighted Salient Region

Further reading: https://towardsdatascience.com/medical-image-analysis-using-probabilistic-layers-and-grad-cam-42cc0118711f Image credit: https://news.yale.edu/2019/11/13/yale-study-reveals-hyperhotspots-identifying-skin-cancer-risk

Why? Feature Importance

- Question
 - Why?
 - What caused this prediction?
- Explains
 - Which features are important for the prediction
 - In what way the features influenced the prediction
- Implementation
 - Weights in Linear / Logistic Regression
 - Surrogate Weights from LIME
 - Saliency Map of CNN

Performance-Interpretability Trade-off

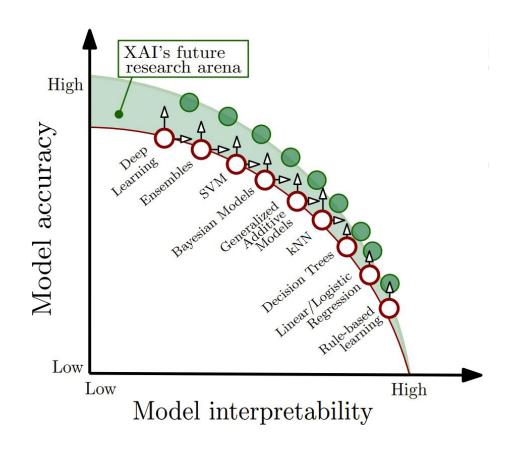
High performance

(Low interpretability)

- Non-Linear relationships
 - $y = w_1 x_1^2 + \log(x_2)$
- Interacting features

•
$$y = x_1 + x_2 + x_1 x_2$$

- Many features or parameters
- Unrelatable features



High interpretability

(Lower performance)

- Linear relationships
 - $y = w_1 x_1 + w_2 x_2$
- Independent features
 - $y = x_1 + x_2$
 - $y = f_1(x_1) + f_2(x_2)$
- Few features (x_r) , and parameters (w_r, θ_r)
- Semantically meaningful features

Arrieta, A. B., Díaz-Rodríguez, N., Del Ser, J., Bennetot, A., Tabik, S., Barbado, A., ... & Herrera, F. (2020). <u>Explainable Artificial Intelligence (XAI): Concepts, taxonomies, opportunities and challenges toward responsible AI.</u> *Information Fusion, 58*, 82-115.

Explainable AI (XAI) Categorization

Explanability

		Glassbox	Model-Agnostic	Model-Specific	Blackbox
Scope	Global	Linear RegressionLogistic RegressionDecision Tree	Collection of local explanations		Deep Neural NetworksHighly non-
	Local	• Examples (e.g., kNN)	• LIME	• Grad-CAM	linear models

<u>Definitions</u>

Glassbox model

- Prediction model is implicitly interpretable
 Model-Agnostic explanation
- Uses surrogate model to provide simple explanations
 Model-Specific explanation
- Derived from calculations in specific prediction model **Blackbox** model
- Very uninterpretable, not transparent

Global explanation

- Explains general behavior for all instances
- Does not change for different instances
 Local explanation
- Explains behavior for specific instance



Interpreting Linear Regression



How would you interpret? Linear Regression

$$\hat{y} = w_0 + w_1 x_1 + w_2 x_2 + \dots + w_n x_n = \sum_{r=0}^{n} w_r x_r$$

= $\mathbf{w} \cdot \mathbf{x} = \mathbf{w}^{\mathsf{T}} \mathbf{x}$

How would you interpret? Linear Regression

$$\hat{y} = w_0 + w_1 x_1 + w_2 x_2 + \dots + w_n x_n = \sum_{r=0}^n w_r x_r$$

$$= \mathbf{w} \cdot \mathbf{x} = \mathbf{w}^{\mathsf{T}} \mathbf{x}$$
If $w_1 = k w_2$, then w_1 is k times more important than w_2

Weighted Sum Interpretation

Bigger w_r means

- Larger weight
- More **importance** for to x_r
- Direction? Supportive (positive) or opposing (negative) influence

Gradient Interpretation

Bigger W_r means

- **Steeper** slope for x_r axis
 - Changes in x_r lead to bigger in \hat{y} changes
- More **importance** for x_r
- Direction indicates increasing or decreasing influence



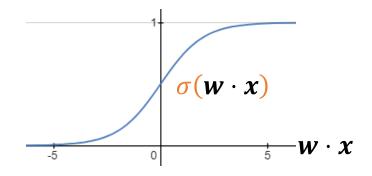
Interpreting Logistic Regression



How would you interpret? Logistic Regression

$$\hat{y} = \sigma(z) = \frac{1}{1 + e^{-z}}$$

$$z = \mathbf{w} \cdot \mathbf{x} = \sum_{r=0}^{n} w_r x_r$$



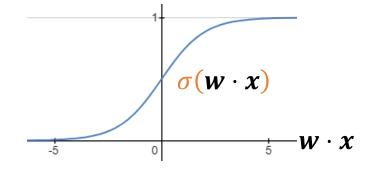
How would you interpret? Logistic Regression

Not proportional, since non-linear If $w_1 = kw_2$, then what is the relationship between w_1 and w_2 ?

$$\hat{y} = \sigma(z) = \frac{1}{1 + e^{-z}}$$

$$z = \mathbf{w} \cdot \mathbf{x} = \sum_{r=0}^{n} w_r x_r$$

$$\hat{y} \not\propto w_r x_r, \forall r$$



Weighted Sum Interpretation

Bigger w_r means

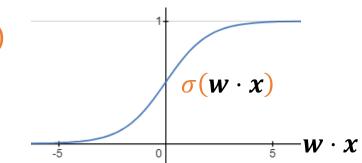
- Larger importance
- Direction indicates influence

$$\hat{y} = \sigma(f)$$
 is positively monotonic, i.e., $f_1 > f_2 \Rightarrow \sigma(f_1) > \sigma(f_2)$ Bigger $f \Rightarrow$ bigger \hat{y}

Interpreting weights in Logistic Regression

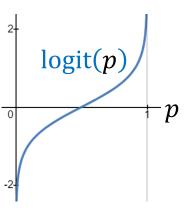
Probability

$$P(\hat{y}) = p = \hat{y} = \frac{1}{1 + e^{-w \cdot x}} = \sigma(p)$$
$$\frac{1}{p} = 1 + e^{-w \cdot x}$$



Odds Ratio

Log Odds Ratio
$$\operatorname{logit}(p) = \log\left(\frac{p}{1-p}\right) = w \cdot x$$



$$\operatorname{logit}(P(\hat{y})) \propto w_r x_r, \forall r$$

If $w_1 = kw_2$, then log odds ratio of w_1 is k times bigger than of w_2

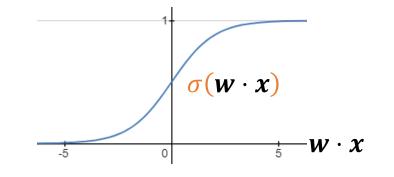
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How would you interpret?

Logistic Regression

$$\hat{y} = \sigma(f) = \frac{1}{1 + e^{-f}}$$

$$f = \mathbf{w} \cdot \mathbf{x} = \sum_{r=0}^{n} w_r x_r$$



 $\operatorname{logit}(P(\hat{y})) \propto w_r x_r, \forall r$

If $w_1 = kw_2$, then \log odds ratio of w_1 is k times bigger than of w_2

Weighted Sum Interpretation

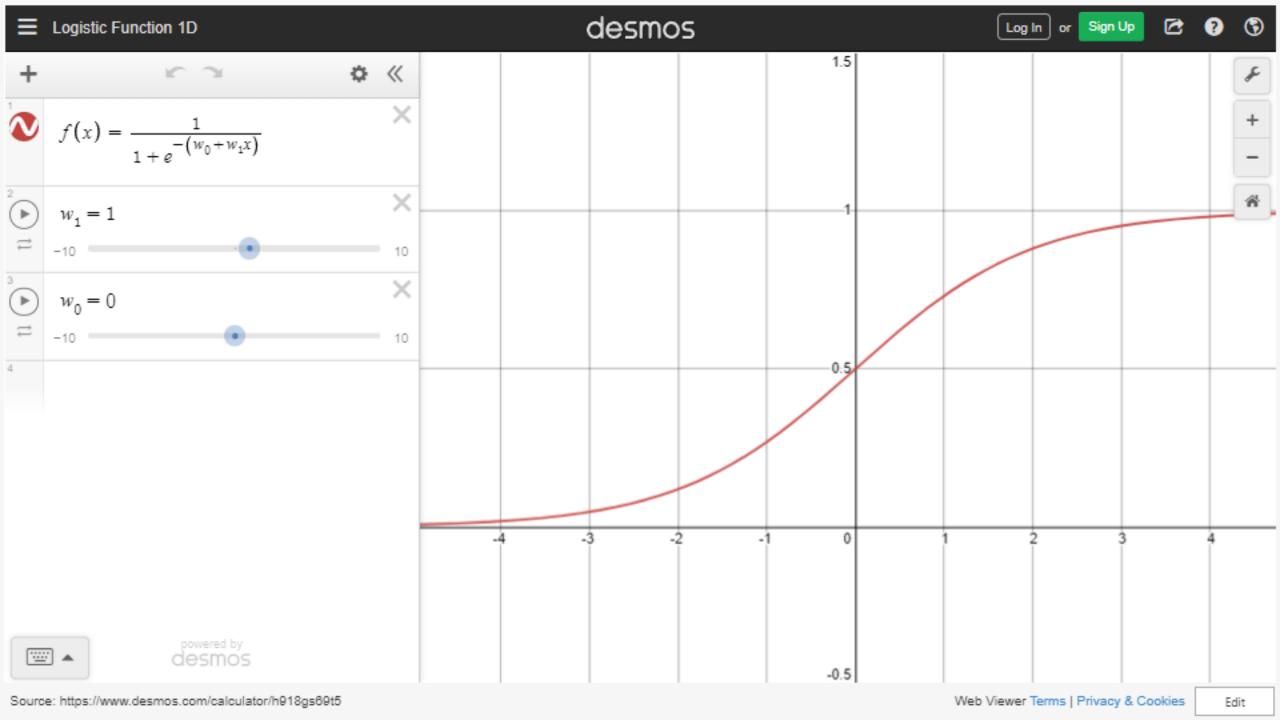
Bigger w_r means

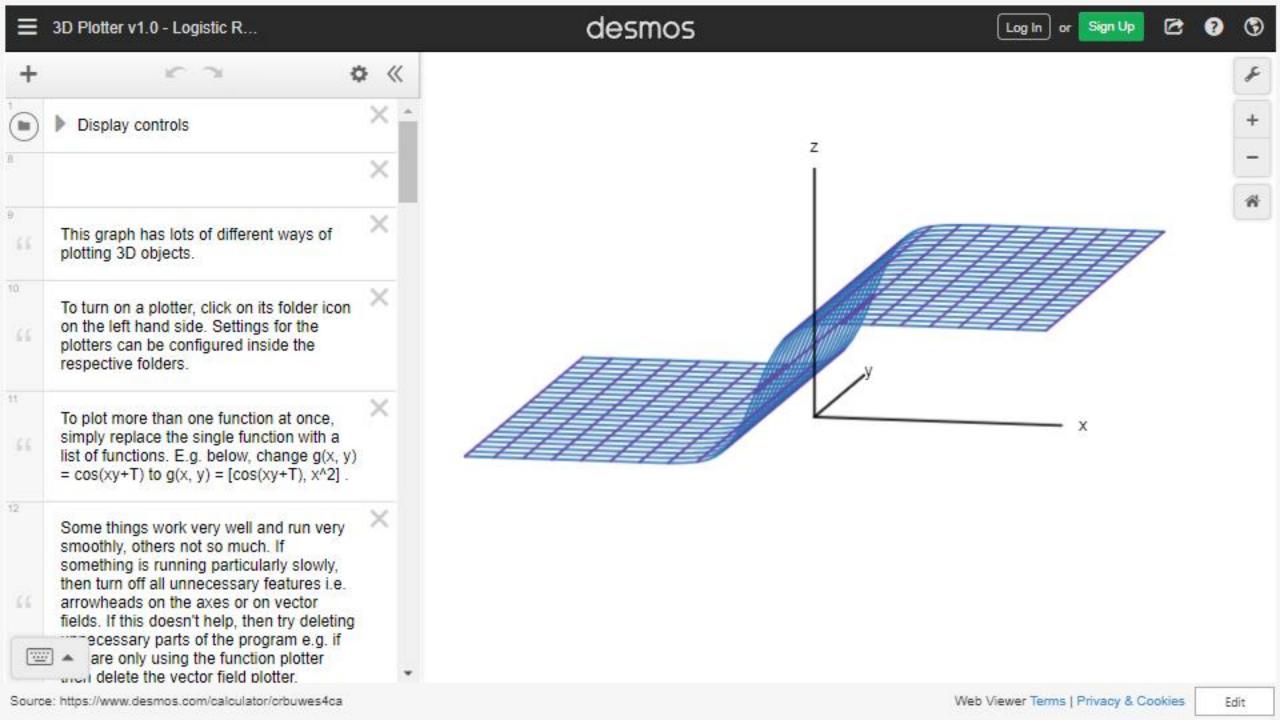
- Larger importance
- Direction indicates influence

Gradient Interpretation

Bigger w_r means?

- Steepness? Sigmoid bounded between 0 and 1
- Direction in 2D (or higher)?





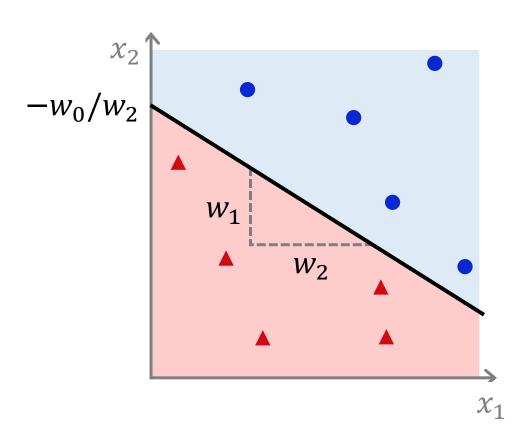
Linear Classification

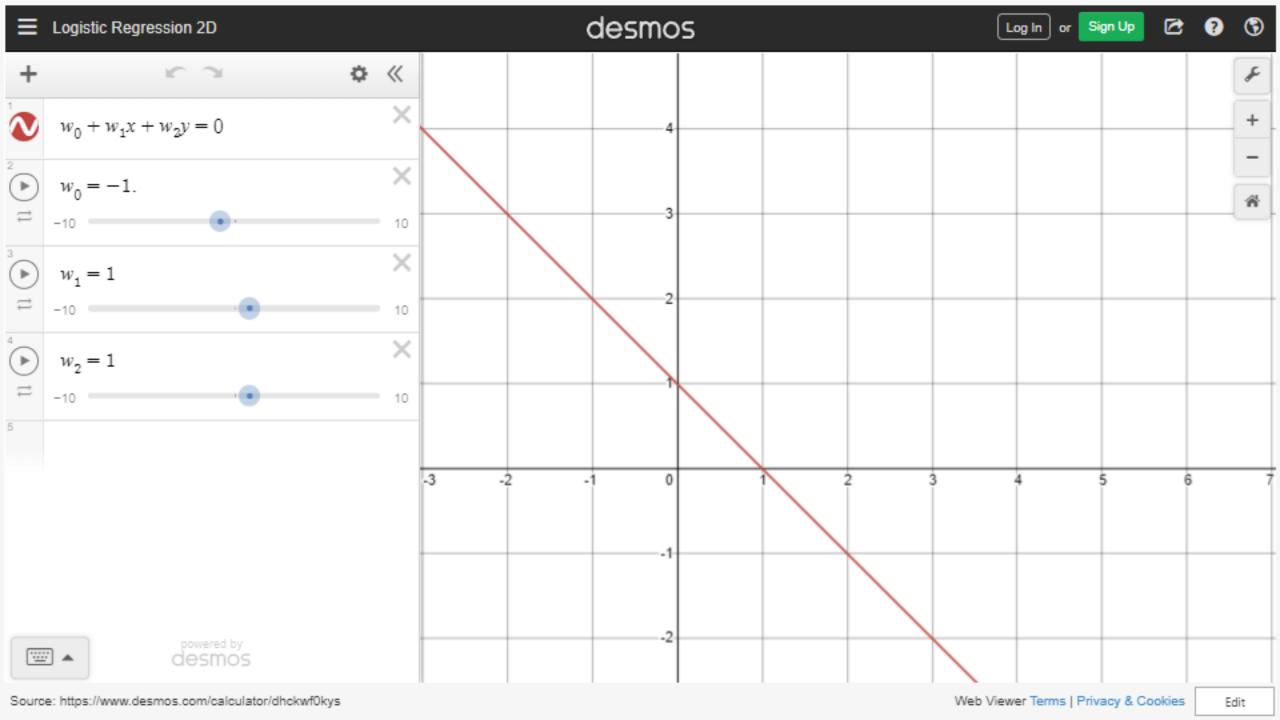
$$w_2 x_2 + w_1 x_1 + w_0 = 0$$

$$\sum_{r=0}^{n} w_r x_r = 0 \ x_0 = 1$$

$$\sum_{r=0}^{n} w_r x_r > 0 \qquad \sum_{r=0}^{n} w_r x_r \le 0$$

$$\hat{y} = \sigma \left(\sum_{r=0}^{n} w_r x_r \right)$$





Linear Classification

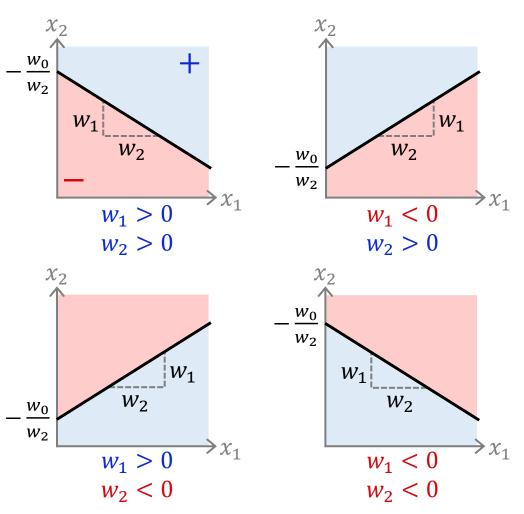
$$w_2 x_2 + w_1 x_1 + w_0 = 0$$

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$$\sum_{r=0}^{n} w_r x_r > 0 \qquad \sum_{r=0}^{n} w_r x_r \le 0$$

$$\hat{y} = \sigma \left(\sum_{r=0}^{n} w_r x_r \right)$$

Weight sign indicates direction towards pos/neg prediction

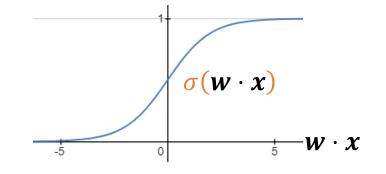


How would you interpret?

Logistic Regression

$$\hat{y} = \sigma(z) = \frac{1}{1 + e^{-z}}$$

$$f = \mathbf{w} \cdot \mathbf{x} = \sum_{r=0}^{n} w_r x_r$$



 $\operatorname{logit}(P(\hat{y})) \propto w_r x_r, \forall r$

If $w_1 = kw_2$, then log odds ratio of w_1 is k times bigger than of w_2

Weighted Sum Interpretation

Bigger w_r means

- Larger importance
- Direction indicates influence

Gradient Interpretation

Bigger w_r means?

- **Steeper** slope for x_r near decision boundary
- **Decision boundary** more *perpendicular* to x_r
- Weight sign indicates direction of pos/neg prediction



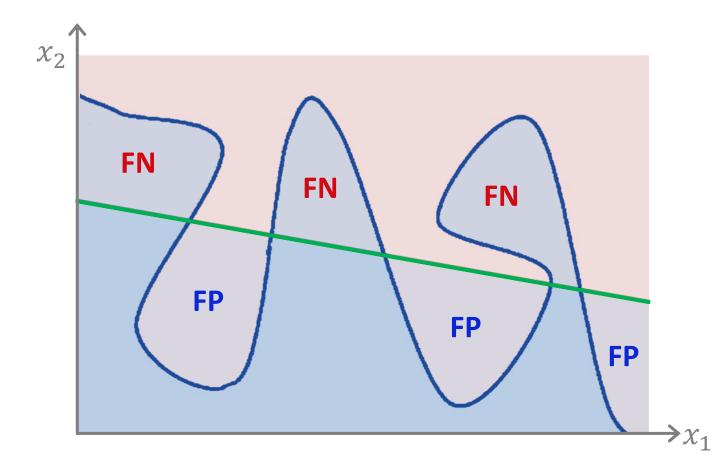


Local Interpretable Model-agnostic Explanations LIME



How to describe with just x_1 and x_2 ?

Non-Linear Decision Boundary f(x)



Prediction Model

- Non-linear model of $\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \end{pmatrix}$
- Shown as curvy decision boundary

Explanation: Linear Model

$$g(\mathbf{x}) = \mathbf{w} \cdot \mathbf{x} = \sum_{r=0}^{n} w_r x_r$$

- Simple to interpret
- But too many errors between g and f

$$L = f(\mathbf{x}) - g(\mathbf{x})$$

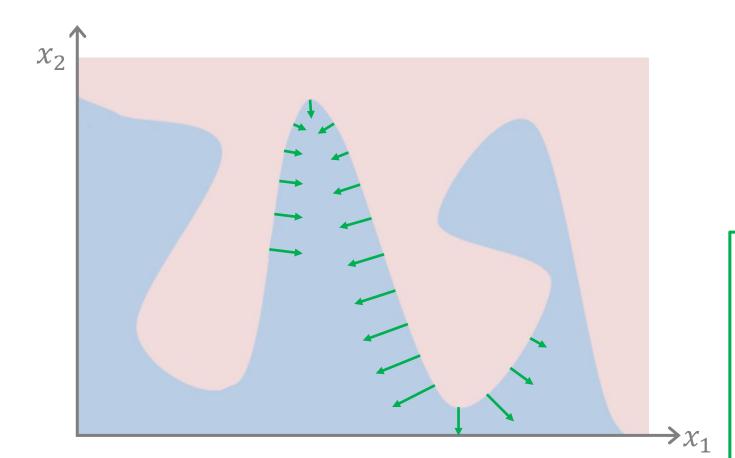
Image Credit: https://santiagof.medium.com/model-interpretability-making-your-model-confess-lime-89db7f70a72b

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How to describe with just x_1 and x_2 ? Non-Linear Decision Boundary

$$\nabla f(\mathbf{x}) \neq \begin{pmatrix} w_1 \\ w_2 \\ \vdots \end{pmatrix} = \mathbf{w}$$

Since f is not linear



Prediction Model

- Non-linear model of $\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \end{pmatrix}$
- Shown as curvy decision boundary

Explanation: Gradients

$$g(\mathbf{x}) = \nabla f(\mathbf{x}) = \frac{\partial f}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \end{pmatrix}$$

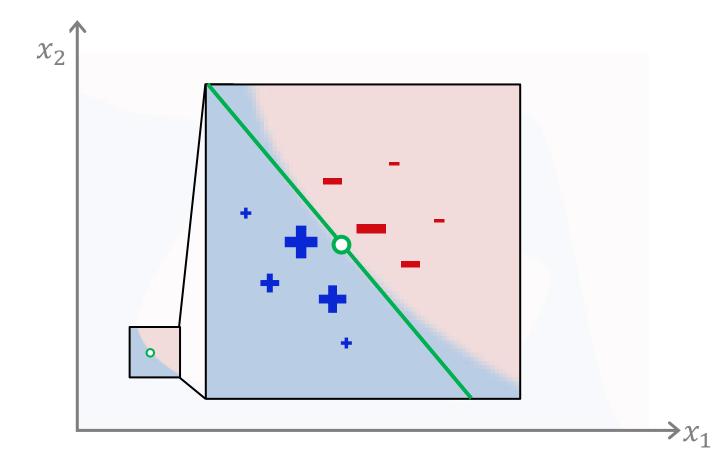
- Steepness for each feature x_r
- Difficult to remember, since gradients are different for each instance (point)

Image Credit: https://santiagof.medium.com/model-interpretability-making-your-model-confess-lime-89db7f70a72b

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LIME

Local Interpretable Model-agnostic Explanations



Prediction Model

- Non-linear model of $\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \end{pmatrix}$
- Shown as curvy decision boundary

Explanation: LIME

- 1. Starting with **instance** x to explain
- 2. Focus on **Local** region
- 3. Training set as **neighbors** $x^{(\eta)} \in X^{(\eta)}$
- 4. Train **surrogate model**, e.g., linear:

$$g(x) = w \cdot x = \sum_{r=0}^{n} w_r x_r$$

Image Credit: https://santiagof.medium.com/model-interpretability-making-your-model-confess-lime-89db7f70a72b

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LIME

Find "best" explainer g that minimizes $\xi(x)$

Python API:

https://github.com/marcotcr/lime

$$\xi(\mathbf{x}) = \underset{g \in G}{\operatorname{argmin}} \left(L(f, g, \pi_{x}) + \Omega(g) \right)$$

f is the **predictor** function (model) g is the **explainer** function (model) $\pi_{x}(x^{\langle \eta \rangle})$ is the neighbor **proximity** function

• E.g., exponential decay $\exp\left(-\left(d(x,x^{\langle\eta\rangle})\right)^2\right)$

 $L(f, g, \pi_x)$ is the <u>locally-weighted error loss</u> function between predictor f and explainer g

$$L(f, g, \pi_{x}) = \sum_{x^{\langle \eta \rangle} \in X^{\langle \eta \rangle}} \pi_{x}(x^{\langle \eta \rangle}) \left(f(x^{\langle \eta \rangle}) - g(x^{\langle \eta \rangle}) \right)^{2}$$

$\Omega(g)$ is the sparsity regularization

- Want simpler explanation
 - \Rightarrow fewer weights
 - ⇒ Lasso (L1 norm)
- Penalizes if total weights is too large
- λ is hyperparameter on how much to penalize

$$\Omega(g) = \lambda ||w_r||_1 = \lambda \sum_{r=1}^n w_r$$

Case 1: Does patient have cancer?

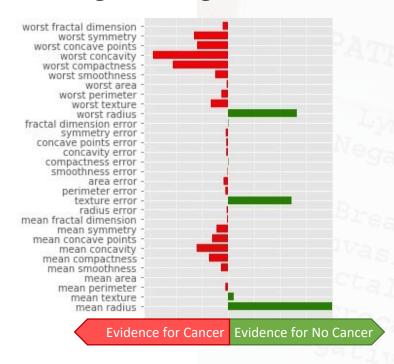
Why do the two set of weights differ?

Instance x

Feature	Value	
worst area	1315.00	
mean radius	16.13	
worst radius	20.96	
агеа еггог	54.18	
worst perimeter	136.80	
worst texture	31.48	
mean perimeter	108.10	
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mean area	798.80	
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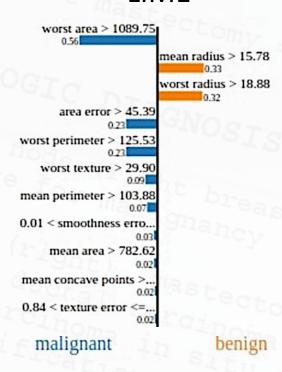
Prediction $\hat{y} = Cancer$

Logistic Regression



Weights **w** of surrogate explanation **f**

LIME



Weights w of surrogate explanation g

Further reading: https://coderzcolumn.com/tutorials/machine-learning/how-to-use-lime-to-understand-sklearn-models-predictions





<u>Gradient-weighted Class Activation Mapping</u>

Grad-CAM



Explaining Image Predictions

- LIME to explain image prediction?
- What are the input features?
 - Feature = Pixels?
 - Too many features
 - Need "super pixels"

- Another way: Attribution → Saliency Map
 - Feature = Activation Map
 - Grad-CAM



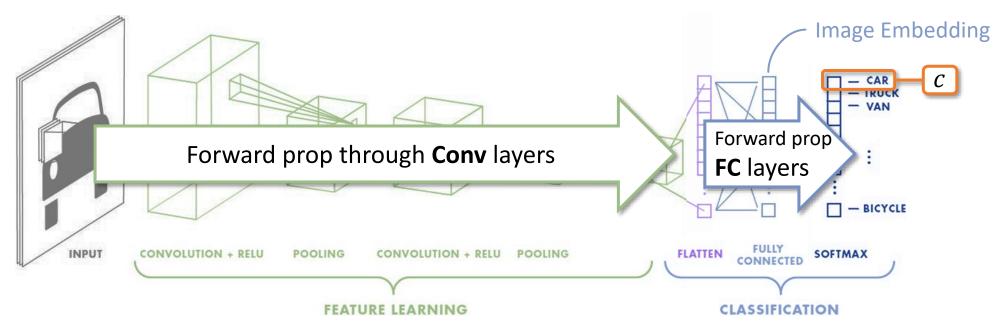
LIME



Grad CAM



Convolutional Neural Network



Key concepts

1 Learn Spatial Feature

- Series of multiple convolution + pooling layers
- Progressively learn more diverse and higher-level features

2 Flattening

Convert to fixed-length1D vector

3 Learn Nonlinear Features

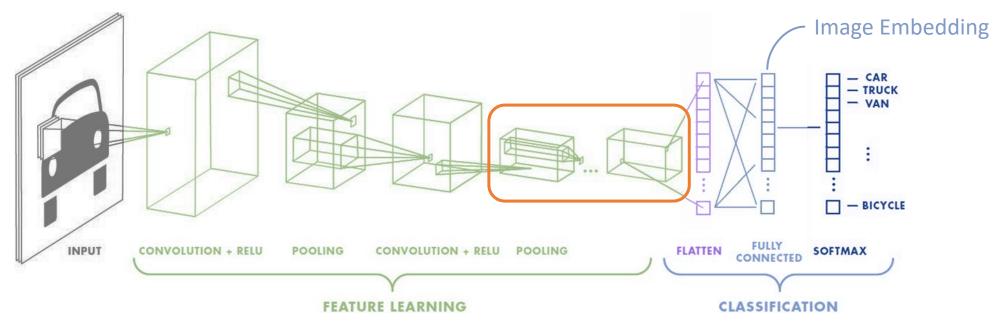
- With fully connected layers (regular neurons)
- Learns nonlinear relations with multiple layers

4 Classification

- Softmax := Multiclass
 Logistic Regression
- Feature input = image embedding vector (typically large vector)

Image credit: https://towardsdatascience.com/a-comprehensive-guide-to-convolutional-neural-networks-the-eli5-way-3bd2b1164a53

Convolutional Neural Network



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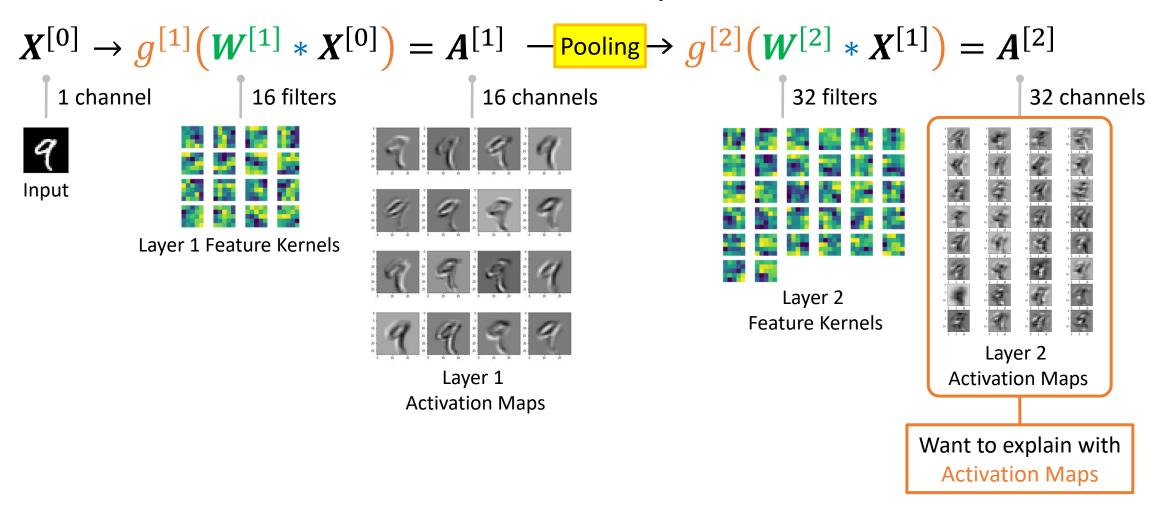
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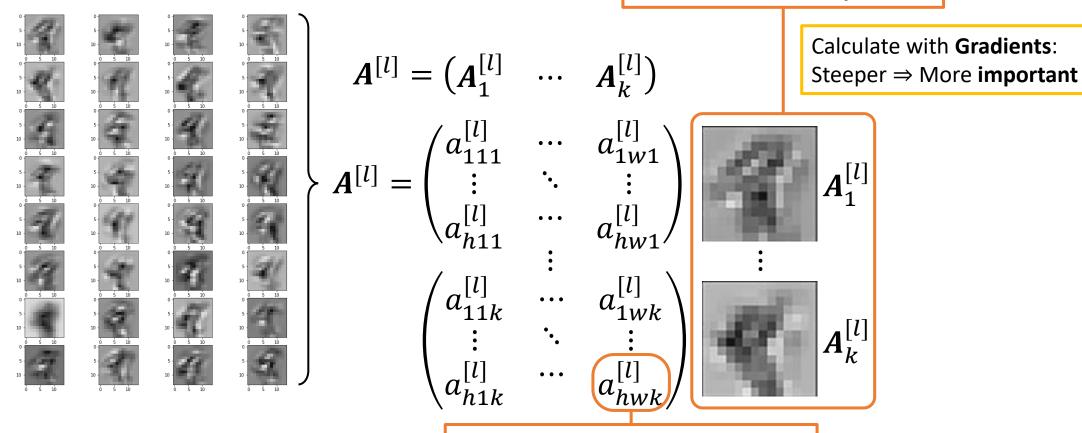
Image credit: https://towardsdatascience.com/a-comprehensive-guide-to-convolutional-neural-networks-the-eli5-way-3bd2b1164a53

Convolutional Layer: Feature Kernels & Feature Maps



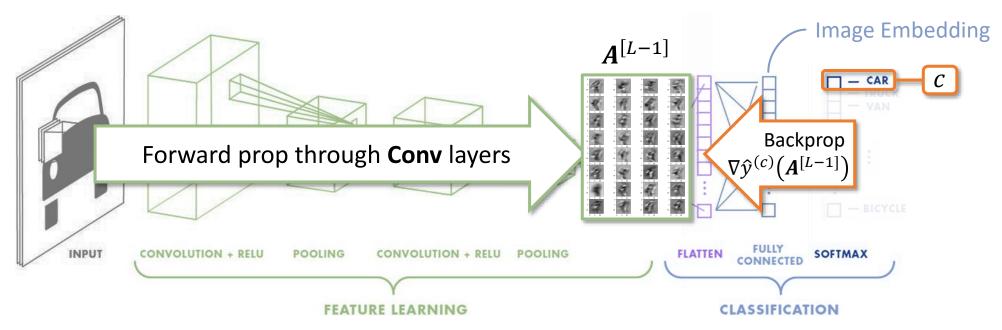
Multi-Channel Activation Maps (layers diagram)

We know the Activation Maps, But which is more **important**?



Activation of kth channel at pixel position (h, w) in layer l

Convolutional Neural Network



Key concepts

1 Learn Spatial Feature

- Series of multiple convolution + pooling layers
- Progressively learn more diverse and higher-level features

2 Flattening

Convert to fixed-length1D vector

3 Learn Nonlinear Features

- With fully connected layers (regular neurons)
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- Softmax := Multiclass
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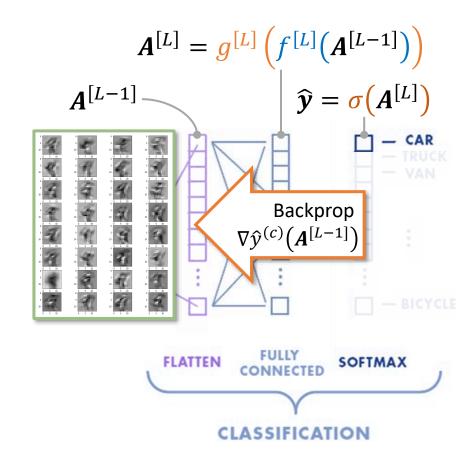
Grad-CAM

Gradient-Weighted Class Activation Maps

$$\frac{\partial \hat{y}^{(c)}}{\partial a_{hwk}^{[L]}} = \frac{\partial f^{[L]}}{\partial a_{hwk}^{[L]}} \frac{\partial g^{[L]}}{\partial f^{[L]}} \frac{\partial \hat{y}^{(c)}}{\partial g^{[L]}}$$

$$\frac{\partial \hat{y}^{(c)}}{\partial \boldsymbol{A}_{k}^{[L]}} = \begin{pmatrix} \partial \hat{y}^{(c)} / \partial a_{11k}^{[L]} & \cdots & \partial \hat{y}^{(c)} / \partial a_{1wk}^{[L]} \\ \vdots & \ddots & \vdots \\ \partial \hat{y}^{(c)} / \partial a_{h1k}^{[L]} & \cdots & \partial \hat{y}^{(c)} / \partial a_{hwk}^{[L]} \end{pmatrix}$$

$$\left\| \frac{\partial \hat{y}^{(c)}}{\partial A_k^{[L]}} \right\|_{1,1} = \sum_{ij} \frac{\partial \hat{y}^{(c)}}{\partial a_{ijk}^{[L]}} = \frac{\partial \hat{y}^{(c)}}{\partial a_{11k}^{[L]}} + \dots + \frac{\partial \hat{y}^{(c)}}{\partial a_{hwk}^{[L]}}$$



 $\{h^{[L]} \times w^{[L]}\}$

$$g(\hat{y}^{(c)}) = \text{ReLU}\left(\sum_{k} \alpha_k^{(c)} A_k^{[L-1]}\right)$$

$$\alpha_k^{(c)} = \left\| \frac{\partial \hat{y}^{(c)}}{\partial A_k^{[L-1]}} \right\|_{1,1}, A_k^{[L]} = \begin{pmatrix} a_{11k}^{[L-1]} & \cdots & \\ \vdots & \ddots & \vdots \\ & \cdots & a_{hwk}^{[L-1]} \end{pmatrix}$$

Weighted Sum

Importance Weight

Activation Map of *k*th filter in the *L*th layer

of kth filter for cth class Keep positive activations only

Selvaraju, R. R., et al. (2017). Grad-cam: Visual explanations from deep networks via gradient-based localization. ICCV'17.

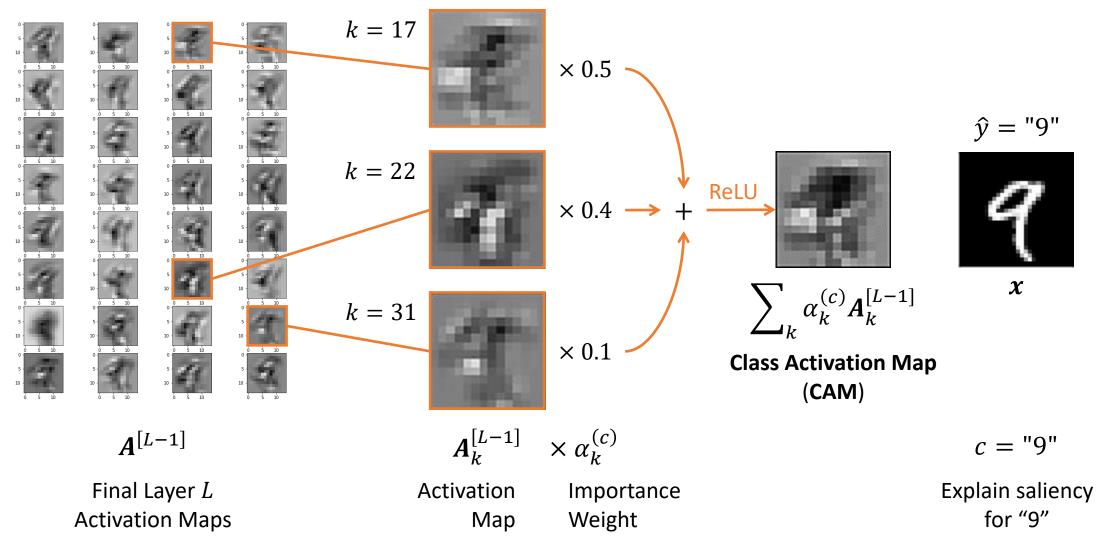
Grad-CAM Steps

- 1. Compute Activation Maps $A^{[L]}$ of last conv layer L
 - 1. via Forward Propagation
- 2. Choose class label c to explain about (e.g., predict "9", "car")
- 3. Filter prediction \hat{y} to be about class c

1. Given:
$$\hat{\boldsymbol{y}} = \begin{pmatrix} \hat{y}^{(1)} \\ \hat{y}^{(2)} \\ \hat{y}^{(c)} \end{pmatrix}$$
, $\boldsymbol{e}^{(c)} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$, then $\hat{\boldsymbol{y}}^{(c)} = \hat{\boldsymbol{y}} \circ \boldsymbol{e}^{(c)} = \begin{pmatrix} 0 \\ 0 \\ y^c \\ 0 \end{pmatrix}$

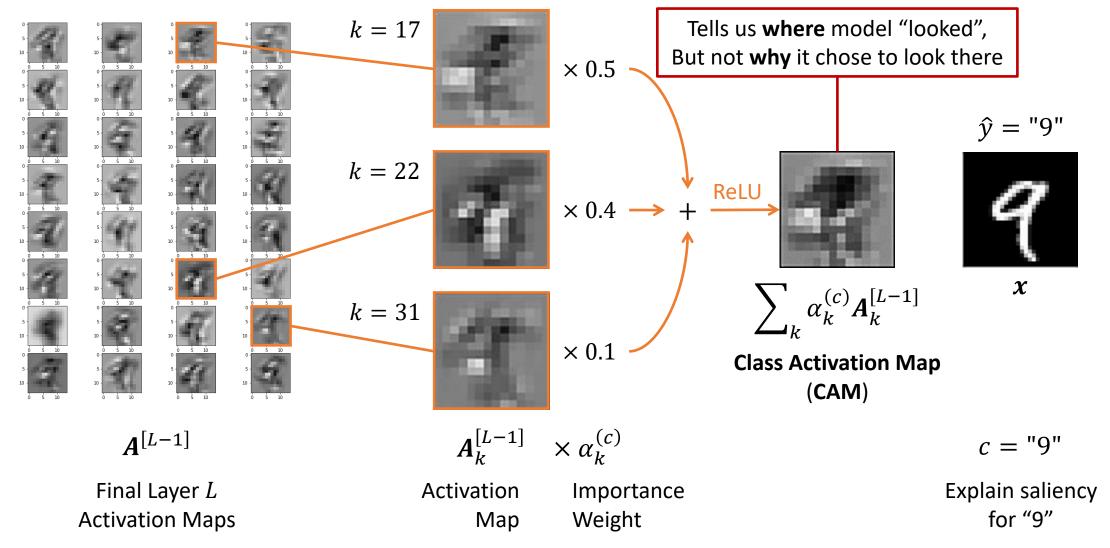
- 2. To generate explanation only for that class c
- 4. Compute importance weight $\alpha_k^{(c)}$ for each Activation Map $A_k^{[L]}$
 - 1. Backprop from $\widehat{\boldsymbol{y}}^{(c)}$ to get gradients at last conv layer
 - Note that gradient is relative to activations, not weights
- 5. Compute weighted sum with ReLU to get Class Activation Map

Grad-CAM example: Why did the CNN predict "9"?





Grad-CAM example: Why did the CNN predict "9"?



W10 Pre-Lecture Task (due before next Mon)

Watch

Who Invented A.I.? - The Pioneers of Our Future by ColdFusion

Play

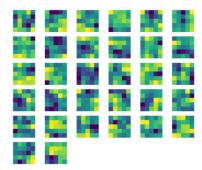
- https://distill.pub/2018/building-blocks/
 - Don't worry about reading the whole article

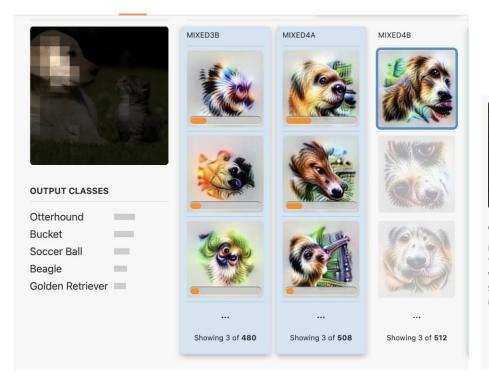
Discuss

- 1. <u>Identify</u> what is strange, funny, or erroneous in the deep learning model in Building-Blocks
- 2. Take a screenshot of the issue and share with your tutorial mates
- 3. Try to explain why the model was behaving as identified
- 3. Post a 2-3 sentence description to the topic in your tutorial group: #tg-xx

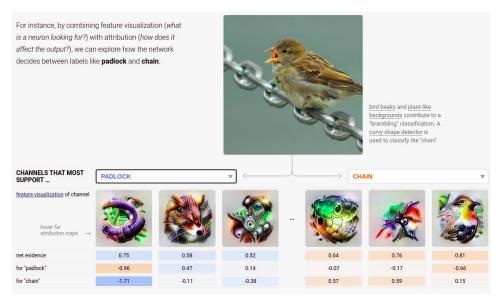
Understanding Filters

Hard to interpret kernels.
They are just matrices used for convolution.







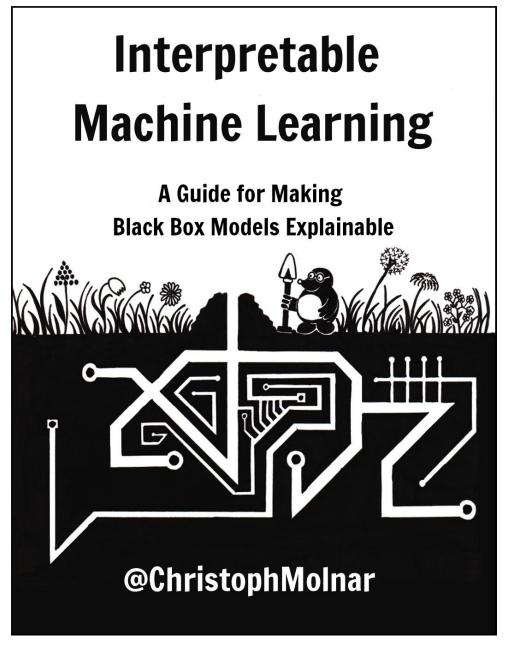


Types of Dogs Bowtie? Chain?

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Further Reading

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





Research in

Human-Centered XAI

(not in exam!)



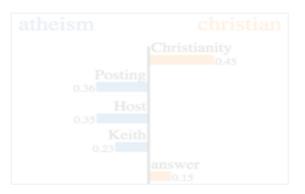






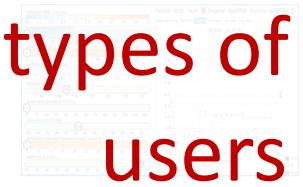
https://ubiquitous.comp.nus.edu.sg

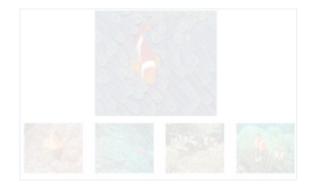








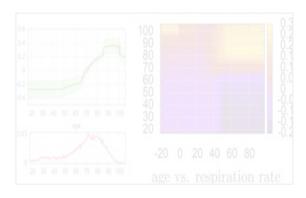






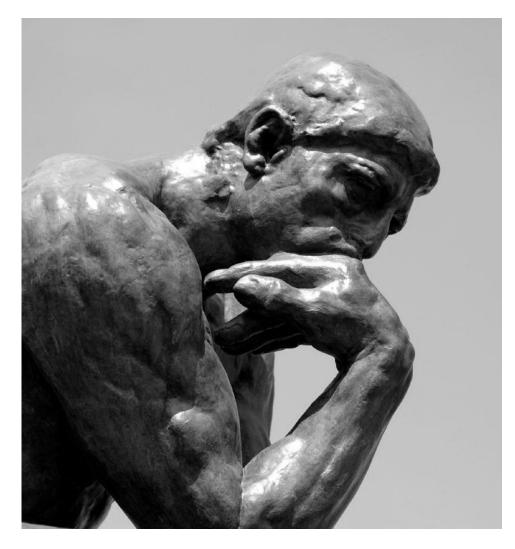








How do people think and explain?

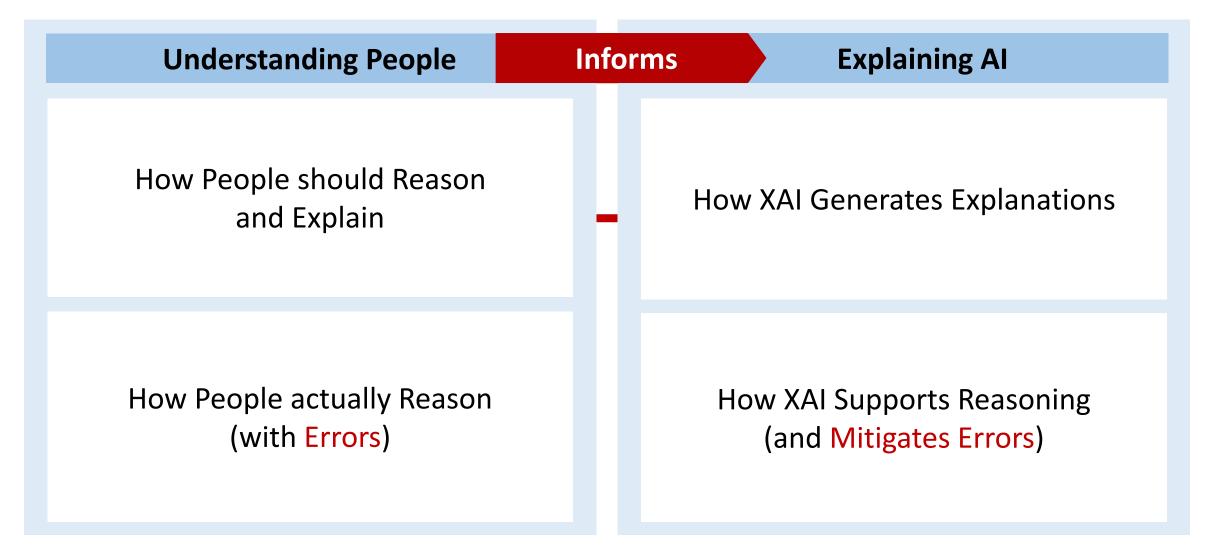


Philosophy

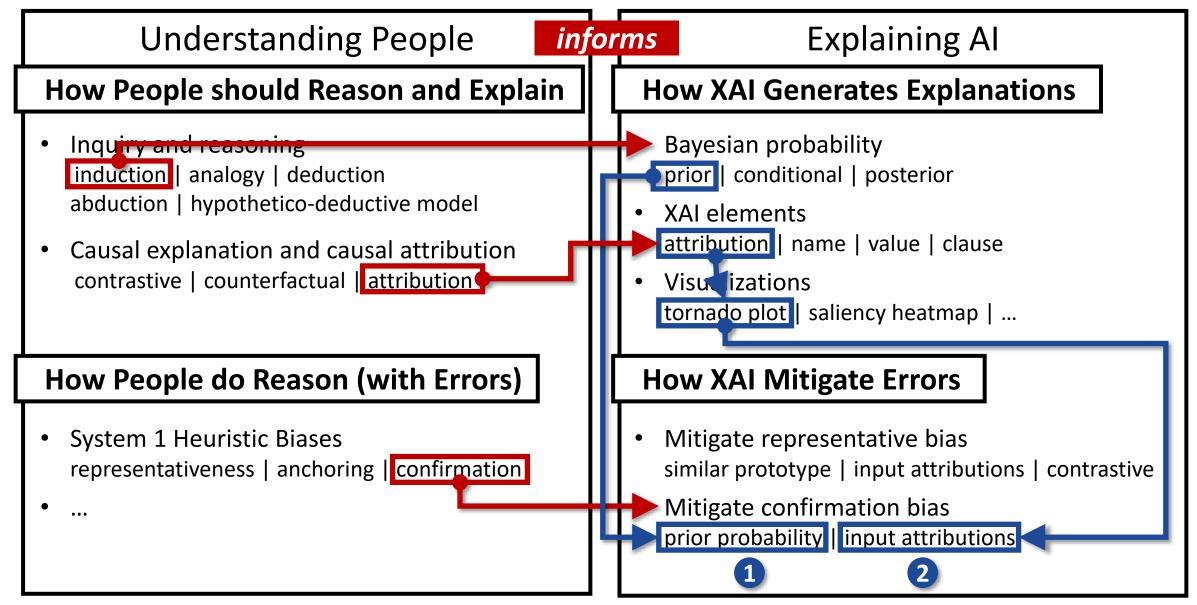


Psychology

Human reasoning theories to inform XAI applications



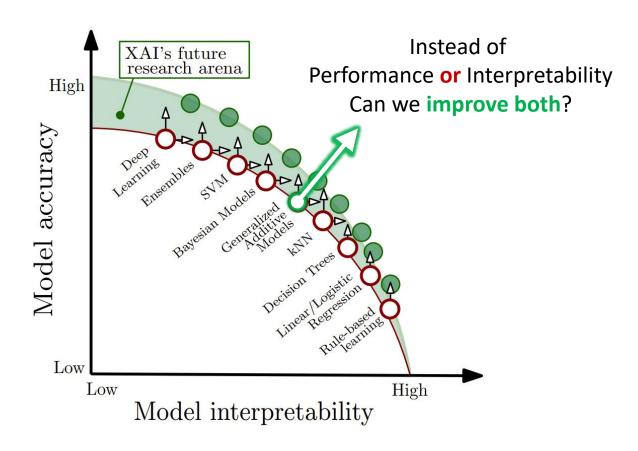
Human reasoning theories to inform XAI applications



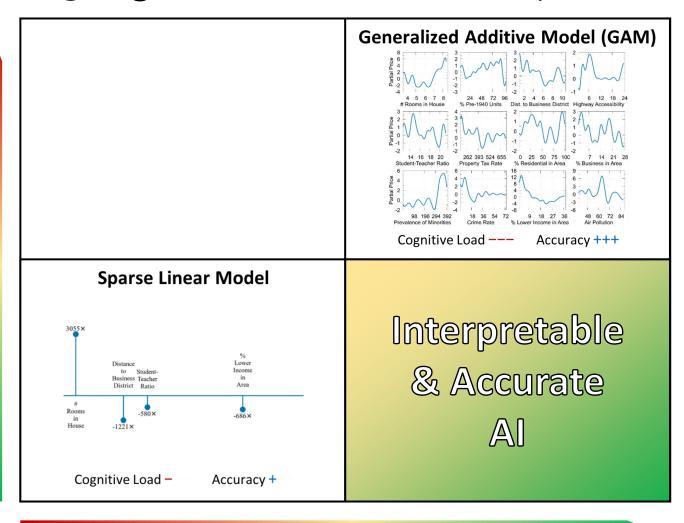
User-Centered Explanations

- Why? Attribution Explanations
- Why Not? Contrastive Explanations
- How To? Counterfactual Explanations

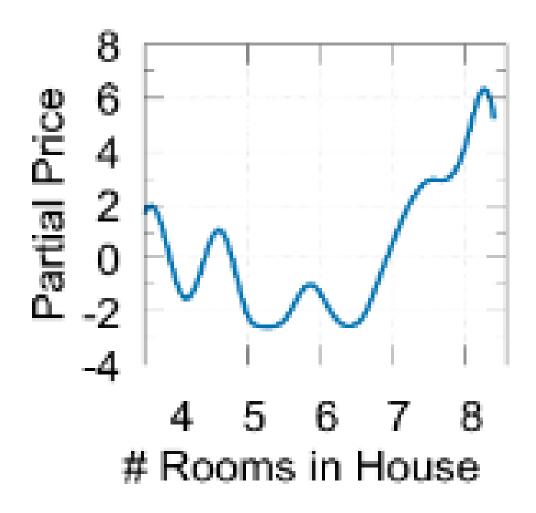
Performance-Interpretability Trade-off

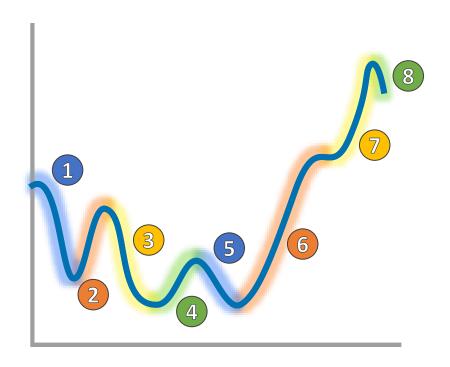


Cognitive Load (Less Interpretable)



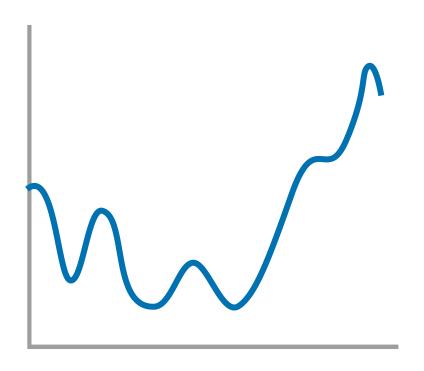






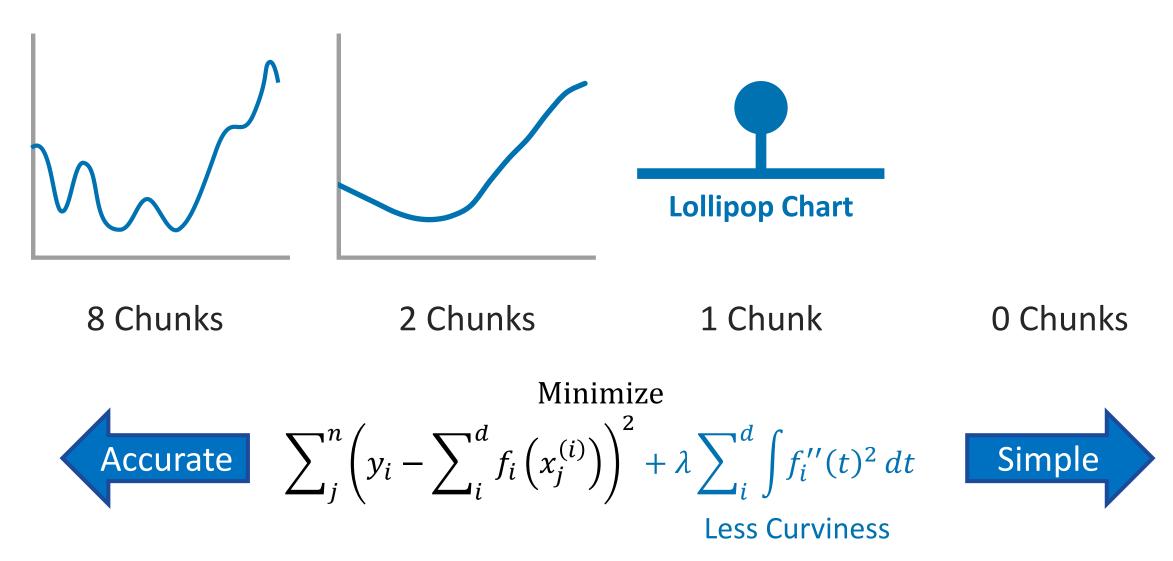
Cognitive Load = Number of Visual "Chunks"

Abdul, A., von der Weth, C., Kankanhalli, M., and Lim, B. Y. 2020.



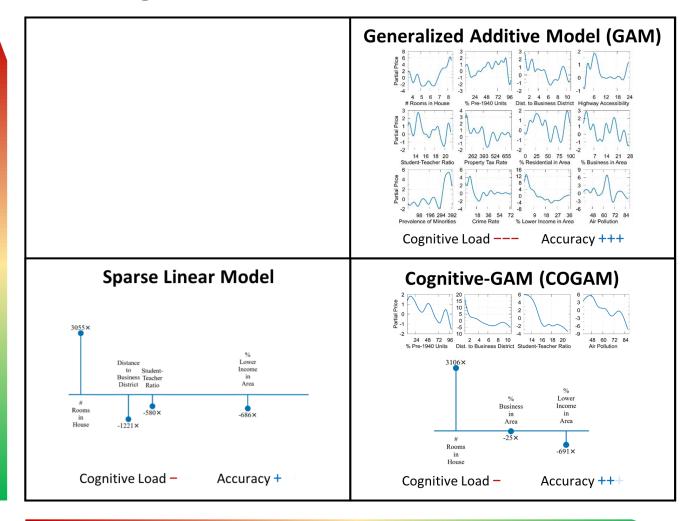
Cognitive Load = Number of Visual "Chunks"

Abdul, A., von der Weth, C., Kankanhalli, M., and Lim, B. Y. 2020.



Abdul, A., von der Weth, C., Kankanhalli, M., and Lim, B. Y. 2020.





Accuracy

Abdul, A., von der Weth, C., Kankanhalli, M., and Lim, B. Y. 2020.

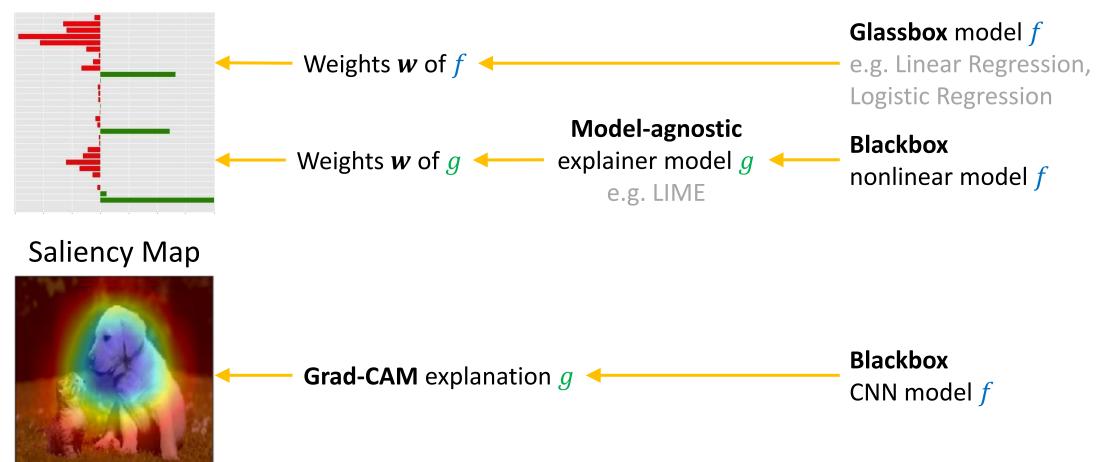


Wrapping Up



What did we learn? Feature Importance Explanations

Feature Attribution





W12 Pre-Lecture Task (due before next Mon)

Read

1. <u>Clustering With More Than Two Features? Try This To Explain Your Findings</u> by Mauricio Letelier

Task

- 1. <u>Describe</u> other use cases where you need to **apply domain knowledge** with data-driven **unsupervised learning** to better understand your business or engineering problem
 - Tip: you can your own projects too; you don't have to be correct
- 2. Post a 1–2 sentence answer to the topic in your tutorial group: #tg-xx