Interpretable and Explainable ML

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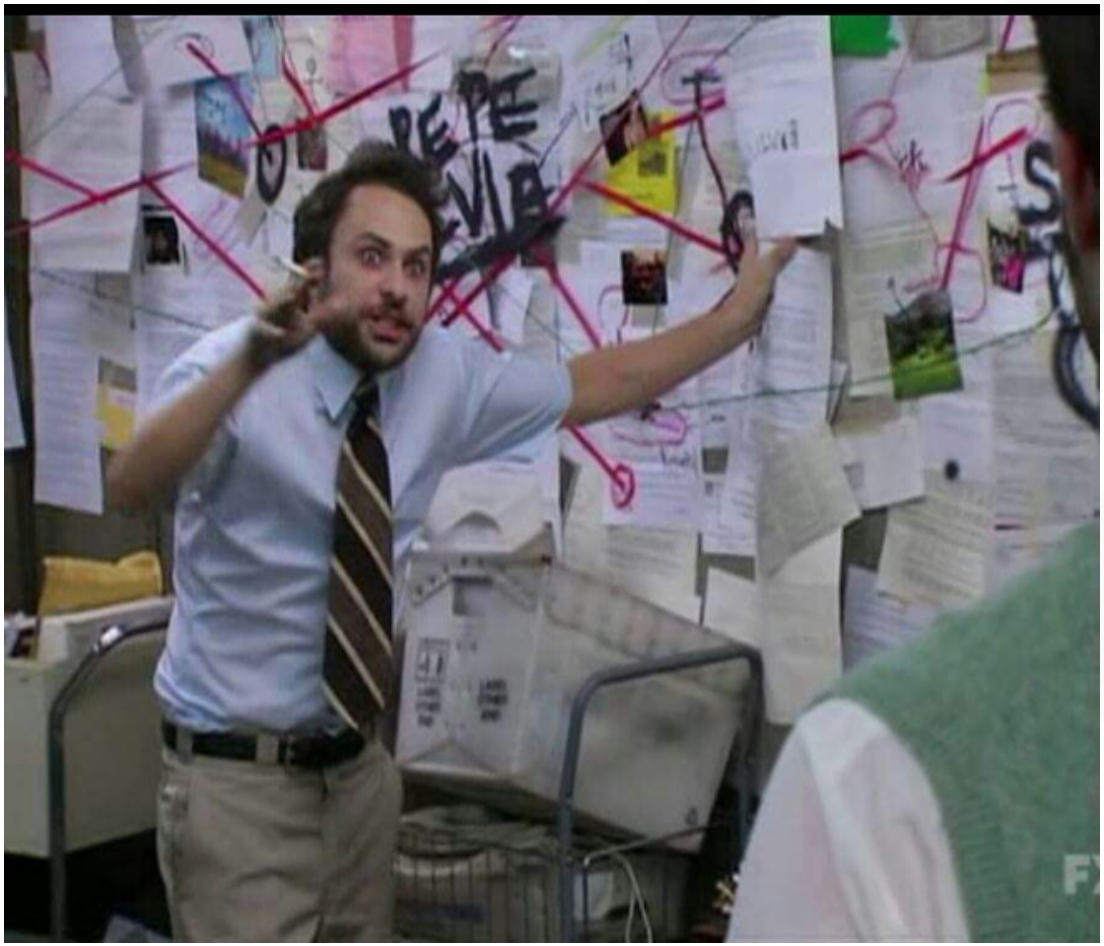
Motivation

- Suppose you spend hours on training your model.
- You are satisfied with your evaluation metric.
- Are you done?

Motivation

The goal of this workshop is to try to answer the following question:

Why does my model predict what it predicts?



Overview

1. Introduction to Explainable ML
2. Model Specific Explanations
3. Model Agnostic

Section 1

1 Introduction to Explainable ML

2 Model Specific Explanations

3 Model Agnostic

Material

The data and code is available

- Materials
- Interpretable Example, Google Colab
- Model Specific, Google Colab

Motivation

- One of the main problems in deploying Machine Learning algorithms is users trust to a prediction and a model.
- Both are highly affected based on the depth of human understanding of a model's behaviour, as opposed to perceiving it as a black box.
- Despite its widespread use, they treated and remain mostly as black boxes that do not explain their predictions in a way that practitioners can understand.

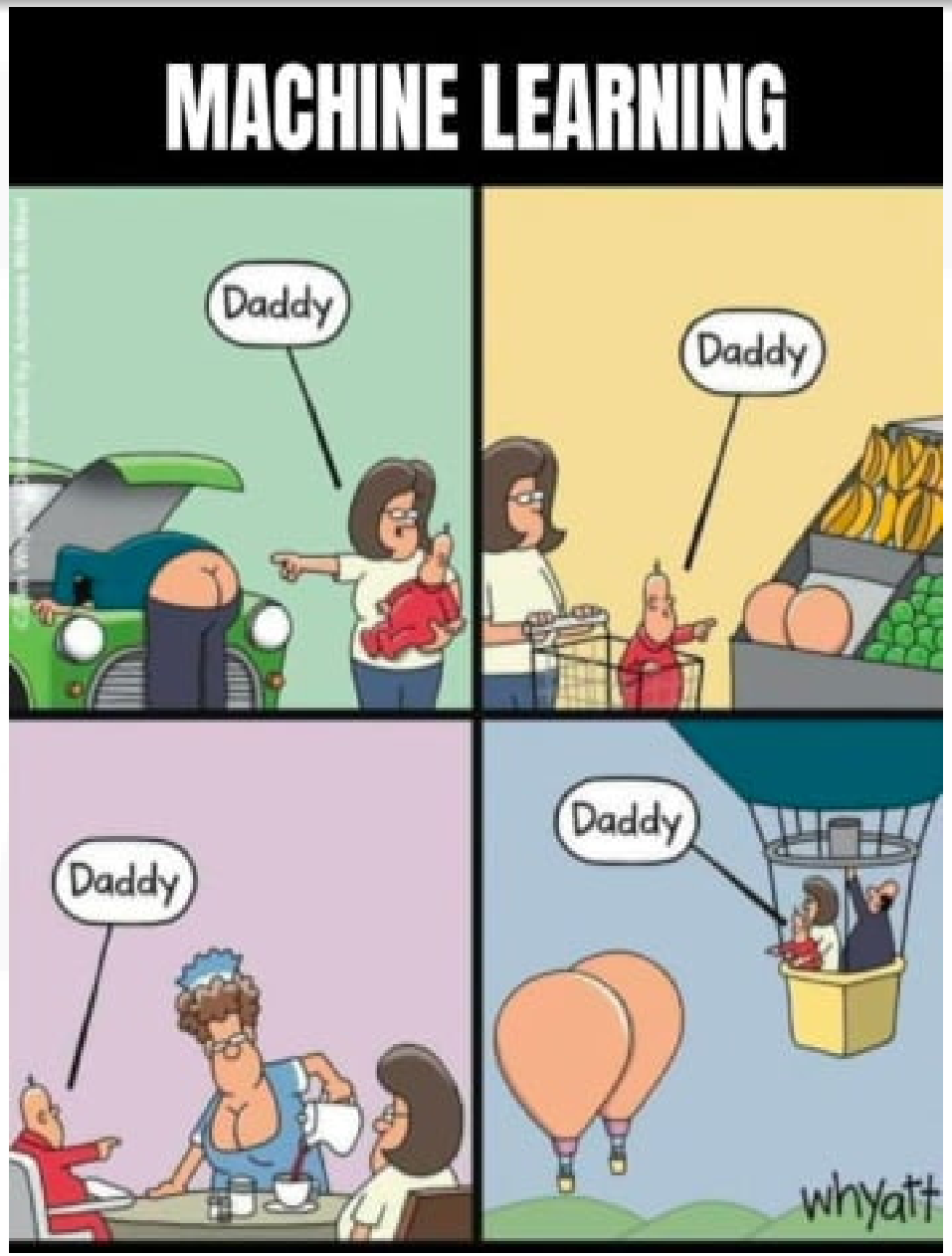
Motivation

1. Currently, most of the models are evaluated using performance metrics on a validation set.
2. However, such metric may not be indicative since the real-world data is often different.
3. **The blind faith to the model** predictions can create discrimination and trust issues.

Why it is important

- COMPAS is a proprietary model that is used in the U.S. Justice system for parole and bail decision.
- Recently it was accused on being racially biased, i.e., "This person is predicted to be arrested because they are black".
- Bank: model to predict who should get a loan or not.
- Computer Vision: Image Classification

What Can Go wrong?



Misuse Example

Models are opinions embedded in mathematics.

- Suppose you are hired at a big tech company to predict employees' performance.
- Available data shows the past performance reviews of individual employees for the past 10 years.
- What can go wrong if you apply black-box model?

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- Available data shows the past performance reviews of individual employees for the past 10 years.
- What can go wrong if you apply black-box model?
- What if that company tends to promote men more than women?
- The model will learn the bias, and predict that men are more likely to be performant.

Misuse Examples

- Suppose now you work for a company whose main job is to classify wolves vs husky.
- The available data is pictures of wolves and huskies,
- What can go wrong if you apply black-box model [7]?

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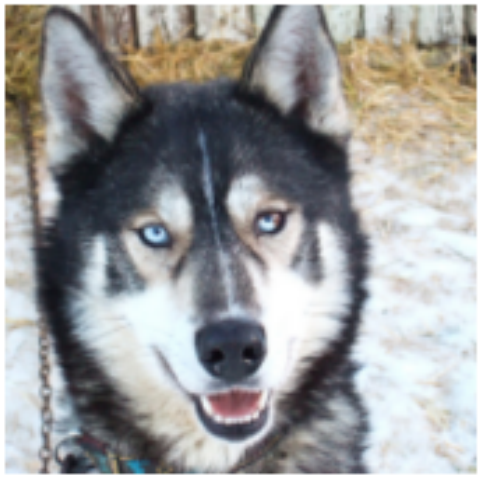

(a) Husky classified as wolf

(b) Explanation

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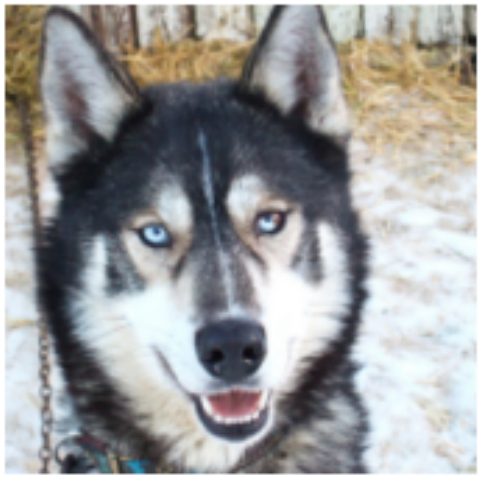


(a) Husky classified as wolf

(b) Explanation

Congratulations you just build a snow detector!!!

Misuse Example

A popular example from [2].

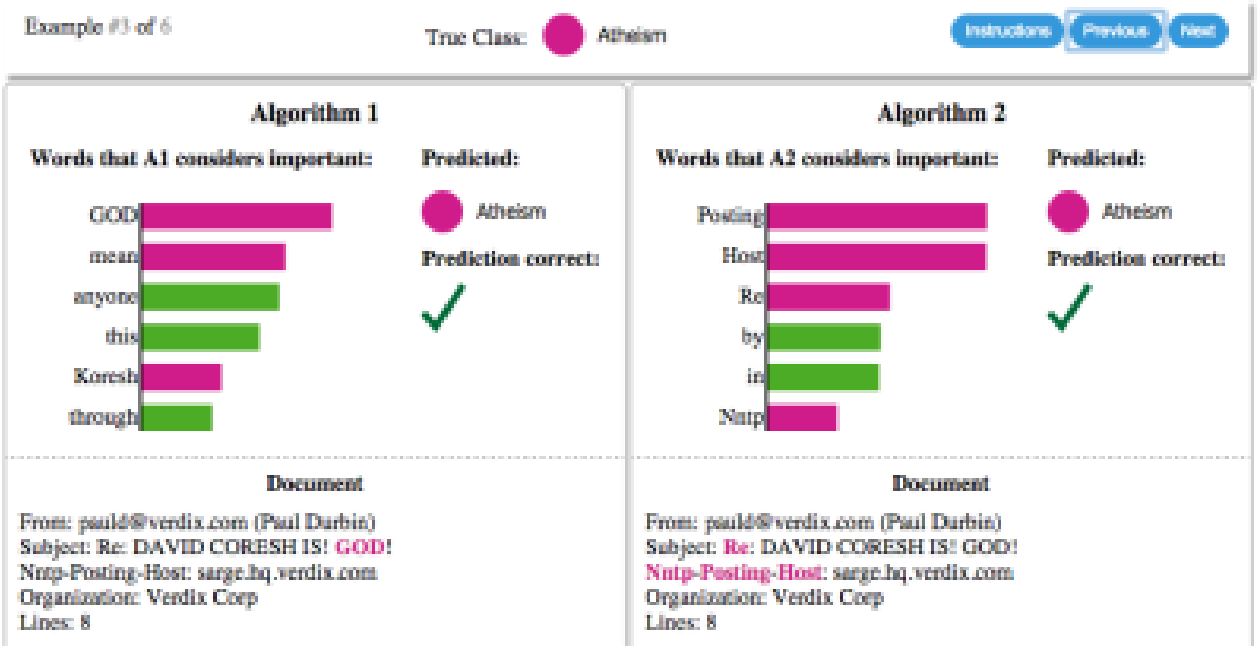
(A) **Cow: 0.99**, Pasture: 0.99, Grass: 0.99, No Person: 0.98, Mammal: 0.98

(B) No Person: 0.99, Water: 0.98, Beach: 0.97, Outdoors: 0.97, Seashore: 0.97

(C) No Person: 0.97, **Mammal: 0.96**, Water: 0.94, Beach: 0.94, Two: 0.94

Misuse Example

- Now we want to predict whether a given document is about Atheism or Christianity.
- Algorithm 1 and Algorithm 2 have prediction accuracy 89%, 95%, respectively. Which one would you choose?



Interpreting your prediction

Interpretable vs Explainable ML

- There is a significant difference between interpretable and explainable models.
- A commonly used interpretable models are linear and logistic regression, decision trees, rule based methods and their extensions.

Interpretability example

- Consider a linear regression

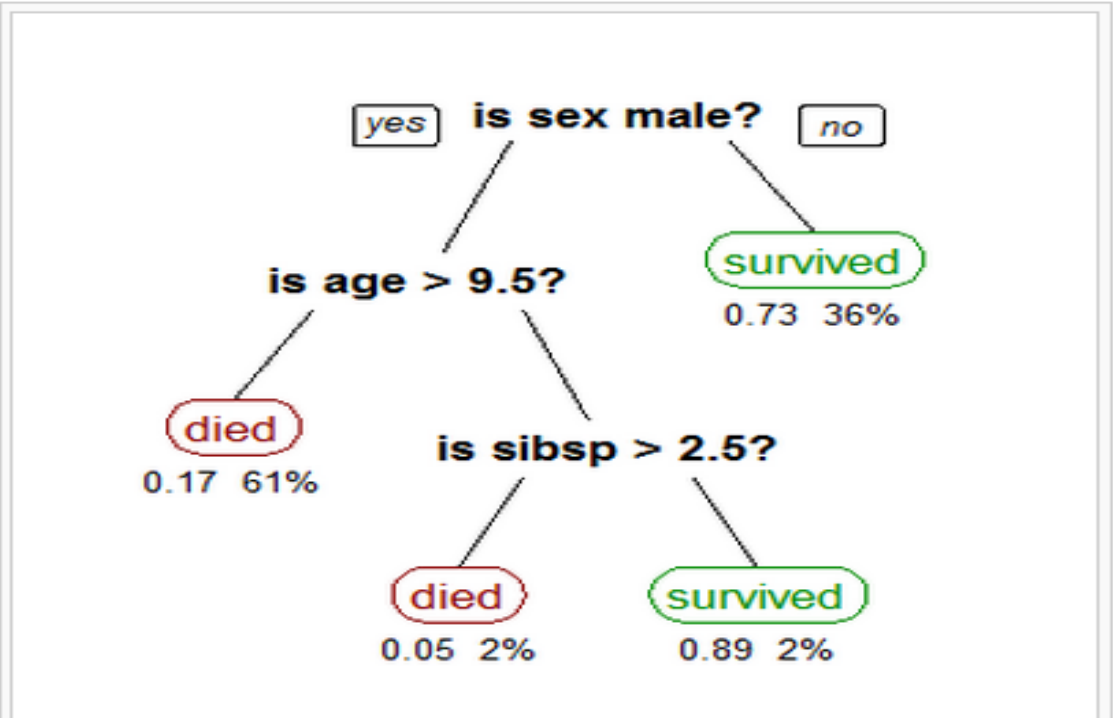
$$y = 5x - 0.6z + \epsilon$$

- or a logistic regression

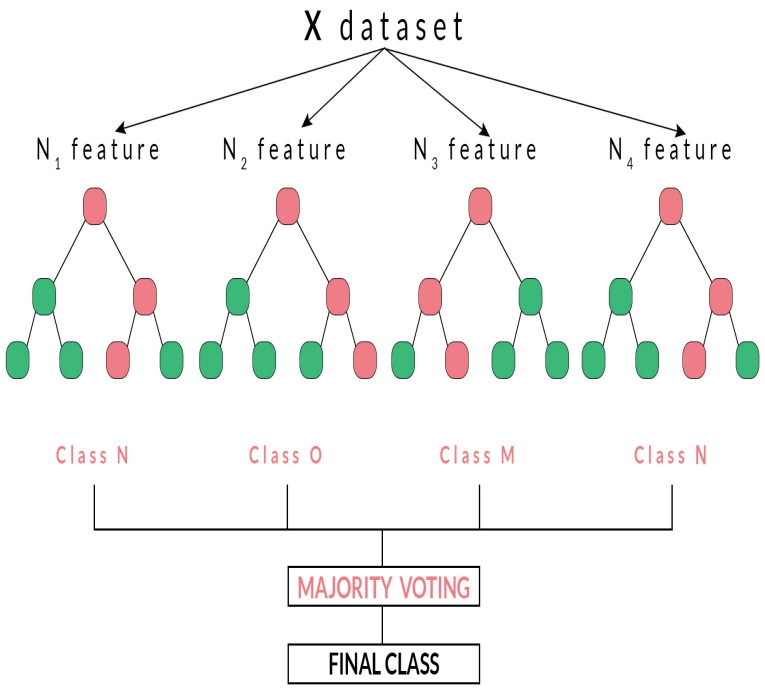
$$\log\left(\frac{P(Y=1)}{1-P(Y=1)}\right) = 6x - 0.5z + \epsilon$$

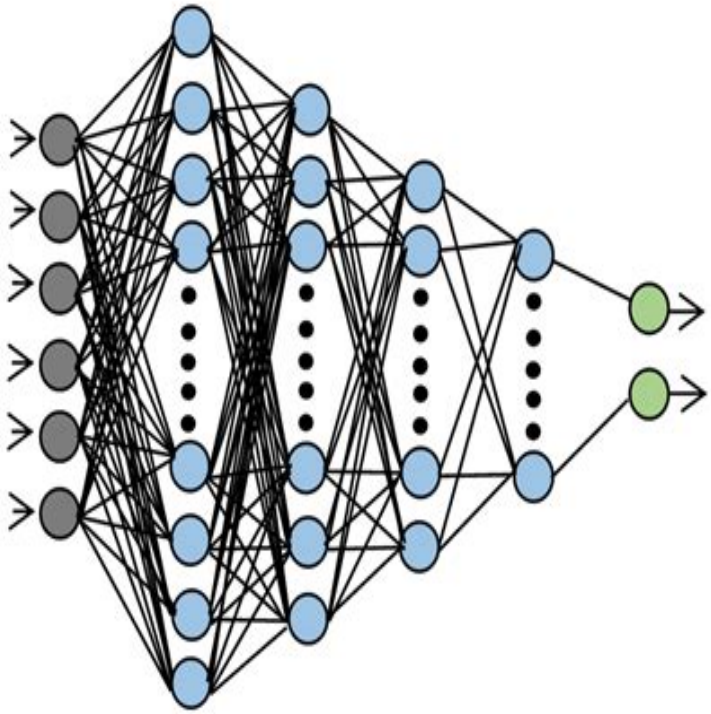
and $P(Y=1) = \frac{1}{1+e^{-(6x-0.5z)}}$

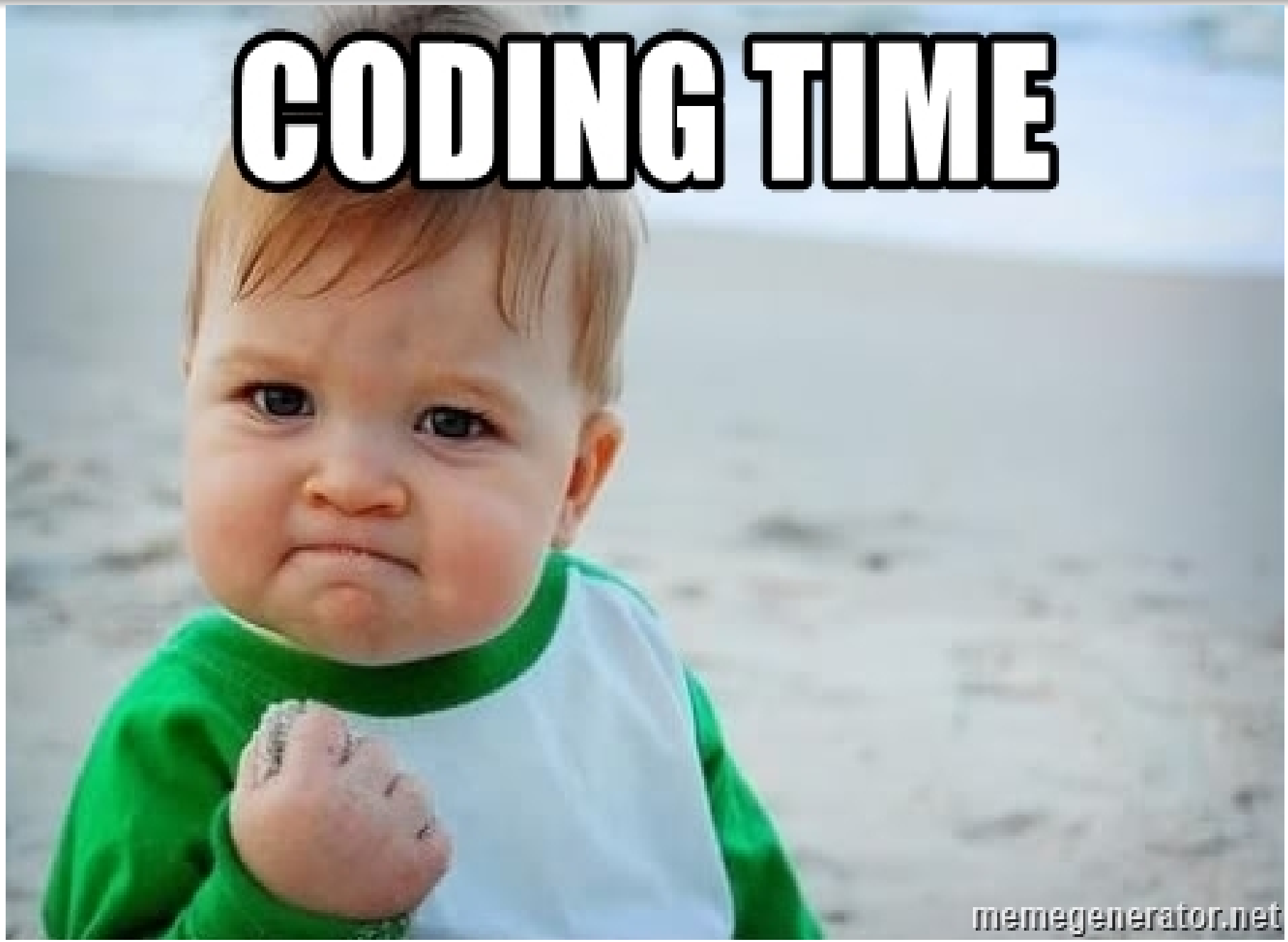
- or a decision tree



Black Box Model





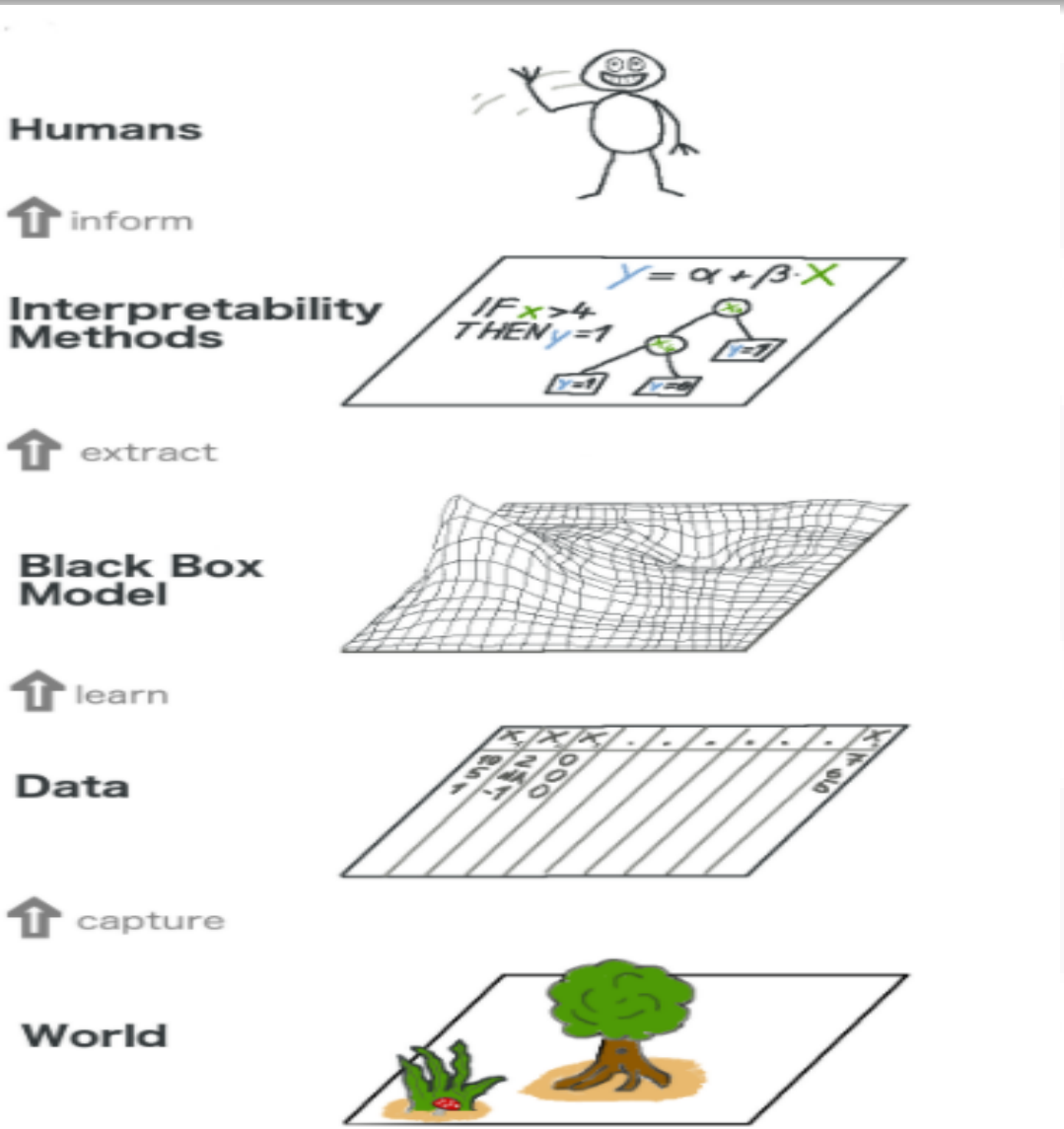


Details

Explainable ML

- In contrast to interpretable models, explainable methods do not create models that are inherently interpretable.
- But a post hoc model that explains the prediction of the original black box model.
- Do not use these methods for high stack decisions, but use as a tool for analysis and algorithmic audit.

Explainable ML



Borrowed from [6]

Explainable ML

- Rather than trying to create models that are inherently interpretable, Explainable ML creates a second(posthoc) model to explain the first black box model [9].
- Pros
  - Easy to construct
  - Model Agnostic: Treats the model as a black-box. Doesn't need to know how it makes predictions
- Cons
  - Can provide explanations that are not faithful to the original model.
  - Often do not provide enough details to understand what the black box is doing.

Explainable Models

Explainable methods are separated into

- Model Specific: Grad-CAM, guided backpropagation, DeepLIFT, etc
- Model Agnostic: LIME, SHAP, surrogate trees, etc.

Explainable ML

- Explanations are also come with two flavors:
  - **Global** describe the average behavior of a machine learning model.
    - Feature Importance,
  - **Local** methods explain individual predictions.
    - Why the loan for the customer X has been denied?

Section 2

1 Introduction to Explainable ML

2 Model Specific Explanations

3 Model Agnostic

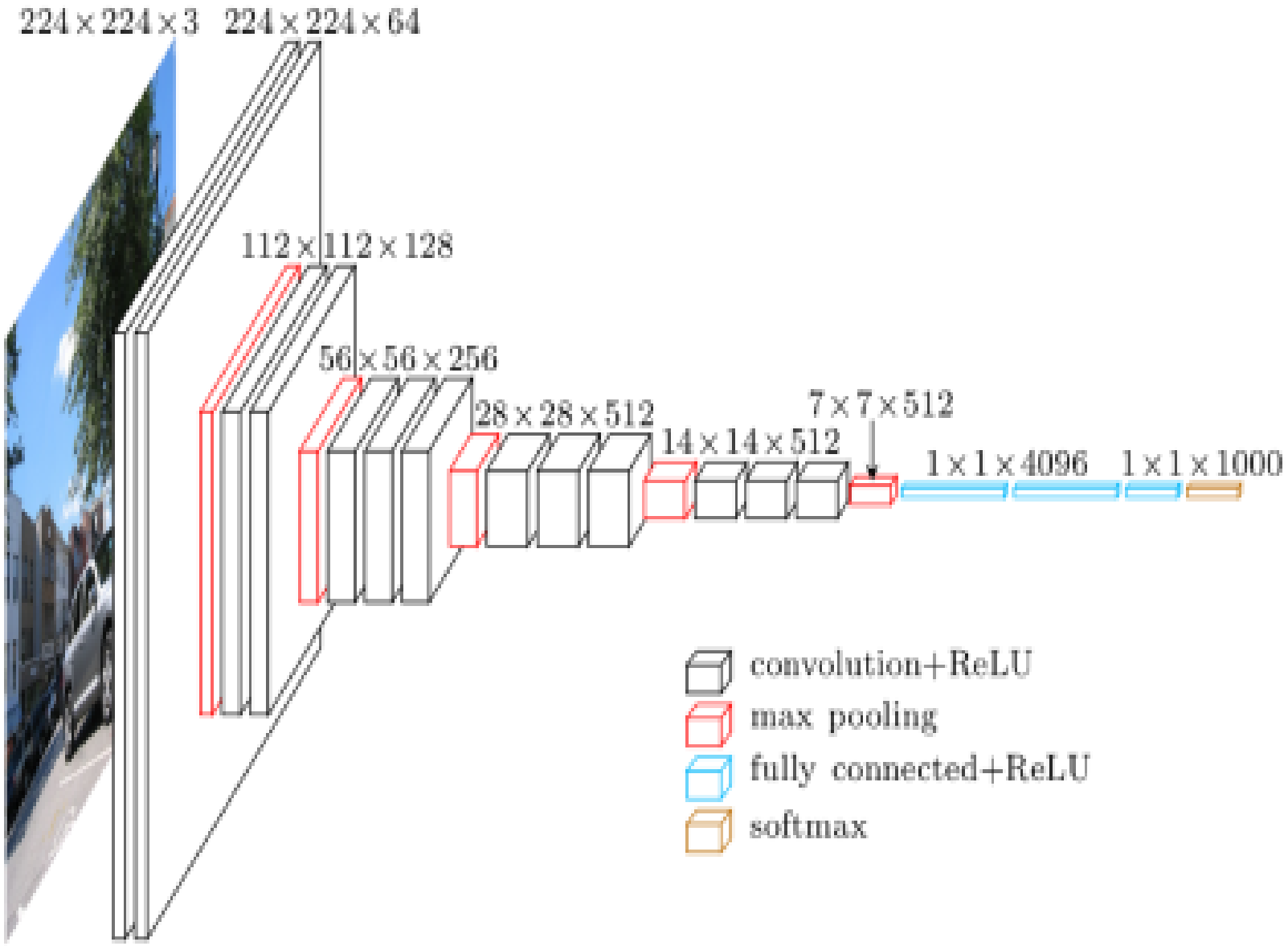
Interpreting ConvNets

- As I mentioned before, deep learning models are "black boxes": they learn representation that are difficult to extract.
- Fortunately, this is not entirely true for the ConvNets.
- Convnets are highly amenable to visualization.

Interpreting what ConvNets learn

- In this part of the workshop, our interest will be on interpreting what ConvNets learn.
- We will focus on two popular methods:
  - Grad-CAM
  - guided backpropagation

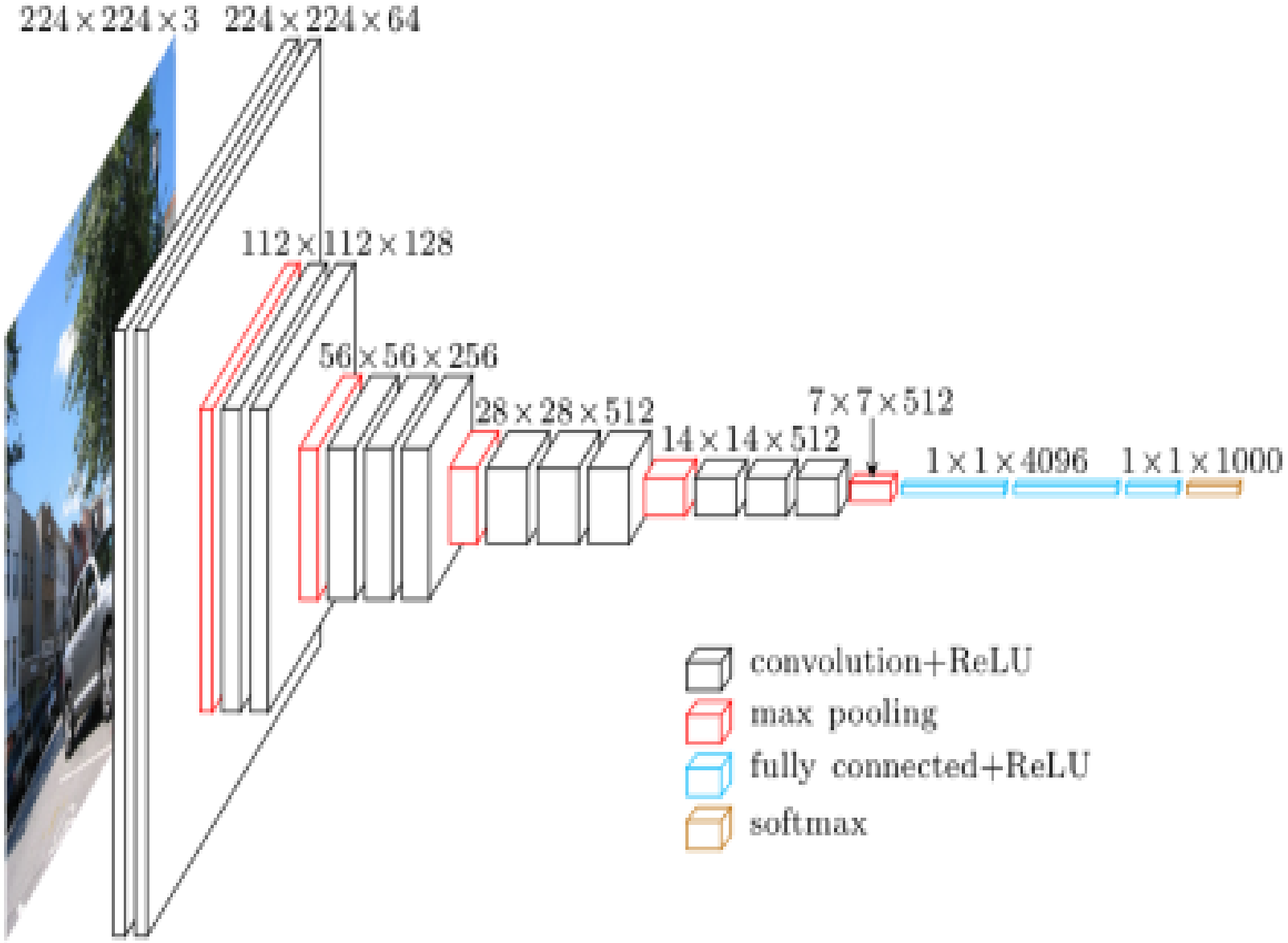
Visualizing Convolutional Networks



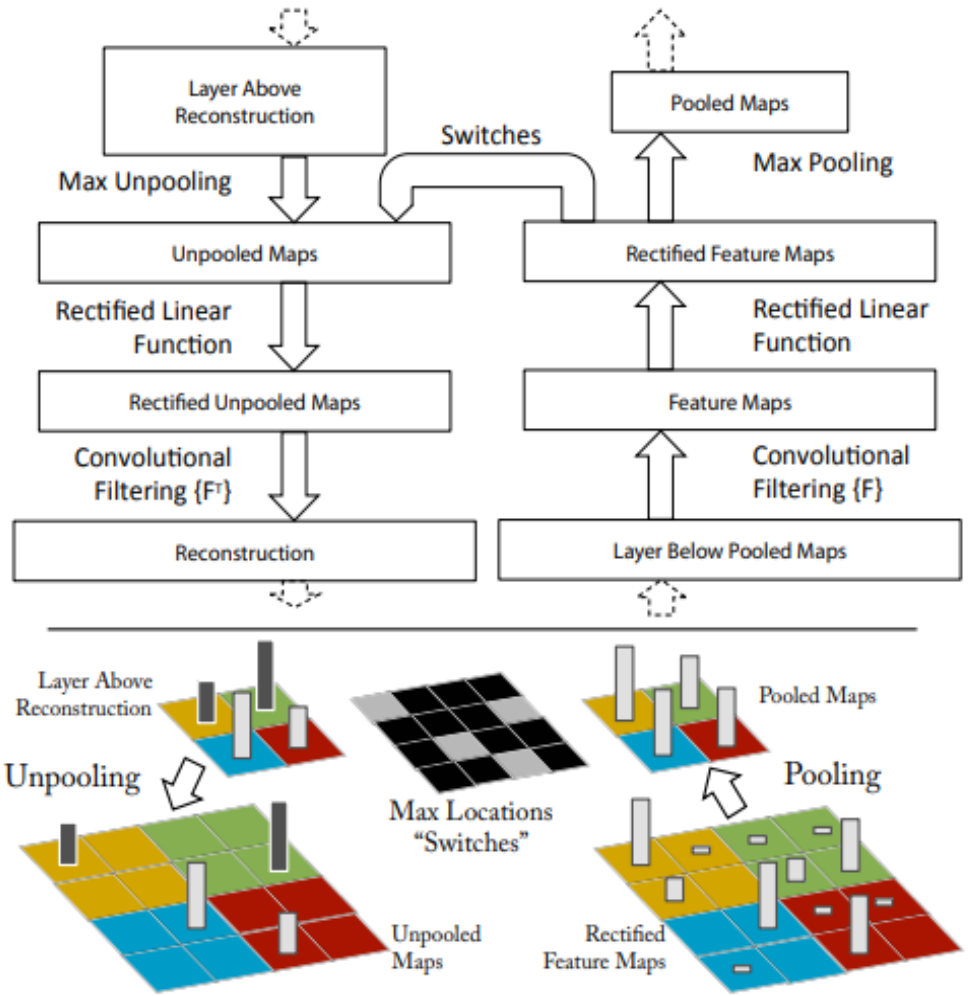
Visualizing ConvNets

- Our goal is to display the values returned by various convolution and pooling layers, given a certain output.
- This tells as how an input is decomposed into the different filters learned by network.
- We want to visualize feature maps with three dimension: width, height, and depth

Different Resolution of layers



Deconvolution



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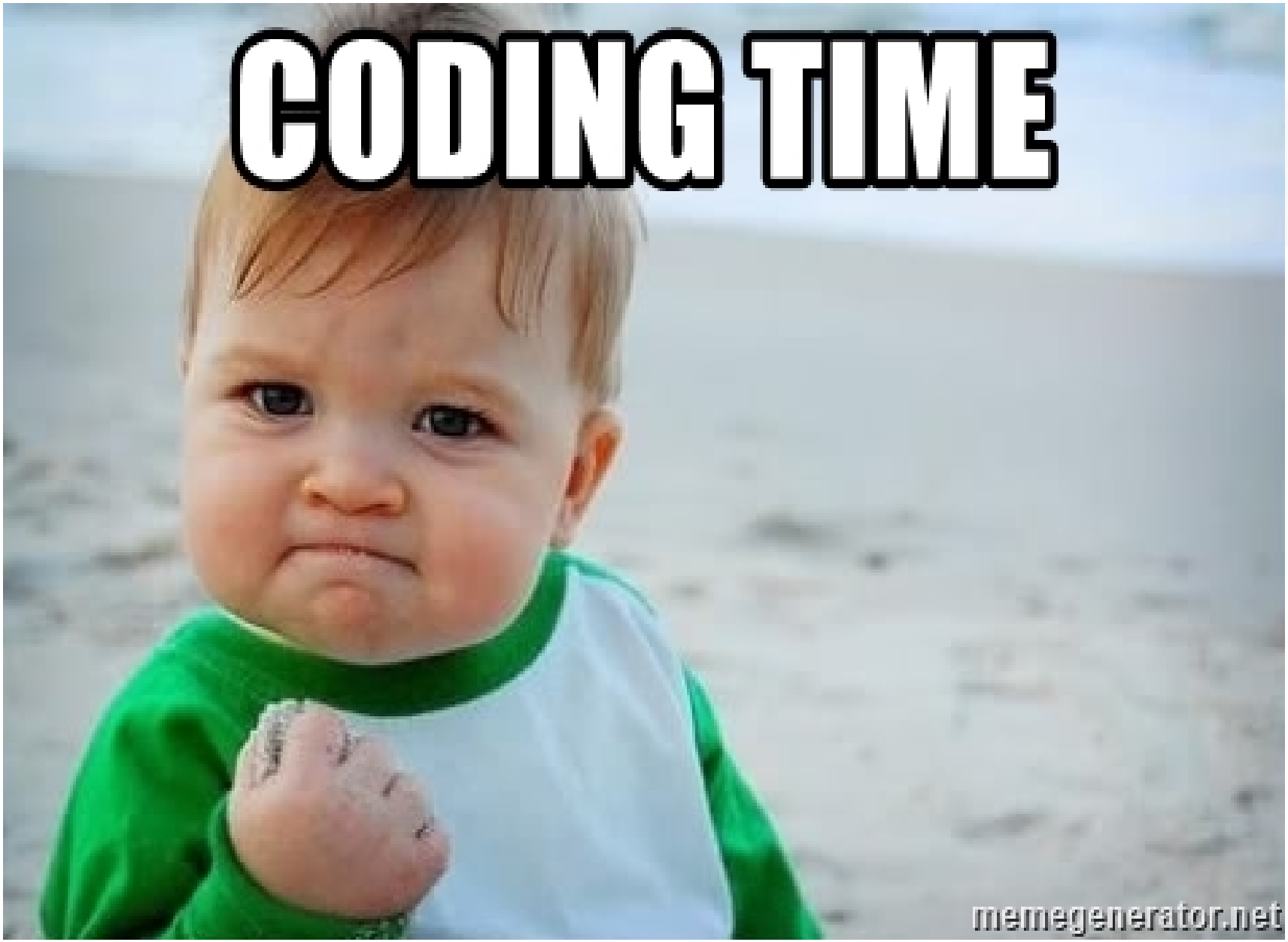
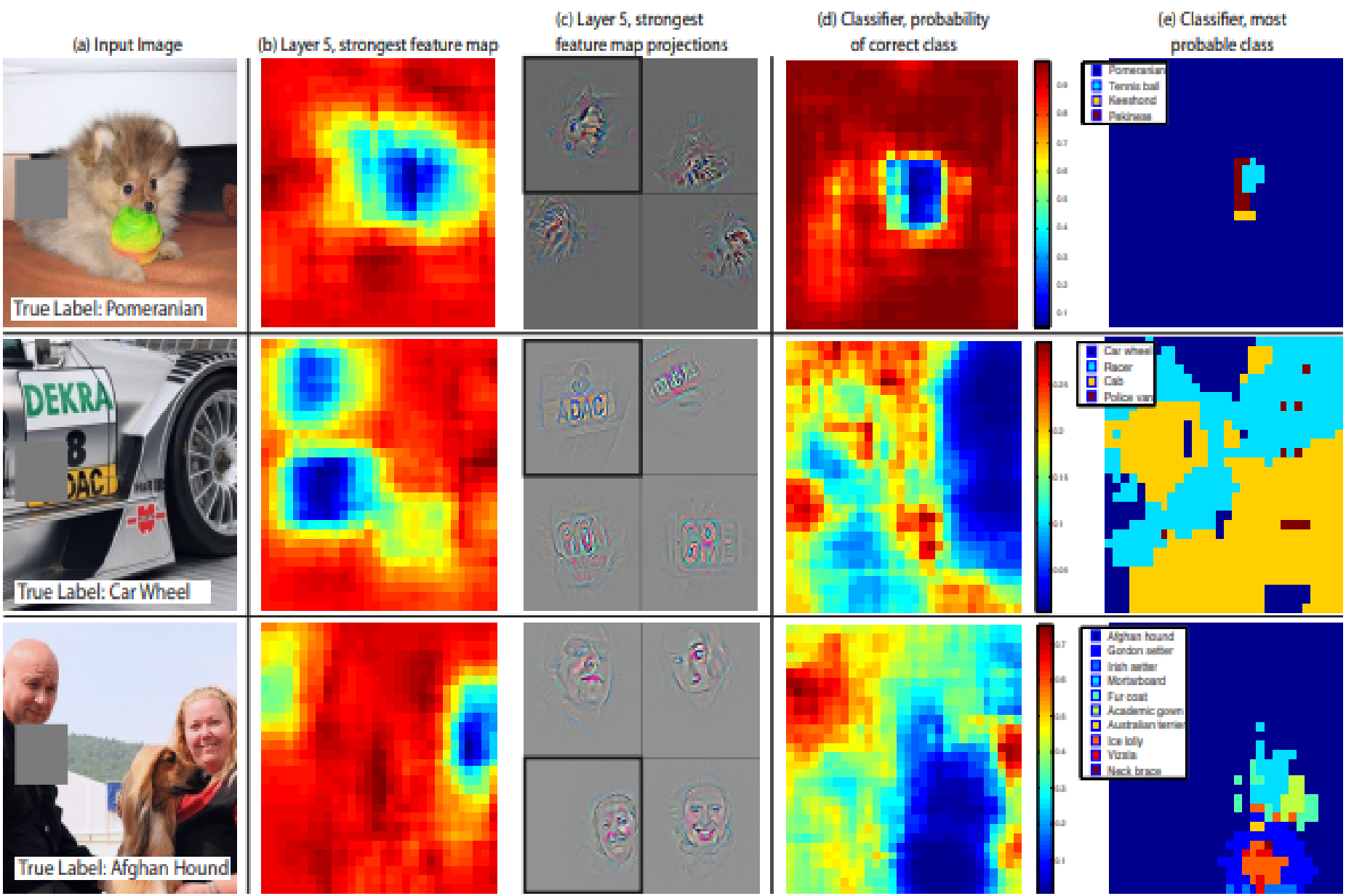
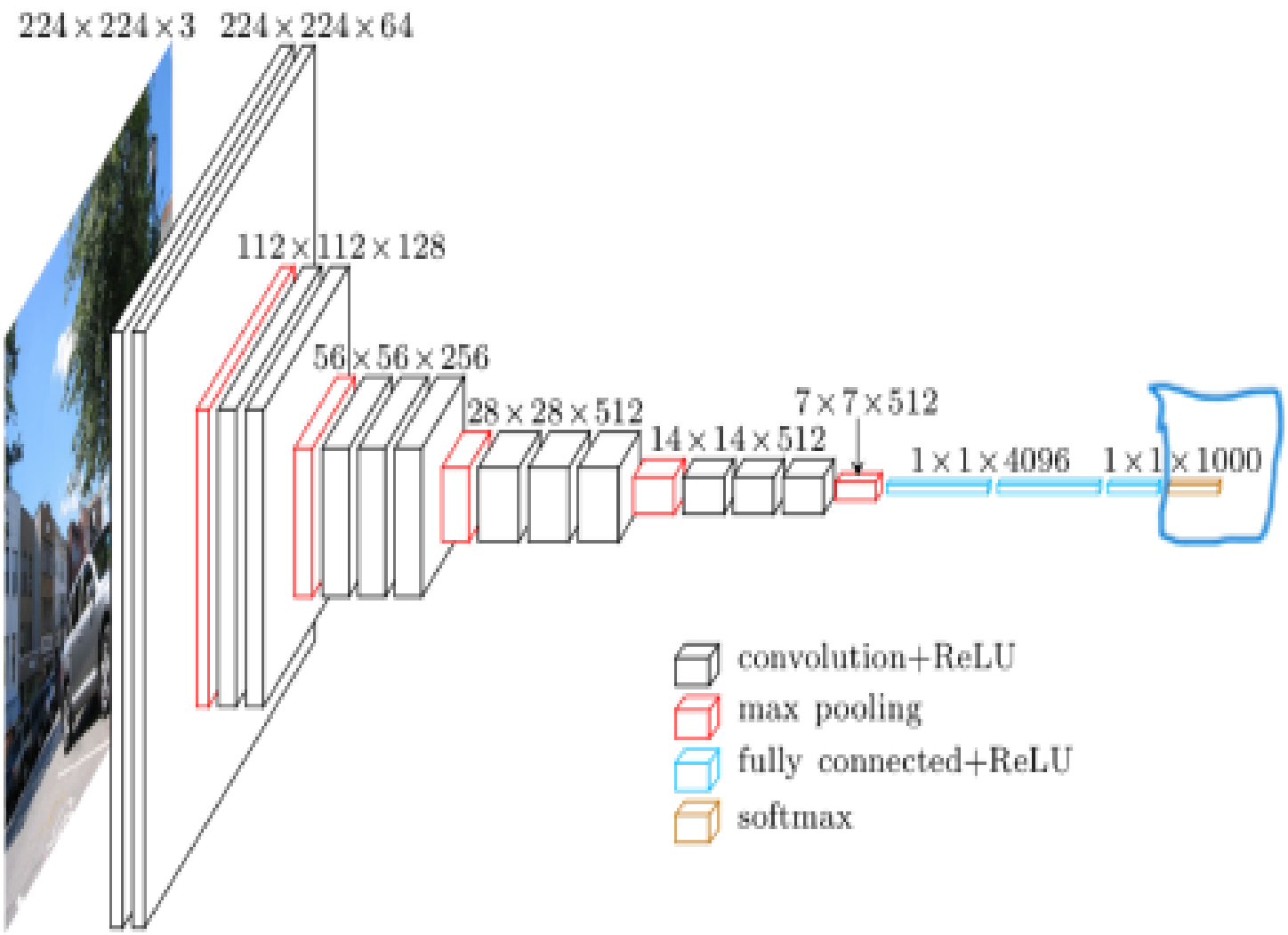


Details

A Potential Good Project



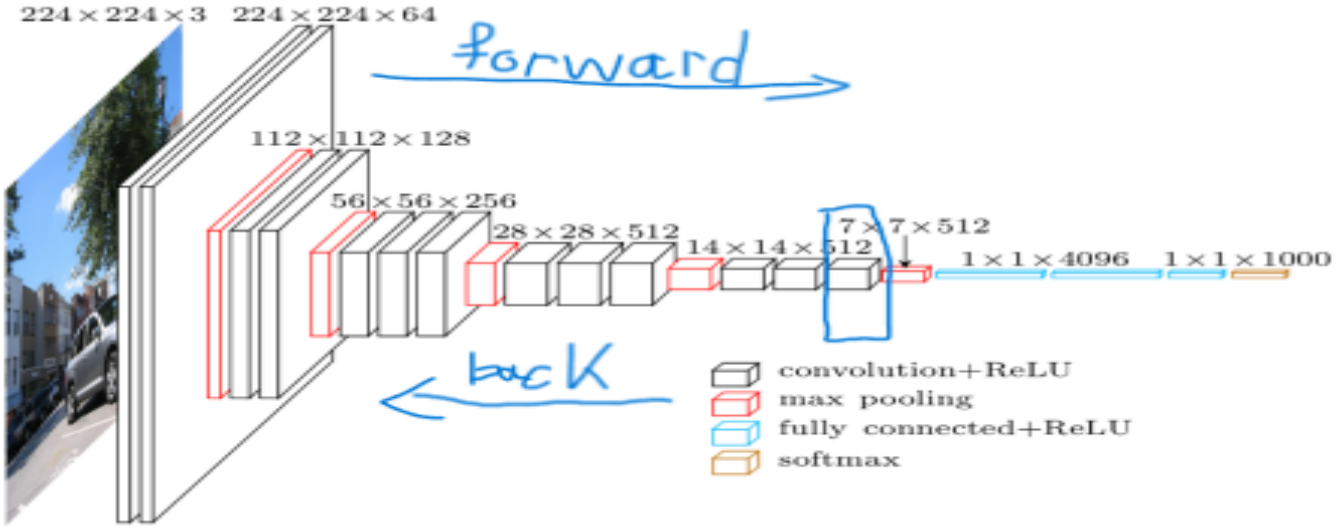
Guided Backpropagation



Question: Can we find an image that maximizes some class score?

Visualize Gradient

A natural idea is to visualize the gradient of the particular layer.



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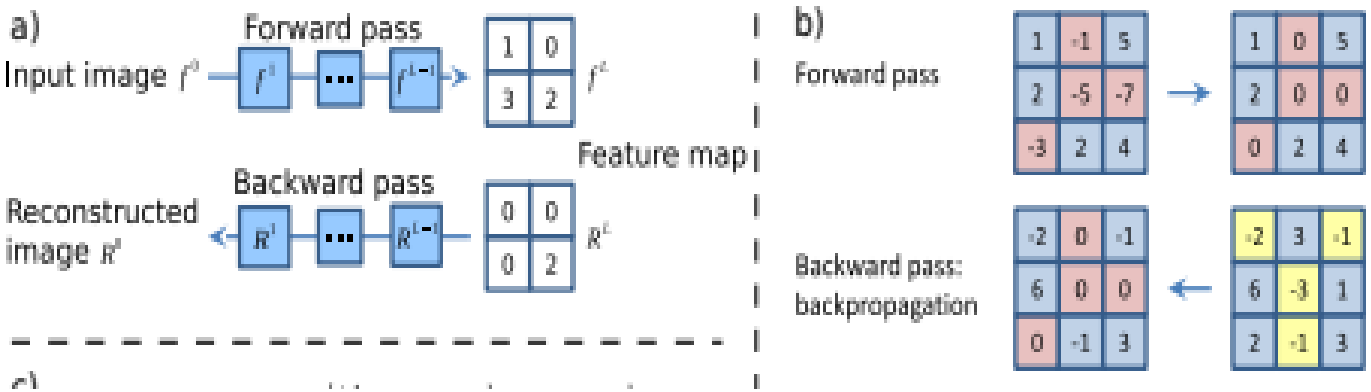
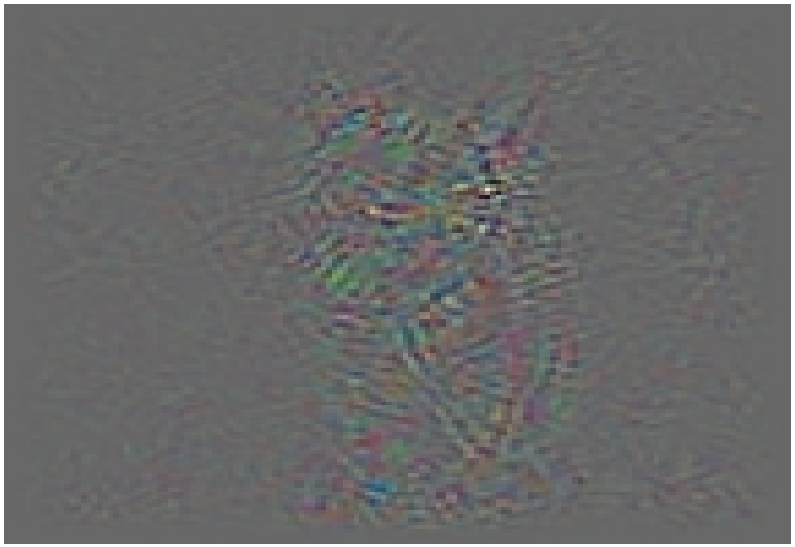


Visualize Gradient

backpropagation



Borrowed from [12]

Visualize Guided Backpropagation

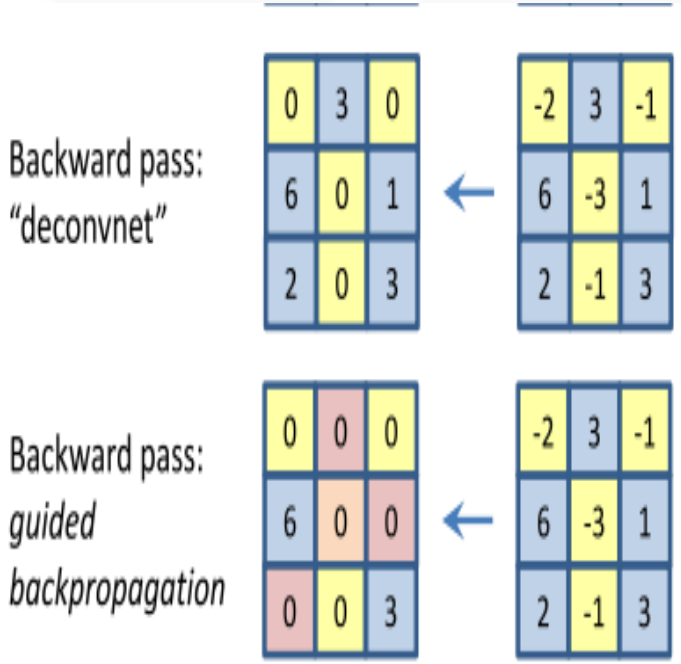
c)

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

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

backward 'deconvnet': $R_i^l = (R_i^{l+1} > 0) \cdot R_i^{l+1}$

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



Borrowed from

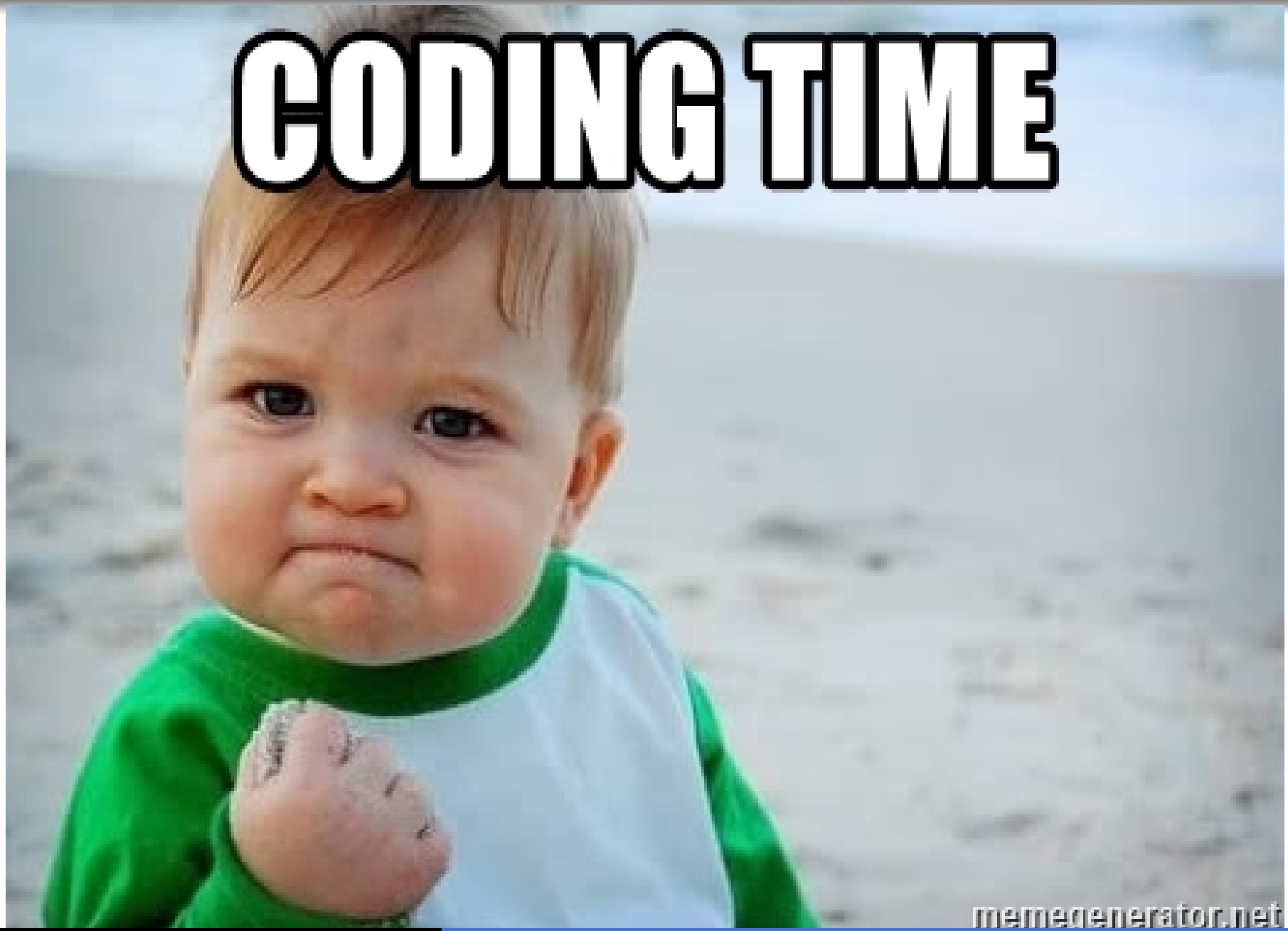
[12]

Visualize Gradient

guided backpropagation

Borrowed from [12]

Grad-CAM



Grad-CAM

- We will now look at what are known as class discriminative saliency maps or class discriminative attribution maps.
- By saliency maps we mean maps or regions in an image that are salient for a given prediction.
- And by class discriminative saliency map, we mean a saliency map that helps distinguish one class from another.
- For example if we had a cat and a dog in an image which part of the image led to it being predicted to be a cat and which part of the same image led to it being predicted as a dog.

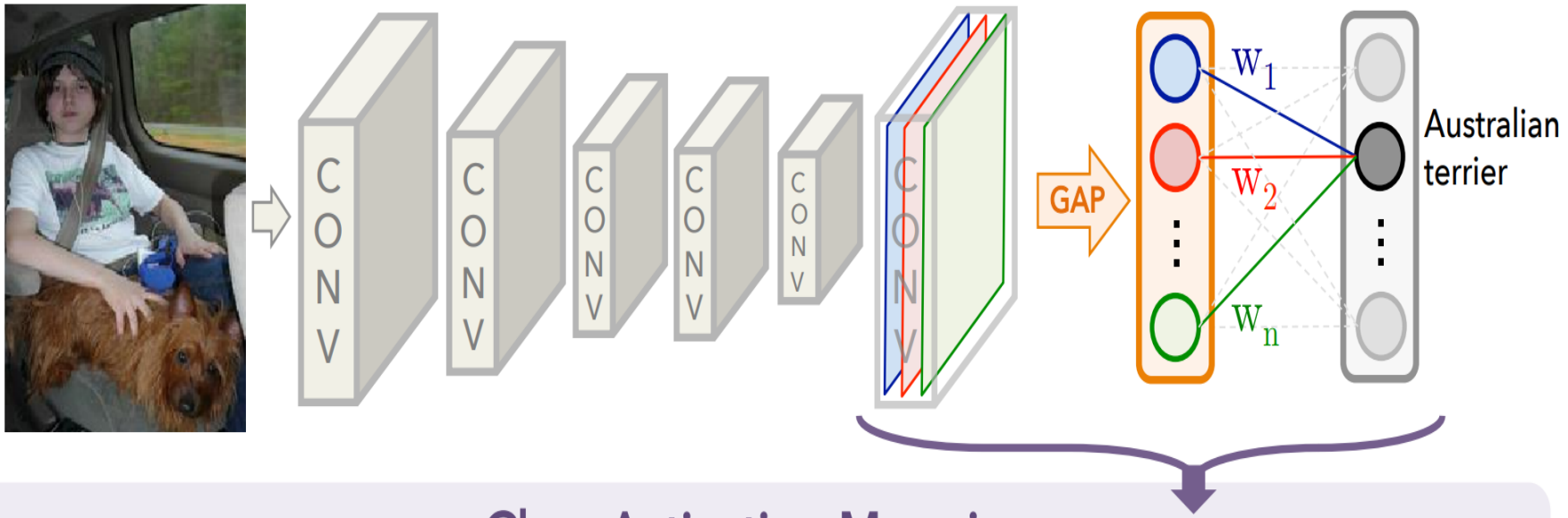
Class Activation Maps

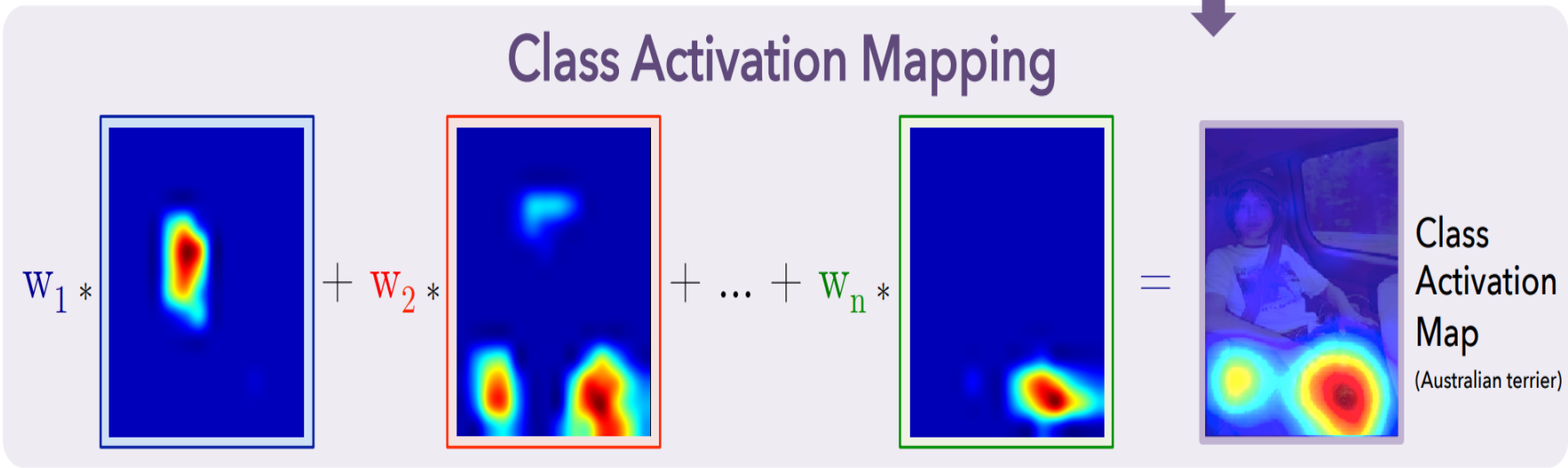
Borrowed from [15]

Class Activation Maps

Borrowed from [15]

Class Activation Maps





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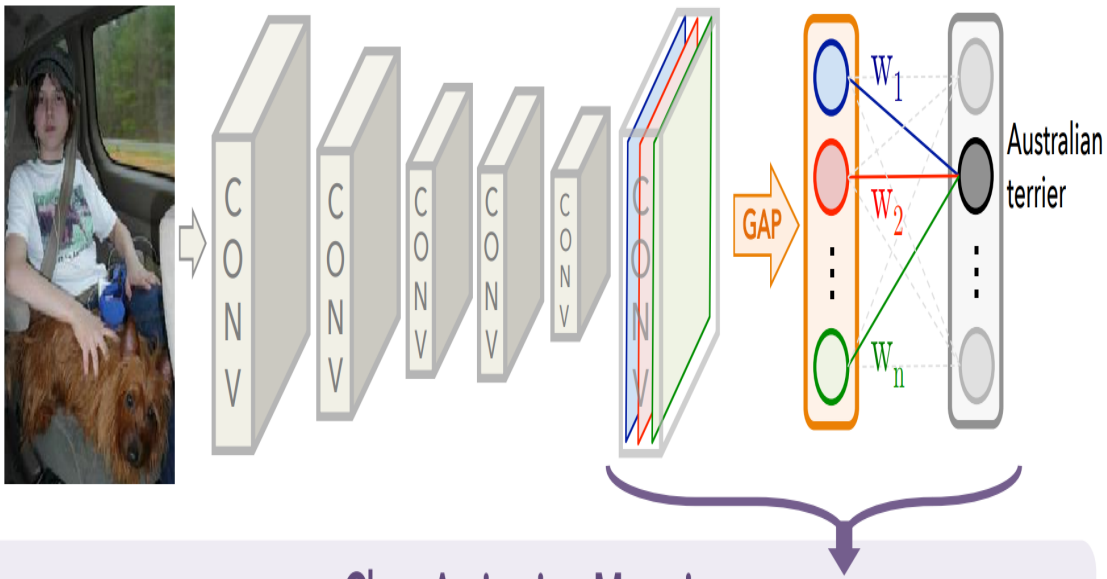
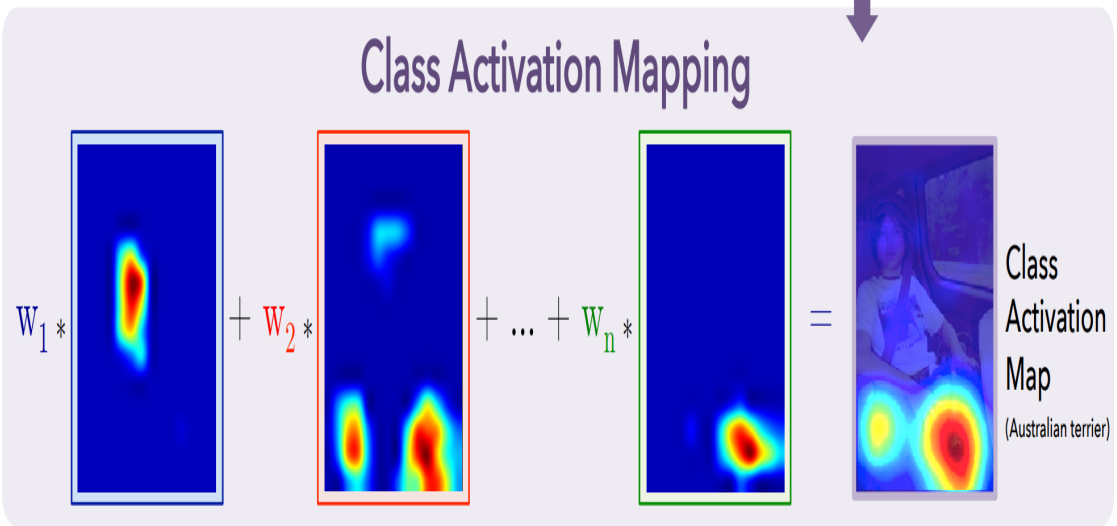
Class Activation Maps





$A_{ij}^k \rightarrow$ activation of unit k in the last convolutional layer.

GAP: $F^k = \frac{1}{Z} \sum_{i,j} A_{ij}^k$

$Y^c = \sum_k w_k^c F^k$, input to the softmax for a given class and w_k^c is a weight corresponding to class c for unit k. It shows importance of F^k for class c.

$$P(Y = c) = \frac{\exp(Y^c)}{\sum_{c'} \exp(Y^{c'})}$$

$$Y^c = \sum_k w_k^c \frac{1}{Z} \sum_{i,j} A_{ij}^k$$

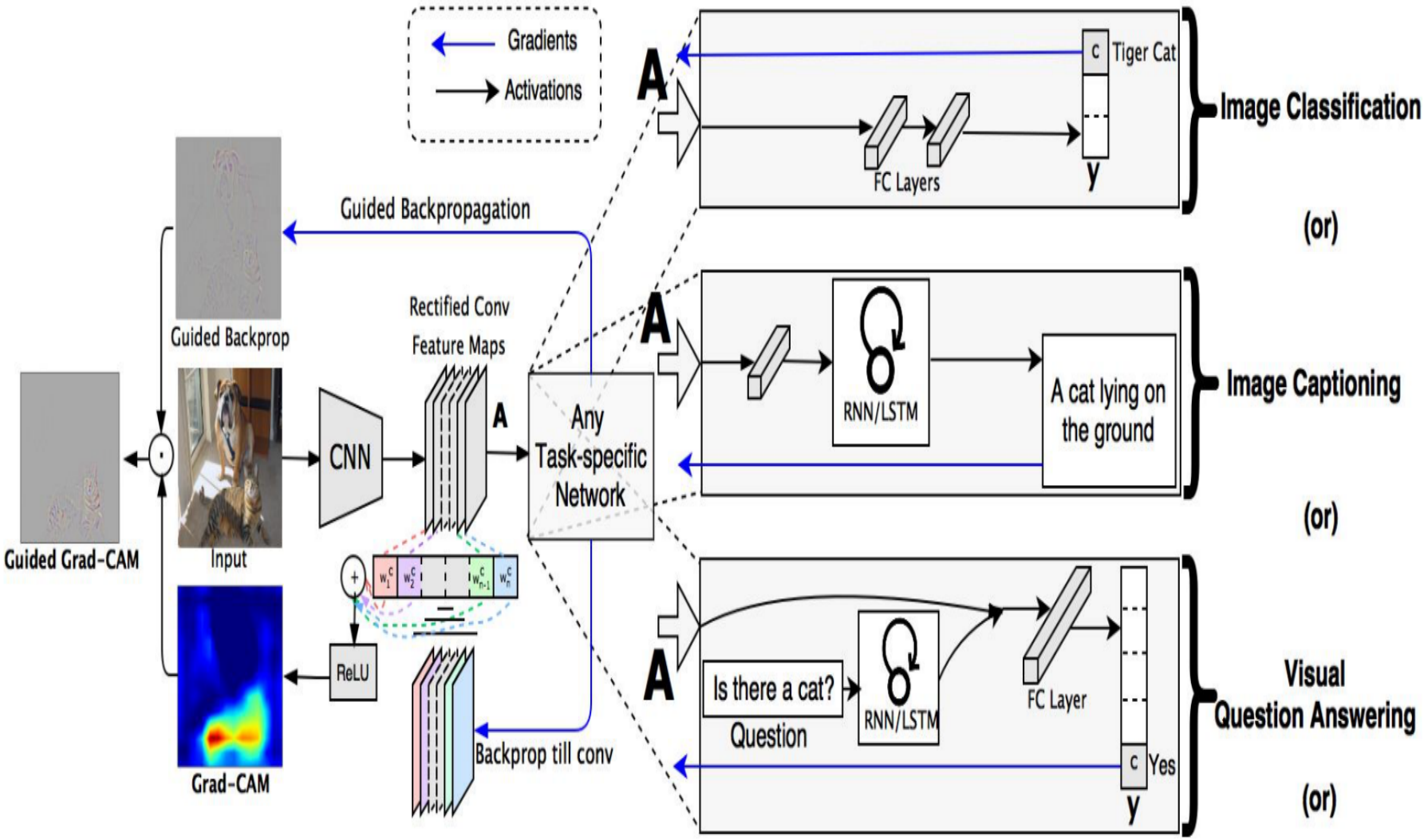
$$= \frac{1}{Z} \sum_{i,j} \sum_k w_k^c A_{ij}^k$$

CAM $= \sum_k w_k^c A_{ij}^k$

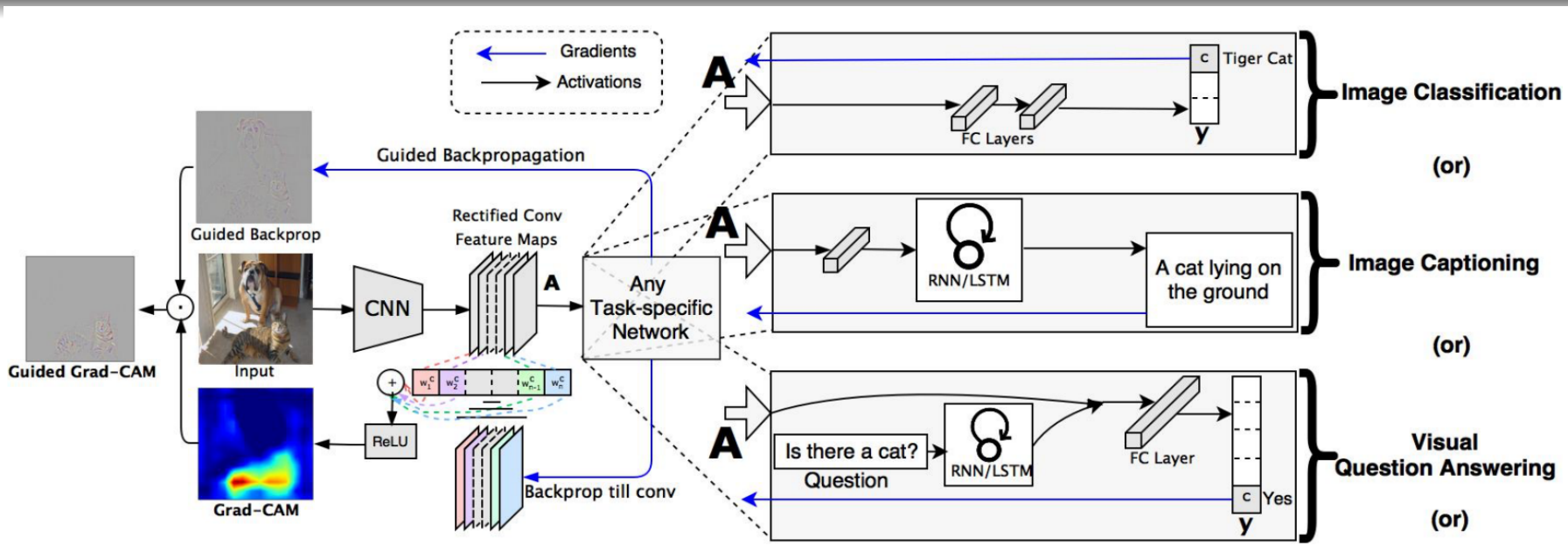
CAM: Pros and Cons

- Advantages
  - It is class discriminative
  - Doesn't require a backward pass.
- Disadvantages
  - GAP imposes constraint on architecture
  - Need retraining to explained trained models.
  - Model may trade off accuracy for interpretability

Grad-CAM


Gradients
Activations
Guided Backpropagation
Guided Backprop
Guided Grad-CAM
Input
Grad-CAM
CNN
Rectified Conv
Feature Maps
A
Any
Task-specific
Network
ReLU
Backprop till conv
A
C
Tiger Cat
FC Layers
y
Image Classification
(or)
A
RNN/LSTM
A cat lying on
the ground
Image Captioning
(or)
A
Is there a cat?
Question
RNN/LSTM
FC Layer
C
Yes
y
Visual
Question Answering
(or)

Grad-CAM



From CAM $Y^c = \sum_k w_k^c F^k$ and $F^k = \frac{1}{Z} \sum_{i,j} A_{ij}^k$, taking derivative

$$\frac{\partial Y^c}{\partial F^k} = \frac{\frac{\partial Y^c}{\partial A_{ij}^k}}{\frac{\partial F^k}{\partial A_{ij}^k}} \implies w_c^k = \frac{\partial Y^c}{\partial A_{ij}^k} Z$$

Summing both sides over i, j

$$Z w_c^k = Z \sum_{i,j} \frac{\partial Y^c}{\partial A_{ij}^k}$$

Class features weights are gradients themselves. No retraining required.

Grad-CAM: Methodology

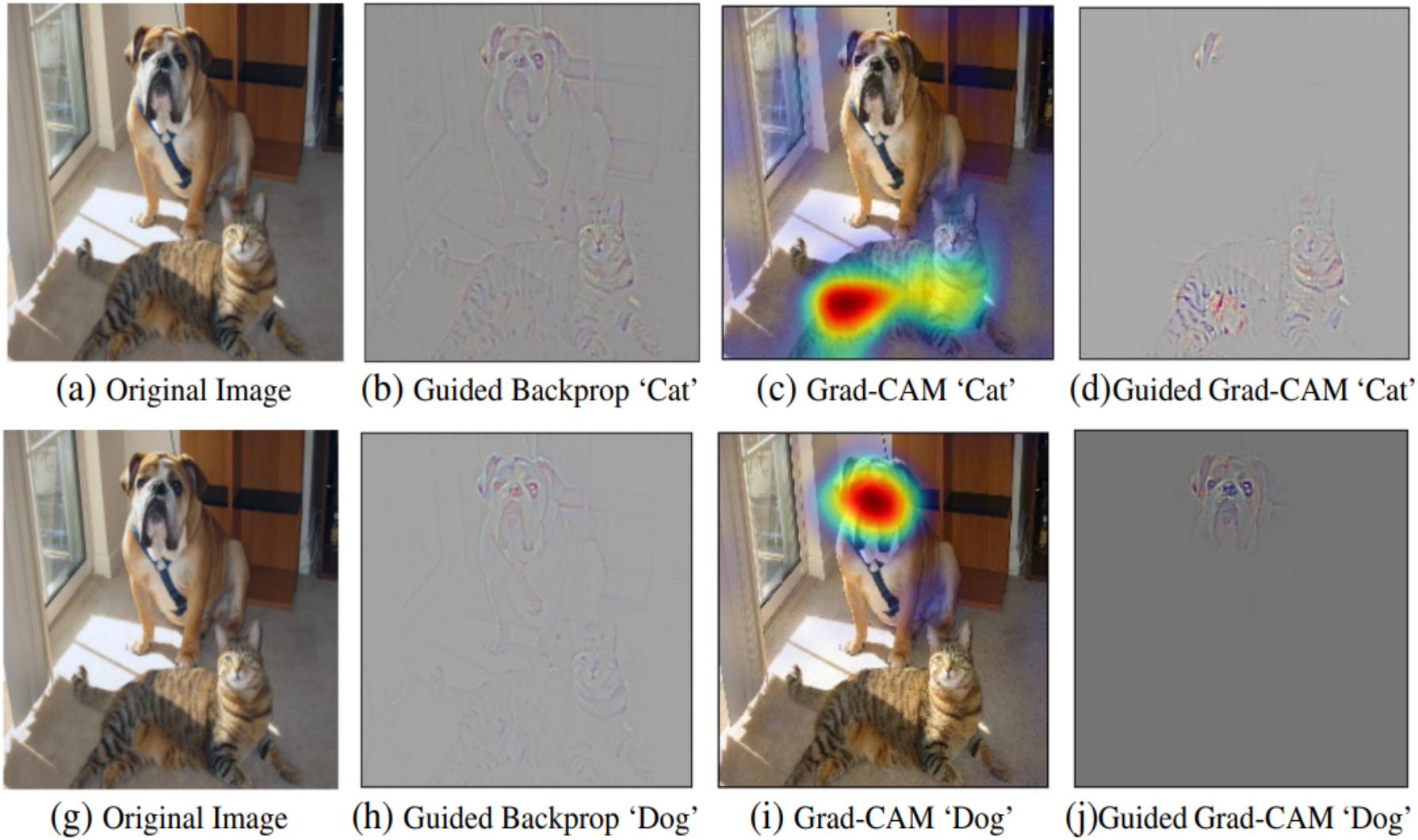
- Uses gradients flowing from output class into activation maps of last convolutional layer as neuron importance weights

$$w_c^k = \sum_{i,j} \frac{\partial Y^c}{\partial A_{ij}^k}$$

- Similar to CAM

$$L_{\text{Grad-CAM}} = \text{ReLU}(\sum_k w_k^c A^k)$$

Grad-CAM



(a) Original Image (b) Guided Backprop 'Cat' (c) Grad-CAM 'Cat' (d)Guided Grad-CAM 'Cat'

(g) Original Image (h) Guided Backprop 'Dog' (i) Grad-CAM 'Dog' (j)Guided Grad-CAM 'Dog'

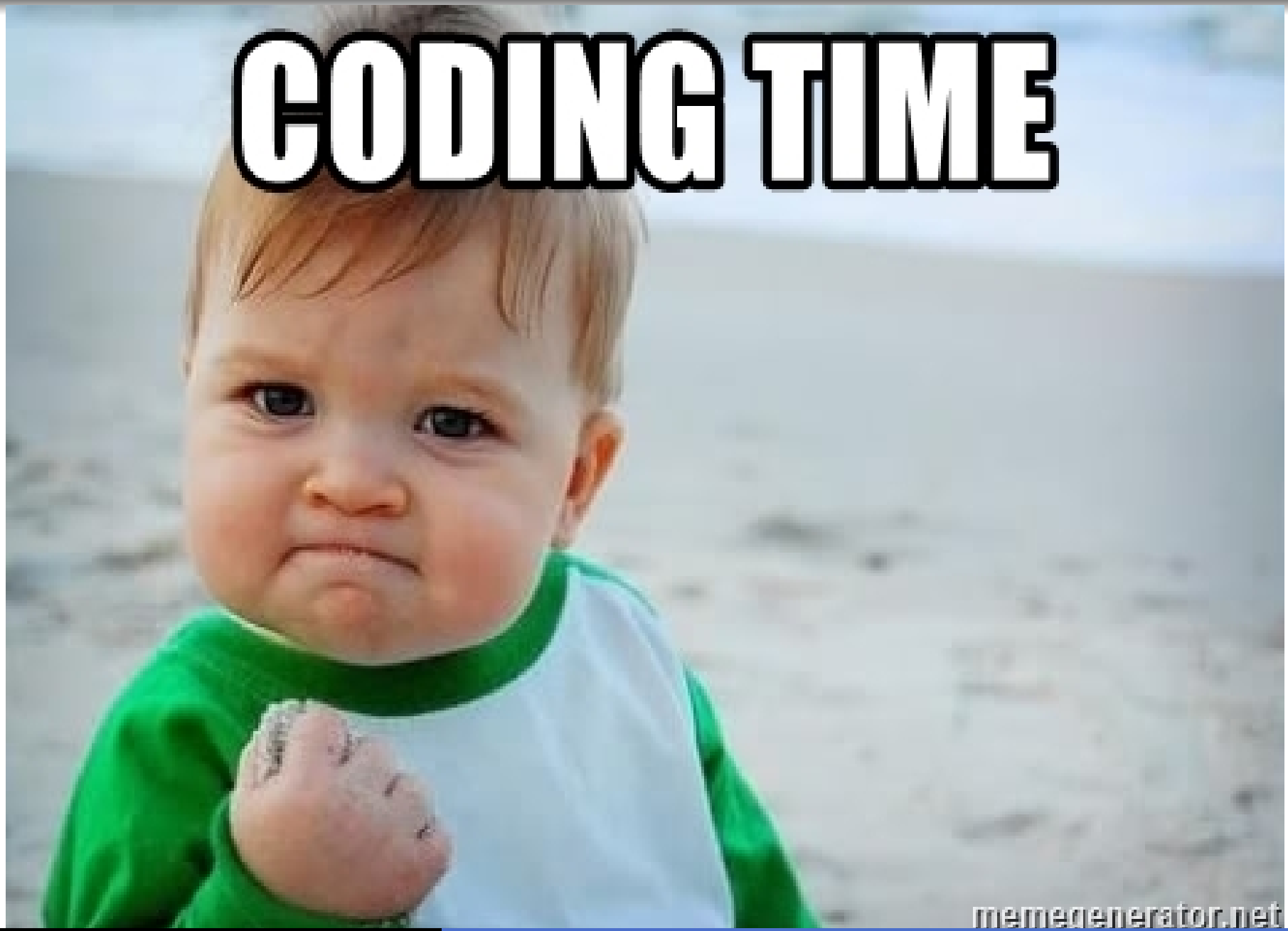
Interestingly, network predicts **Tiger Cat**, but Grad-CAM does not why. Guided Grad-CAM answers the question.

Counterfactual Explanations

- By negating the value of gradients used in w_k^c we can visualize image patches that have adversarial affects.
- By removing or suppressing features occurring in such patches may improve model performance

(a) Original Image (b) Cat Counterfactual exp (c) Dog Counterfactual exp

Grad-CAM

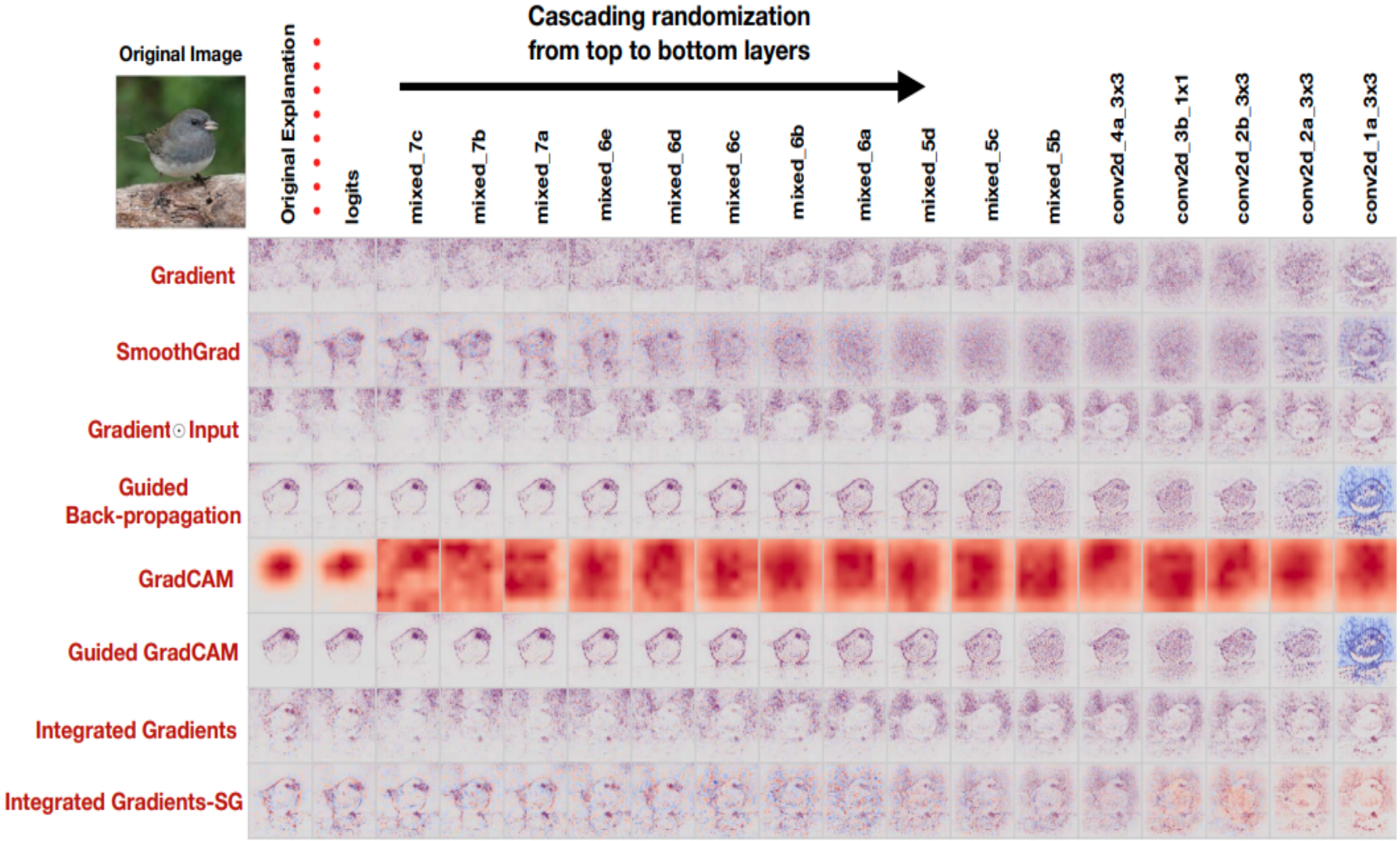


Recent Model Specific Methods

- Grad-CAM++ [4]: Improved version of Grad-CAM
- DeepLIFT [10]: Instead of gradient looks on how perturbation of inputs change the output.
- Integrated Gradient [13]: Gives different activation to gradients and then integrates over the results.
- SmoothGrad [11]: Adds gaussian noise to inputs and measures activation changes.
- XRAI [5]

Warning on using Explainable Methods

One need to be extremely careful on visual interpretation of the explainable methods. See [1].



Section 3

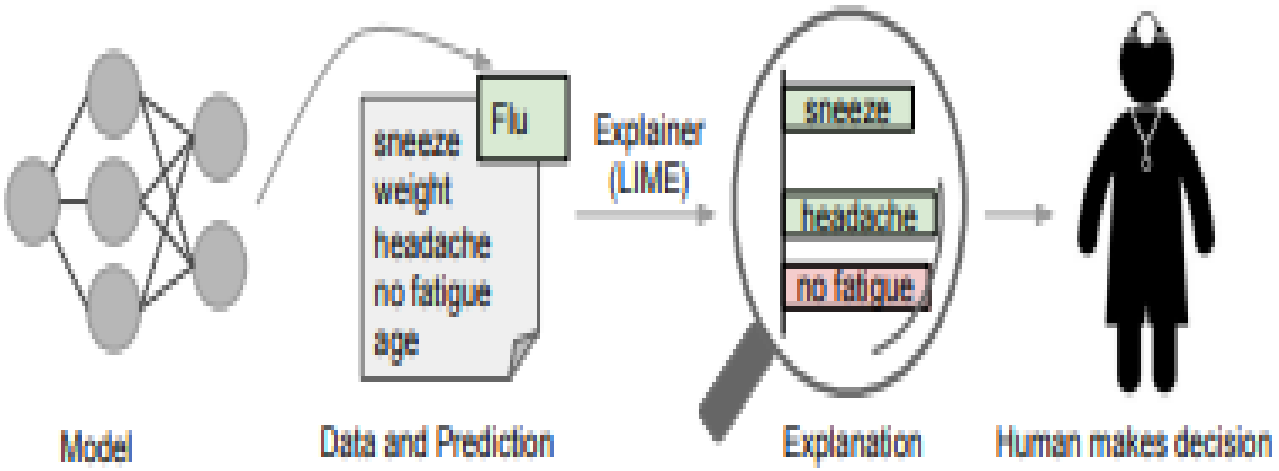
1 Introduction to Explainable ML

2 Model Specific Explanations

3 Model Agnostic

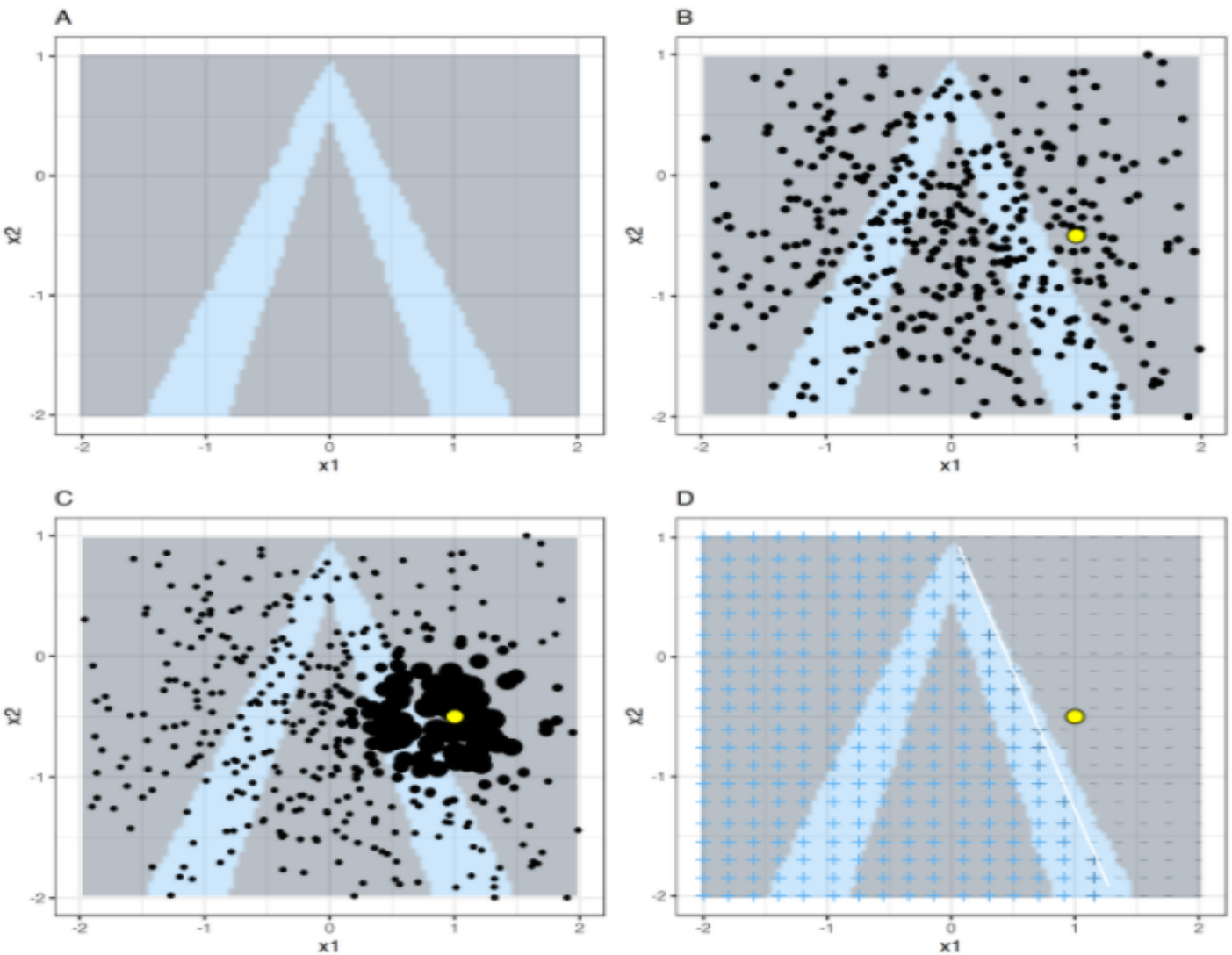
LIME Algorithm

- Local interpretable model-agnostic explanations (LIME) [8] focuses on training local surrogate models to explain individual predictions.



Borrowed from "Why Should I Trust You?: Explaining Prediction for Any Classifier" [8]

How does it work?



A little bit Math

- Recall that We want to find a model that locally approximates a black-box model $f(\cdot)$ around the instance of interest x_*
- We consider a class of G simple models, for example linear models $g(\tilde{X}) = \tilde{X}\beta$
- To find the approximation, we minimize

$$\hat{\beta} = \arg\min_{\beta} L(f, g, \pi(x_*)) + \lambda\|\beta\|,$$

where $\pi_x(x_*)$ defines a neighborhood of x_* and $L(\cdot)$ is a loss function. **What is the most popular loss function?**

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- In practice we choose K feature and there is no need for $\|\beta\|$.

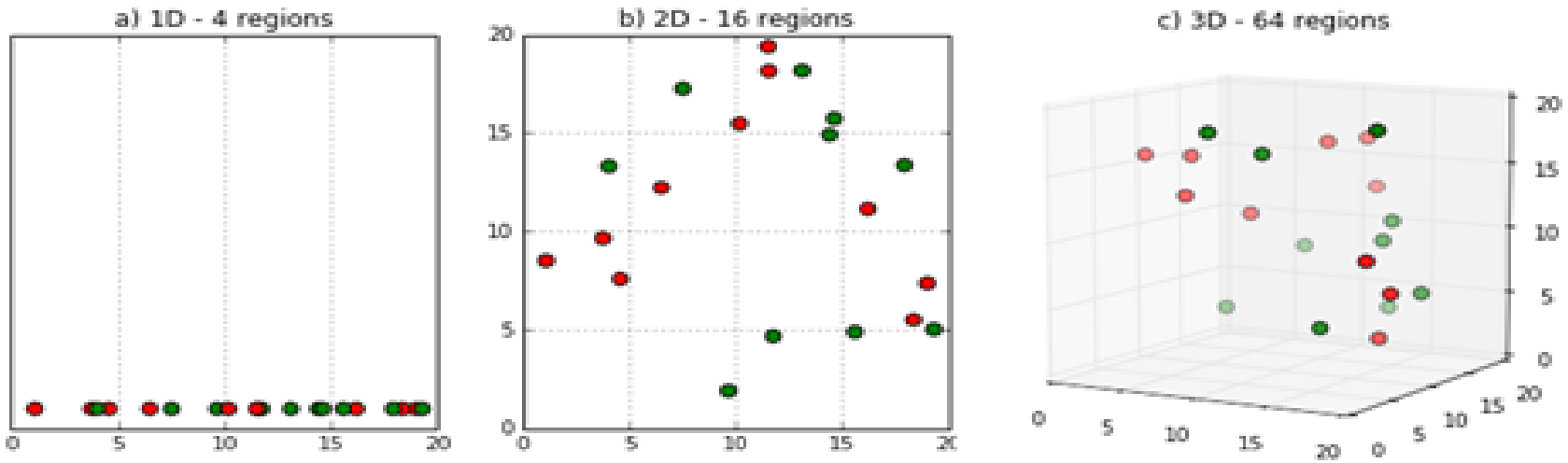
$$\hat{\beta} = \arg\min_{\beta} \sum_{z,z'} \pi_x(z)(f(z) - g(z'))^2$$

LIME algorithm

Require: x^*- observation to be explained
Require: sample size - N, complexity - K
Let $x^{'} = h(x^*)$ lower-dimensional representation
for $i = 1 \dots N$ **do**
$z'[i] =$ sample_around(x')
$z[i] = h(z'[i])$ recover obervation to original space
$y[i] = f(z[i])$ prediction for the new observation
$\pi[i] = \pi_x(z)$ estimate similarity
end for
return $\hat{\beta} = \arg\min_\beta \sum_{z,z'} \pi_x(z)(f(z) - g(z'))^2$

More Details

- Why do we need a lower-dimensional representation?
- Consider an image with 244×244 pixels, i.e. the original space is $3 \times 244 \times 244$ and input space is $178,608$-dimensional.
- Recall for the LIME we need to sample around x which is a hard task for high dimensional problems (**Curse of Dimensionality**)



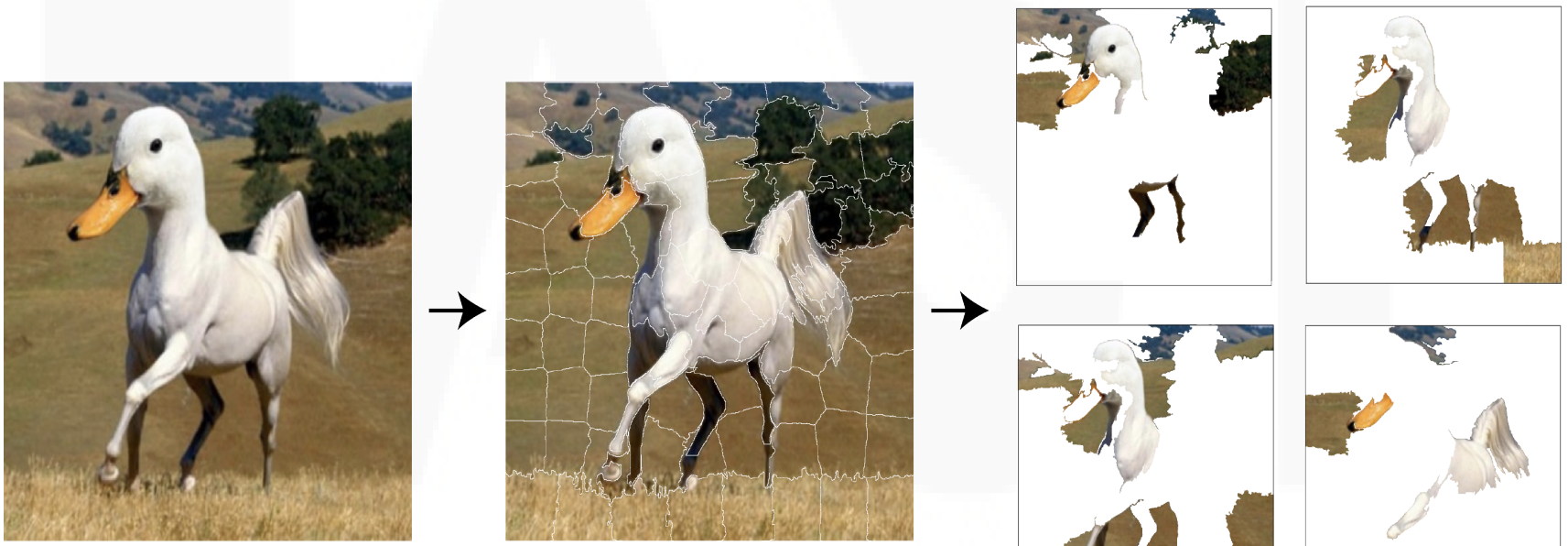
More Details

- To avoid curse of dimensionality the space can be transformed into superpixels, which are treated as binary features that can be turned on or off.
-   [1]
- Thus in this case the black-box model $f()$ operates on $178,608$-dimensional space and $g()$ in $\{0,1\}^{100}$

[1] Picture is borrowed from [3]

Sampling around the instance

- Due to high-dimension usually we cannot sample from the original data, which is sparse.
- In practice, we create new data points by perturbing the instance we want to explain.
-



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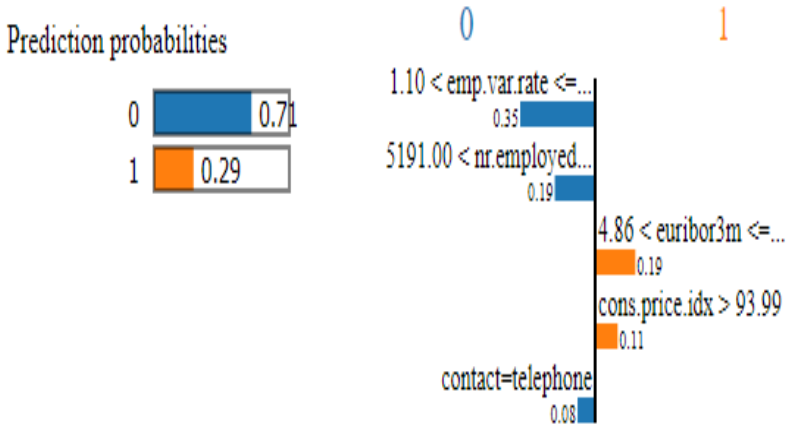
[2]Picture is borrowed from [3]

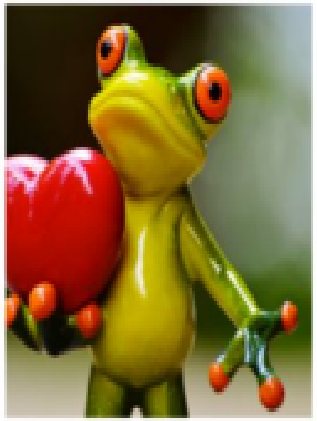
Explanation

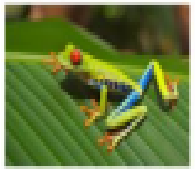
- Central plot shows importance of the top features for this prediction
  - Value corresponds to the weight of the linear model
  - Direction corresponds to whether it pushes in one way or the other
- Numerical features are discretized into bins
  - Easier to interpret: weight == contribution / sign of weight == direction

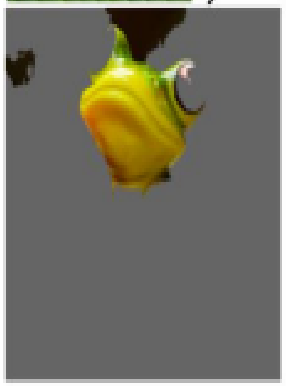


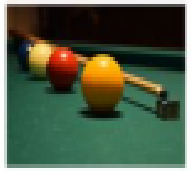
Feature	Value
emp.var.rate	1.40
nr.employed	5228.10
euribor3m	4.95
cons.price.idx	94.47
contact=telephone	True

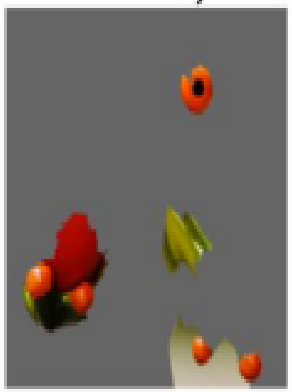
LIME for Images



P() = 0.54



P() = 0.07



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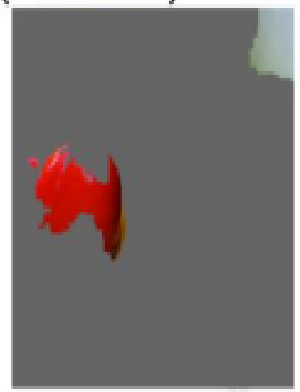


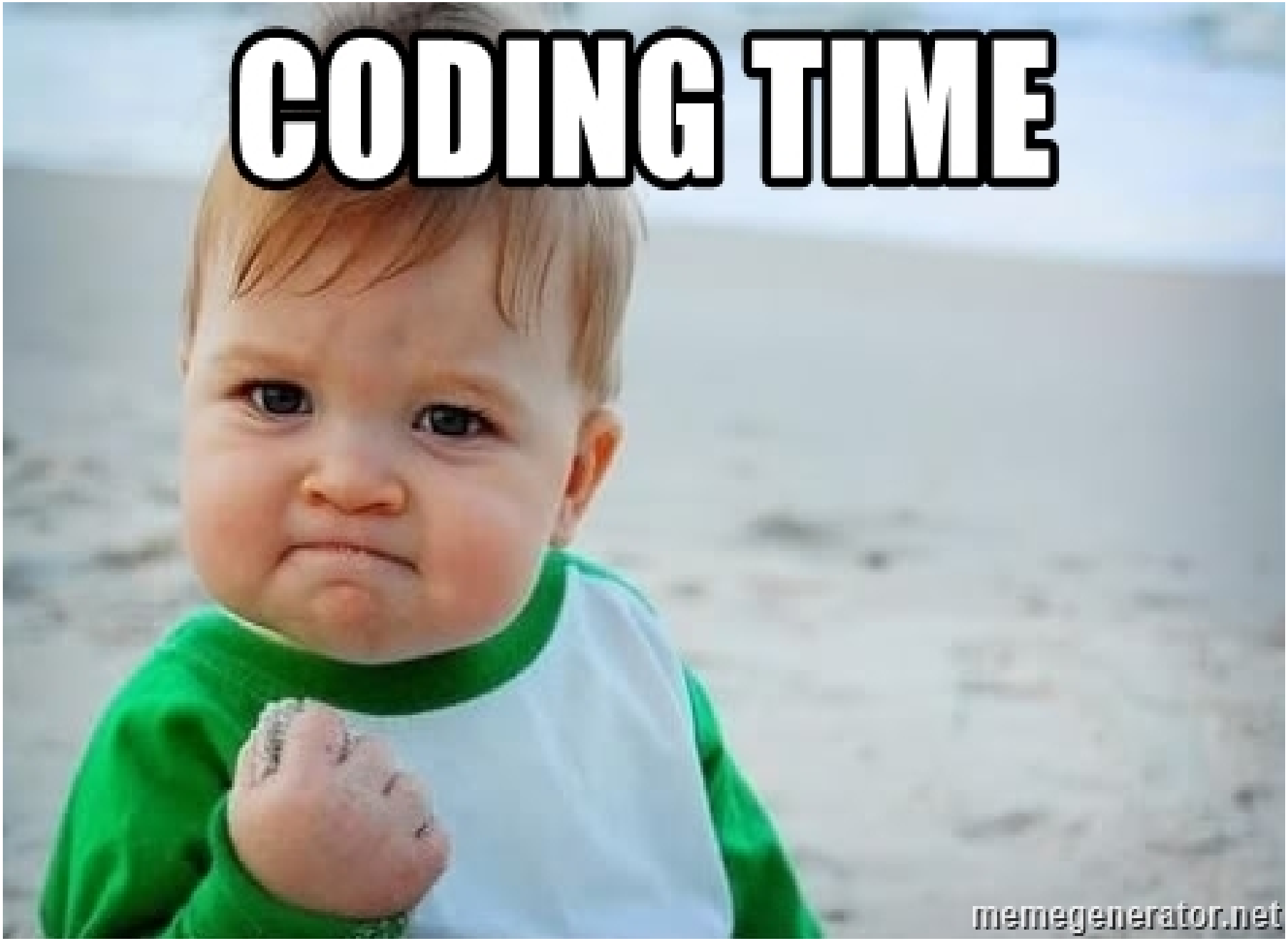
Some drawbacks

- Depends on the random sampling of new points, so it can be unstable
- Fit of linear model can be inaccurate
  - But we can check the r-squared score to know if that's the case
- Relatively slow for a single observation, in particular with images

Types of Data

Lime supports many types of data:

- Tabular
- Recurrent Tabular
- Image
- Text


CODING TIME
memegenerator.net

SHAP values

References I

J. Adebayo, J. Gilmer, M. Muelly, I. Goodfellow, M. Hardt, and B. Kim.
Sanity checks for saliency maps.
In *Proceedings of the 32nd International Conference on Neural Information Processing Systems*, NIPS'18, page 9525–9536, 2018.

S. Beery, G. Van Horn, and P. Perona.
Recognition in terra incognita.
In V. Ferrari, M. Hebert, C. Sminchisescu, and Y. Weiss, editors, *Computer Vision – ECCV 2018*, 2018.

P. Biecek and T. Burzykowski.
Explanatory Model Analysis.
Chapman and Hall/CRC, New York, 2021.

A. Chattopadhyay, A. Sarkar, P. Howlader, and V. N. Balasubramanian.
Grad-cam++: Generalized gradient-based visual explanations for deep convolutional networks.
CoRR, 2017.

References II


A. Kapishnikov, T. Bolukbasi, F. B. Viégas, and M. Terry.
Segment integrated gradients: Better attributions through regions.
CoRR, abs/1906.02825, 2019.


C. Molnar.
Interpretable Machine Learning.
2 edition, 2022.


M. T. Ribeiro, S. Singh, and C. Guestrin.
"why should i trust you?": Explaining the predictions of any classifier.
In *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, page 1135–1144, 2016.


M. T. Ribeiro, S. Singh, and C. Guestrin.
"why should i trust you?": Explaining the predictions of any classifier.
In *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, page 1135–1144, 2016.

References III


C. Rudin.
Nature Machine Intelligence, 1(5):206–215, 2019.


A. Shrikumar, P. Greenside, and A. Kundaje.
Learning important features through propagating activation differences.
CoRR, abs/1704.02685, 2017.


D. Smilkov, N. Thorat, B. Kim, F. B. Viégas, and M. Wattenberg.
Smoothgrad: removing noise by adding noise.
CoRR, 2017.


J. T. Springenberg, A. Dosovitskiy, T. Brox, and M. Riedmiller.
Striving for simplicity: The all convolutional net, 2014.


M. Sundararajan, A. Taly, and Q. Yan.
Axiomatic attribution for deep networks.
CoRR, abs/1703.01365, 2017.


M. D. Zeiler and R. Fergus.
Visualizing and understanding convolutional networks, 2013.

References IV


B. Zhou, A. Khosla, A. Lapedriza, A. Oliva, and A. Torralba.
Learning deep features for discriminative localization, 2015.

Example Details

- Logistic regression models a relationship between predictor variables and a categorical response variable.
- Logistic regression helps us estimate a probability of falling into a certain level of the categorical response given a set of predictors.
- The multiple binary logistic regression model is the following:

$$P(Y=1) = \frac{1}{1+\exp\left(-(\beta_0+\beta_1 X_1+\cdots+\beta_k X_k)\right)}$$

- and its logit transformation

$$\log\left(\frac{P(Y=1)}{P(Y=0)}\right) = \beta_0+\beta_1 X_1+\cdots+\beta_k X_k$$

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