

# NCAR Summer School – AI4ESS

## Peering Inside the Black Box of Machine Learning for Earth Science - Part 2

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# Wonderful Collaborators on this topic



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All at Colorado State University

# NN Interpretation – Initial Thoughts

## Gaining insights into an NN is

- An **iterative, scientist-driven discovery process**,
- Driven by old fashioned methods of experimental design, and hypothesis generation and testing,
- **NN visualization tools simply provide additional tools to *assist* this process** (but they are not driving this process).

So far there is no such thing as an automated, one-size fits-all visualization method. And there *might* never be.

→ Earth scientist always remains crucial in the entire process.

→ You will see that in the examples.

# Acronyms

ANN = (Artificial) Neural Network = NN

Heat map = Heatmap = Attribution map (used interchangeably)

XAI = Explainable AI

= common term used by computer scientists to denote interpretation/visualization methods for AI algorithms.

# NN Interpretation Tools – Part 2

Two methods beyond what Amy McGovern just covered in Part 1:

## 1) Layer-Wise Relevance Propagation (LRP):

*A method for identifying strategies the NN uses by looking into decision process for specific samples.*

## 2) Receptive Field of CNNs:

*A property of NN architecture – helpful for NN architecture selection and interpretation.*

**Let's get started with #1 ...**

# Motivation

## ANNs

- Have emerged as promising tool in countless earth science related applications.
- **Perform amazingly well at many complex tasks.**
- **ANNs are generally treated as black box:** it's considered too difficult a task to understand how they work.
- *Why is that a problem?*  
*If ANNs work fine, why do we care how they work?*

# Example: Problematic strategies

Insights from a study of strategies utilized by a neural network.

Reference (also source of images on the following slides):

*Lapuschkin et al. "Unmasking Clever Hans Predictors and Assessing What Machines Really Learn." Nature Communications, vol. 10, no. 1, Mar. 2019, p. 1096, doi:10.1038/s41467-019-08987-4.*

Inventors of  
LRP method



**Task:**

- Given an ANN trained for object recognition in images.
- Decide whether there is a **horse** in a given image.

**Methodology used in that paper:**

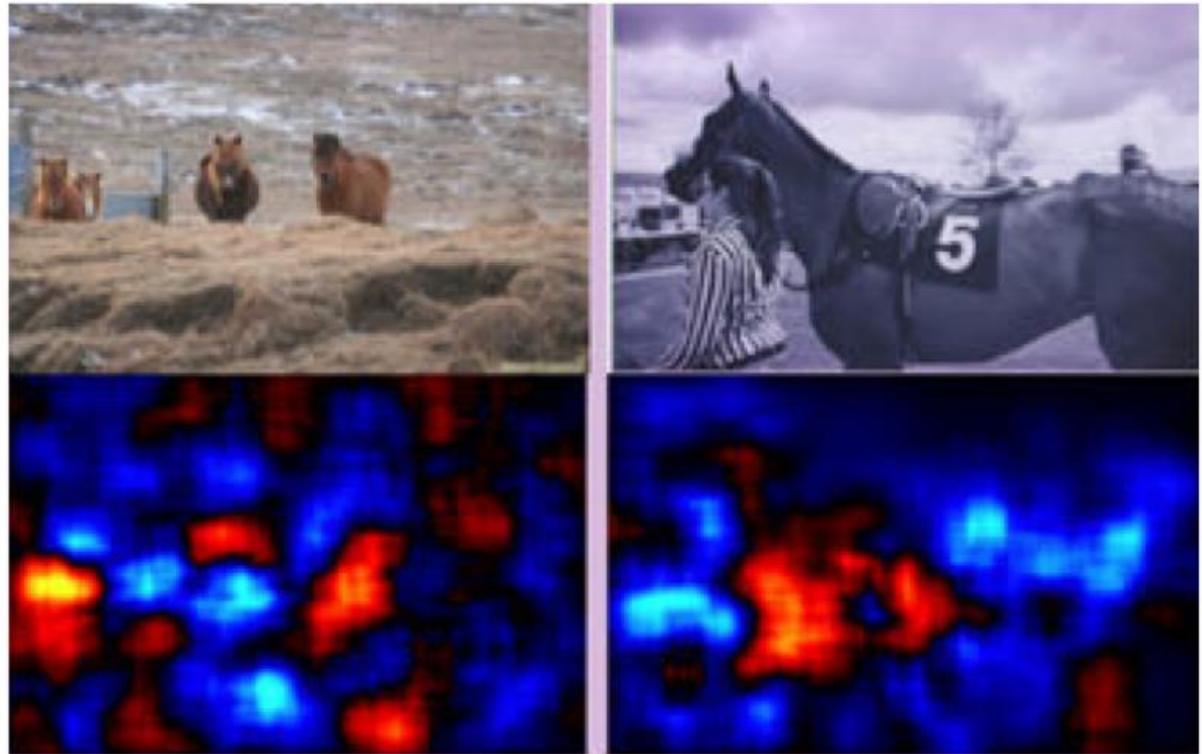
- Step 1: Train neural network to decide whether there's a horse.
- Step 2: Apply visualization technique (LRP) to analyze network's strategies.

The following slides provide two things:

1. An example of **problematic strategies** an ANN might use.
2. A **way to identify such strategies: visualization in action.**

# Detecting horses – Strategy 1 of algorithm

Input Images



Attribution maps (aka heat maps)

Attribution maps (from LRP):  
In red is where the NN is  
looking to decide whether  
there is a horse.

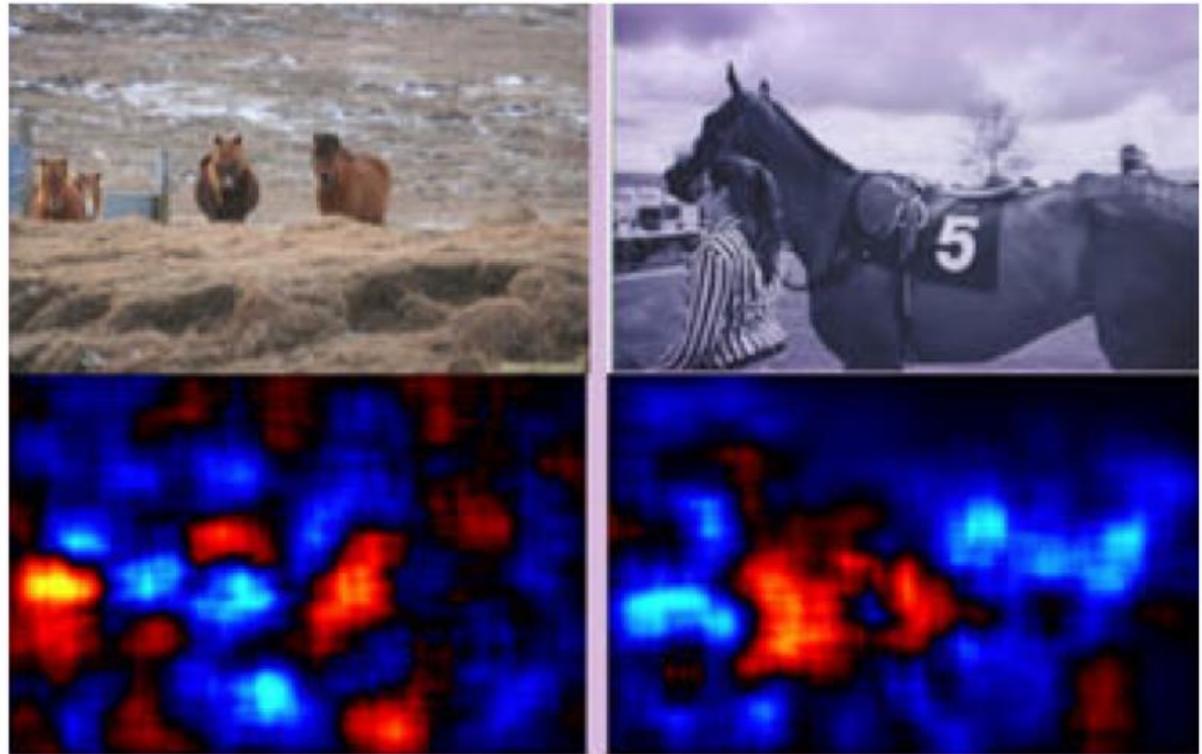


Red areas: increase confidence  
Blue areas: decrease confidence  
Black areas: not useful

**Strategy 1: What does ANN detect in *these* images?**

# Detecting horses – Strategy 1 of algorithm

Input Images



Attribution maps:  
In red is where the NN is  
looking to decide whether  
there is a horse.

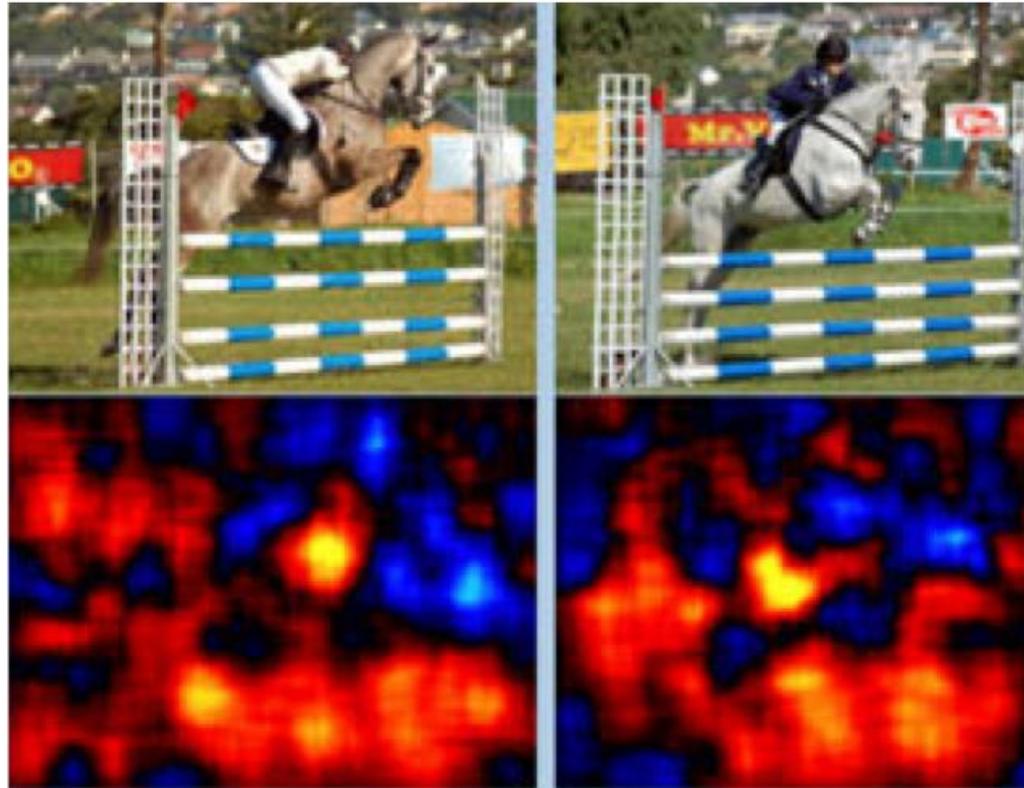


Red areas: increase confidence  
Blue areas: decrease confidence  
Black areas: not useful

Strategy 1: What does ANN detect? **MAINLY PARTS OF HORSES. Great!**

# Detecting horses – Strategy 2 of algorithm

Input Images



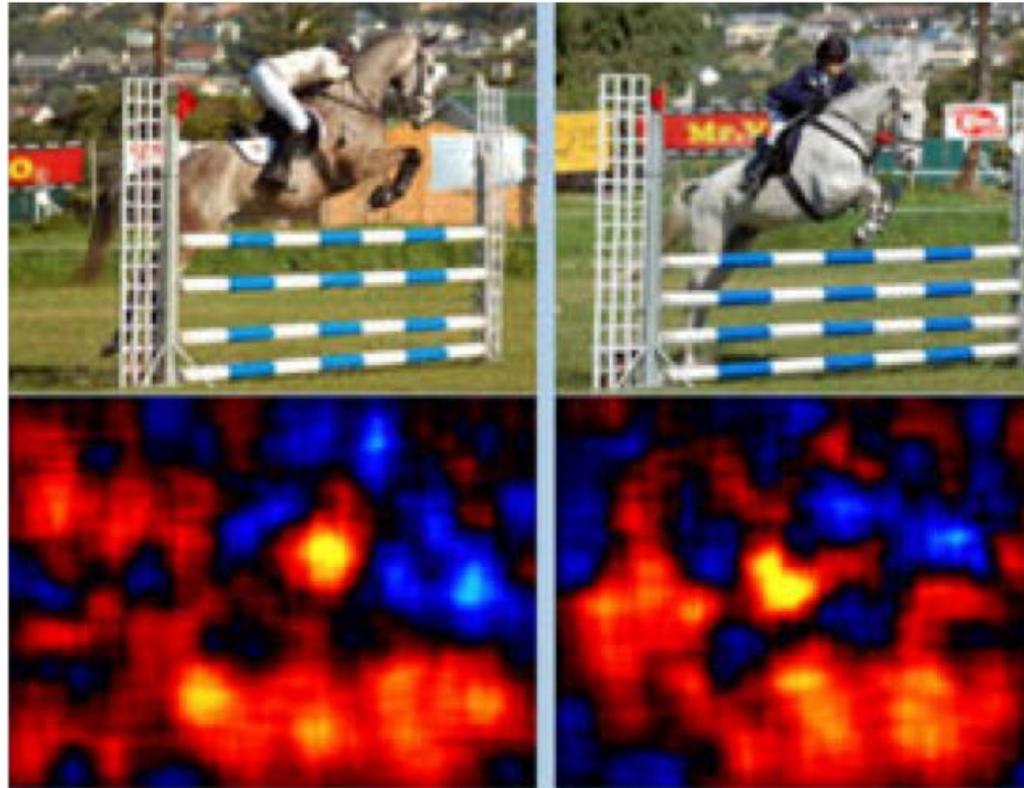
This is where the NN is looking to decide.



Strategy 2: What does ANN detect in *these* images?

# Detecting horses – Strategy 2 of algorithm

Input Images



This is where the NN is looking to decide.



**Strategy 2: What does ANN detect?**

**Poles = items correlated with horses.**

**Not a great strategy.**

**What happens for an image containing poles but no horse?**

**False positive!**

## Detecting horses – Strategy 3 of algorithm



**Strategy 3: What does ANN detect in *this* image?**

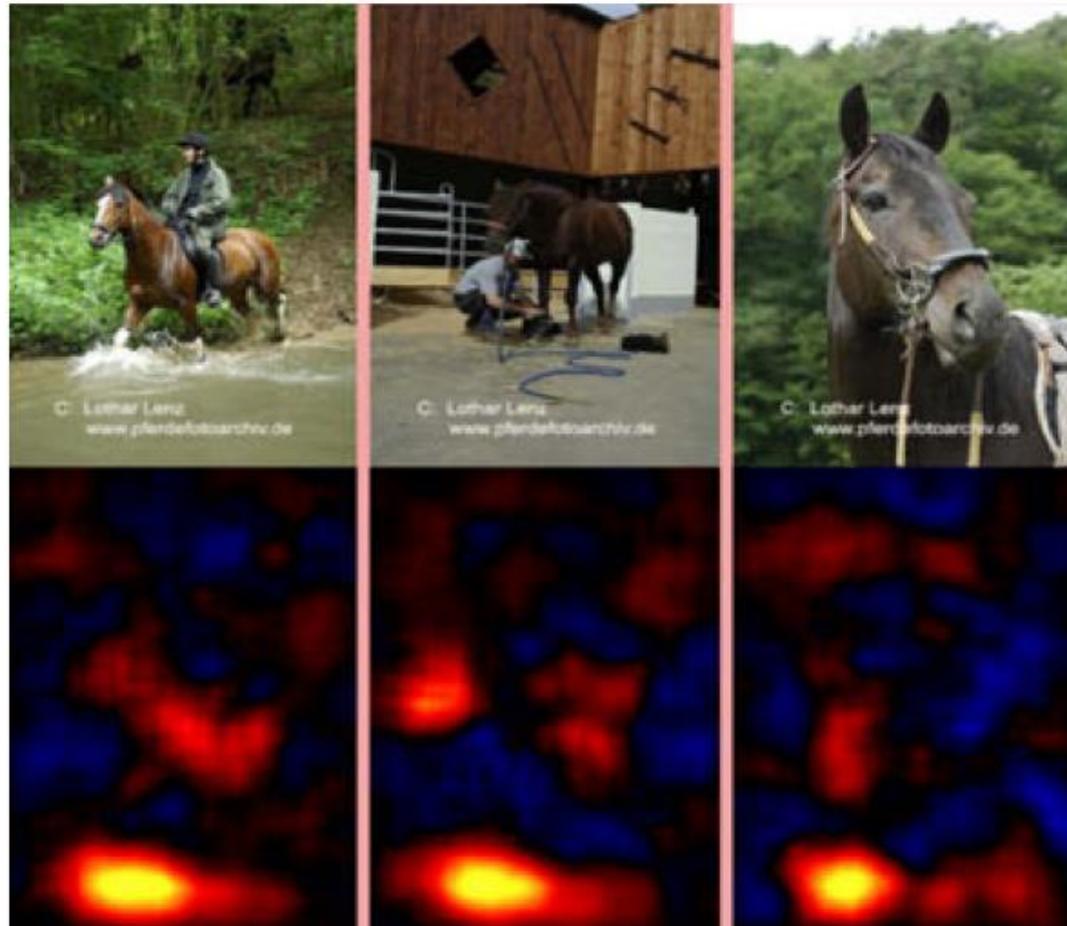
## Detecting horses – Strategy 3 of algorithm



Look at attribution map for a hint!

**Strategy 3: What does ANN detect in this image?**

## Detecting horses – Strategy 3 of algorithm



Attribution maps  
as hint.

**Strategy 3: What does ANN detect in *these* images?  
The html tags! Definitely do NOT want *this* strategy!  
There are no html tags in the real world! Would result in false negatives.**

# What happened?

**Don't blame the algorithm – it did exactly what it was supposed to do:**

- **Algorithm correctly learned *correlations present in the data* to achieve its objective.**
- But some of the correlations were not representative of correlations in real world (e.g., poles can occur without horse, no html tags in real world!).
- Can call this the “*Inadvertent-correlation-present-only-in-data*” problem.

**→ Algorithm seems to perform well, but its reasoning does not generalize to the world.**

- **Conclusion: Using ANN as black box can be a problem.**

**But also learned:**

- **Visualization method proved useful to detect correct & incorrect strategies.**
- Can we use such methods to find strategies learned by ANNs trained for earth science applications?

# How visualization methods can help

## Using visualization tools can:

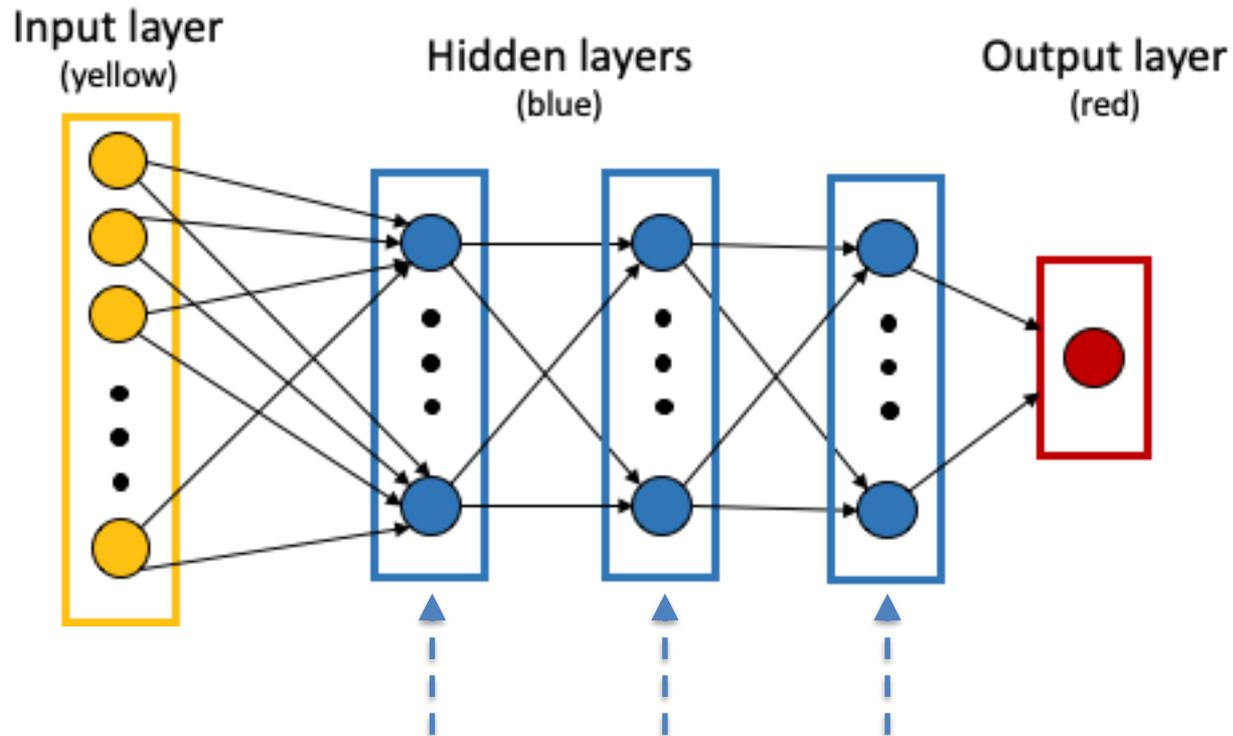
Provide information on ANN's reasoning, e.g., in form of attribution maps, as shown above.

In turn that provides:

1. **Increased trust in ANN – you're more likely to use a method you understand.**
2. Important information for **design of ANNs**, enables physics-guided machine learning.
3. **Provides new role for ML:** visualization output can even be used to **discover new science!** (*See REFs at end of this presentation*).

# Visualization – Type A: Feature Visualization

**Philosophy:** Seek to understand all internal components of ANN.



Seek to understand the meaning of all intermediate (blue) nodes.

# Visualization – Type A

## Visualizing individual neurons – two sample methods:

**Method 1:** Identify training samples that yield high activation of that neuron.

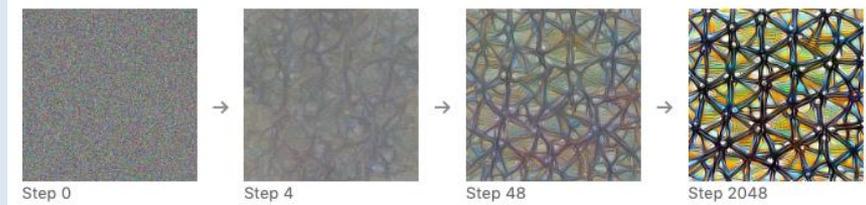


- But *what* in the image triggered activation - the building or the sky?
- Strategies might still not be obvious.
- Nevertheless very useful method.
- Excellent application paper:

Xie, M., Jean, N., Burke, M., Lobell, D., & Ermon, S. (2016, March). "Transfer learning from deep features for remote sensing and poverty mapping". In Thirtieth AAAI conference on artificial intelligence. [LINK TO PAPER](#) .

**Method 2:** Generate synthetic image that maximizes activation of considered neuron.

- Uses built-in derivatives + gradient descent tools of ANN framework. Easy to do.
- Start with random image or input sample.
- Gradient descent to max. neuron activation.



Recommended reading/video:

- Olah, C., Mordvintsev, A., & Schubert, L. (2017). Feature visualization. *Distill*, 2(11), e7. [LINK TO PAPER](#)
- CVPR 2020 Tutorial on Interpretable Machine Learning for Computer Vision, June 15, 2020. [LINK TO VIDEO](#)  
See Lecture #4: Christopher Olah, **Introduction to Circuits in CNNs**.

**Related topic - backward optimization by Amy:**

- McGovern, Amy, et al. "Making the black box more transparent: Understanding the physical implications of machine learning." *Bulletin of the American Meteorological Society* 100.11 (2019): 2175-2199.

# Visualization – Type A

We know that layers in a CNN represent increasingly complex spatial patterns, in increasing size.

But – those types of patterns tend to be more pronounced for cats and dogs than for atmospheric rivers and cold fronts, because we deal with

- Fuzzy boundaries,
- Few distinct parts, such as eyes, ears and noses.

That's why we often prefer Type B for earth science applications.  
So what's Type B?

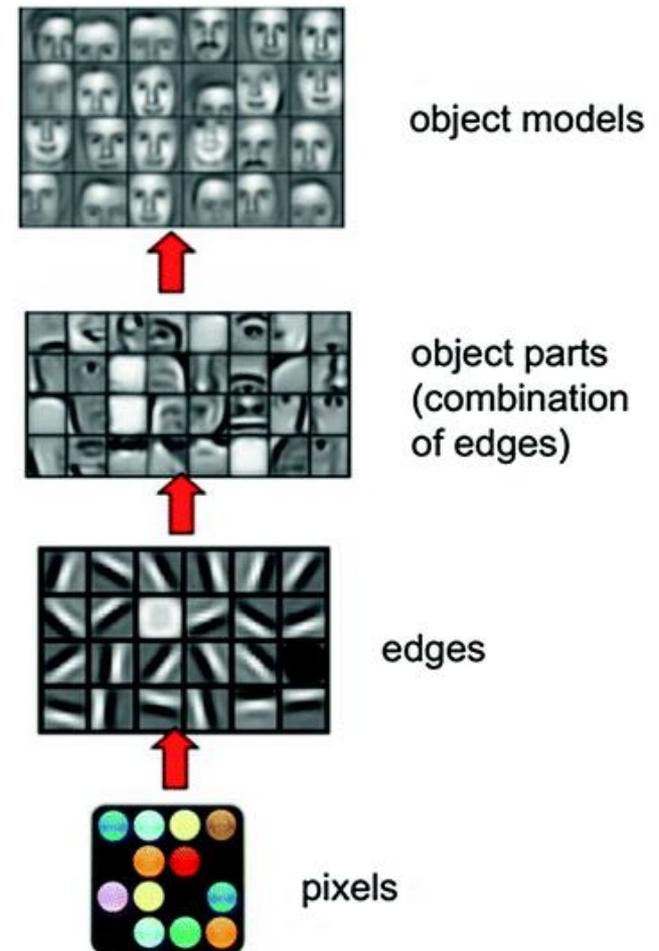
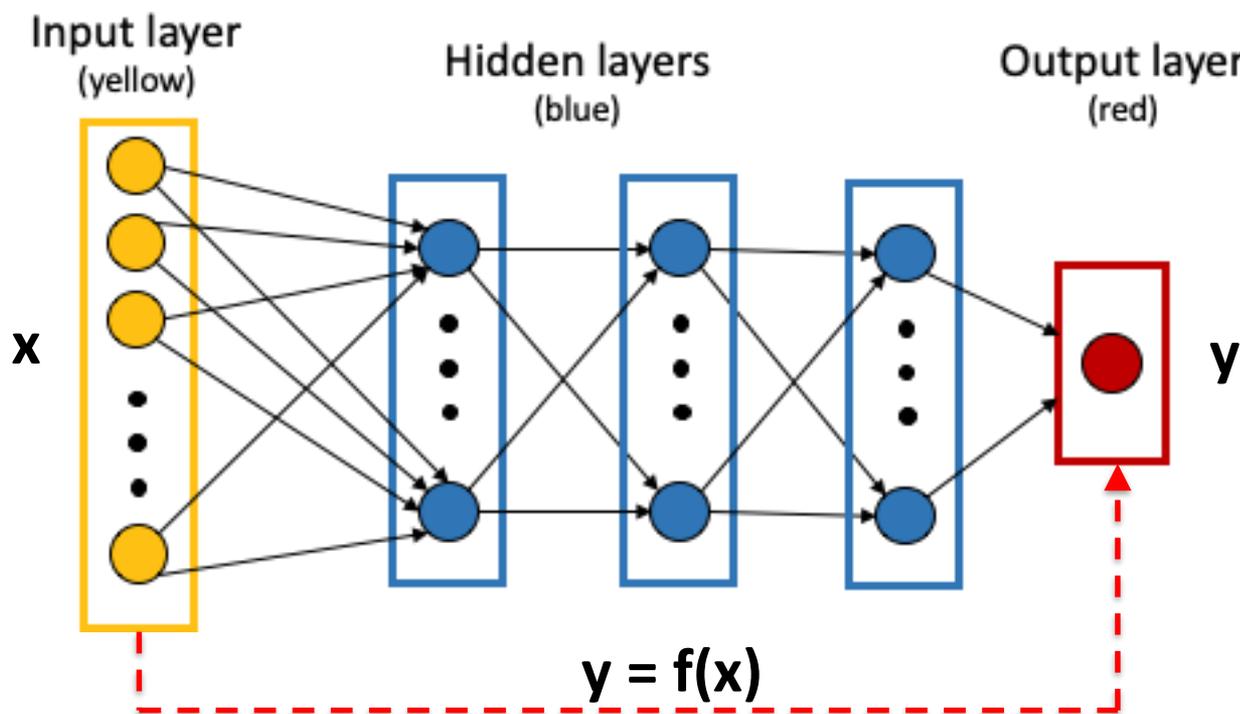


Image source: Garg, D., & Kotecha, K. (2018). Object Detection from Video Sequences Using Deep Learning: An Overview. In *Advanced Computing and Communication Technologies* (pp. 137-148).

# Type B: Attribution / Explaining Decisions

**Philosophy:** Understand the ANN's overall decision making for specific input.



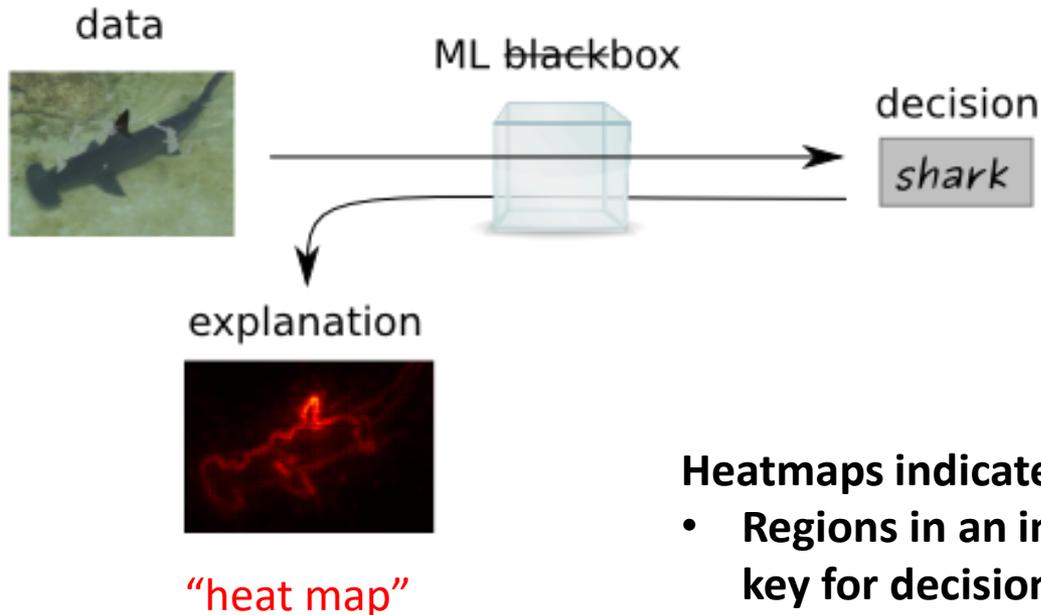
- **Seek to understand the reasoning of entire NN algorithm - for a specific input.**
- **Study overall input-output function of ANN,  $y = f(x)$ , where  $x$  = input,  $y$  = output.**
- **HERE: Do NOT worry about meaning of intermediate (blue) nodes.**

# Type B: Common Means of explanation = Heat maps (aka Attribution maps)

Example: Visualization to explain classification of a *specific image*

Question answered in this example:

*Which pixels of the input image are most important for NN to decide that this is a shark?*



**Heatmaps indicate:**

- **Regions in an input sample that are key for decision/estimate made by NN for this input.**

Source: [www.heatmapping.org](http://www.heatmapping.org).

# Heat maps / attribution maps

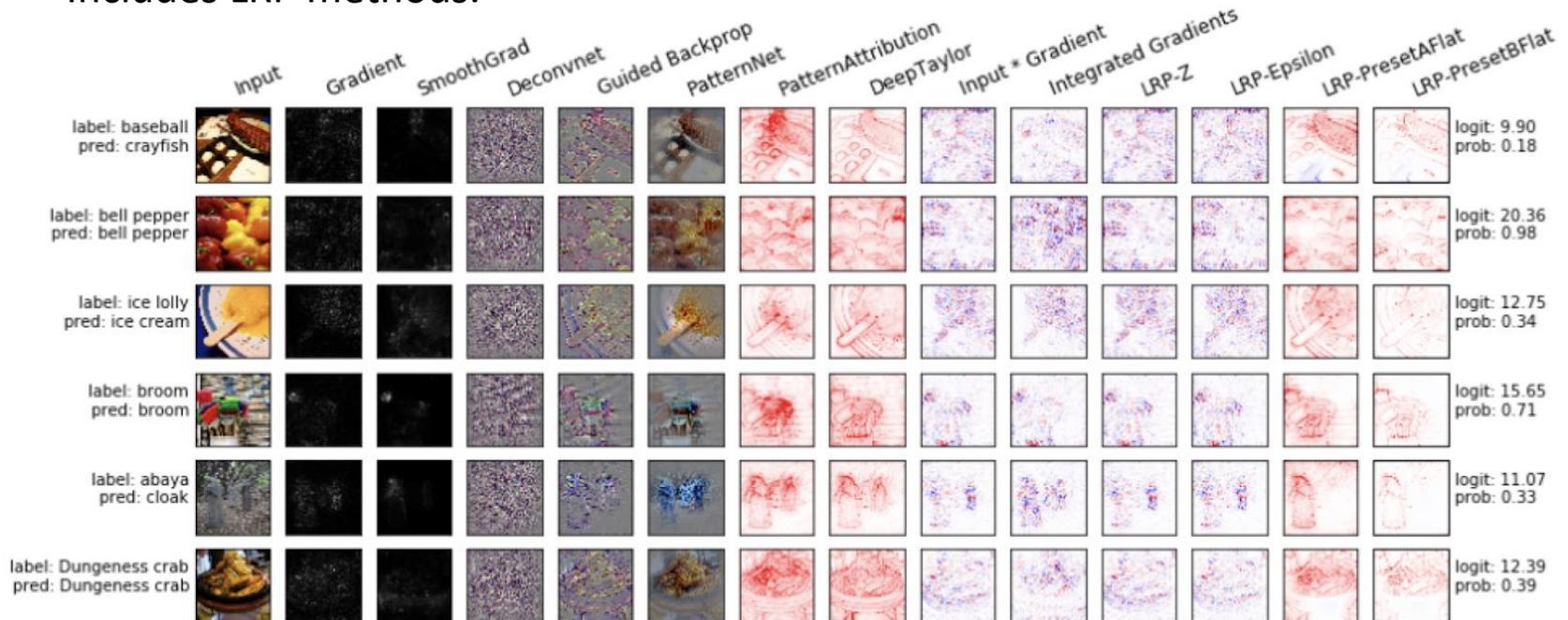
- Heat maps can be calculated with many different algorithms.
- Examples (see also Amy's talk this morning):
  - Saliency maps
  - GradCAM
  - Occlusion Sensitivity
  - Layer-Wise Relevance Propagation (LRP)
  - many others.
- New methods are being developed as we speak.
- Each type of heatmap has different interpretation.
- Each method has its pros and cons.
- Not every method works for every architecture.
- Choice depends on application and question you're trying to answer.
- The purpose of this presentation
  - Is not to promote LRP as “the best method”.
  - Is to show what visualization methods in general can do for the community
    - using LRP as an example.
- We use images as input here for illustration, but input can be anything.
- **Heatmap = overlay for all input elements – regardless of input format.**

Visualization  
toolboxes  
available!

# Visualization toolboxes

## Package 1: **iNNvestigate** (NN + investigate = iNNvestigate)

- Available at [www.heatmapping.org](http://www.heatmapping.org)
- Implementations: pytorch & TF/Keras (TF2.0 version coming soon)
- Includes LRP methods.



These are “**attribution**” methods for image classification:  
identify what the network finds important in input image for certain task

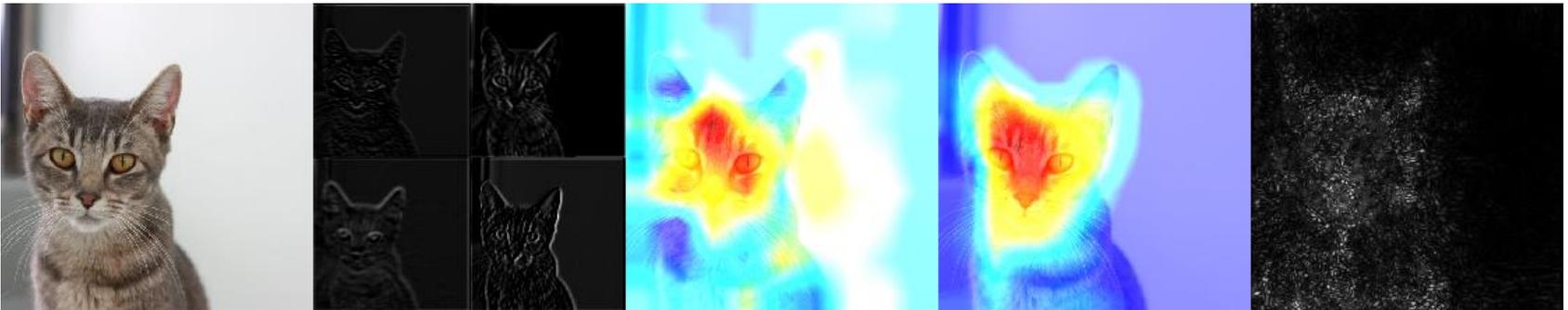
# Visualization toolboxes

## Package 2: **tf-explain**

Available at <https://tf-explain.readthedocs.io/en/latest/>.

Implementation: Tensorflow (Compatible with TF2.0!)

Sample result for network VGG16:



Input

Activation  
visualizations

Occlusion  
sensitivity

Grad CAM

SmoothGrad

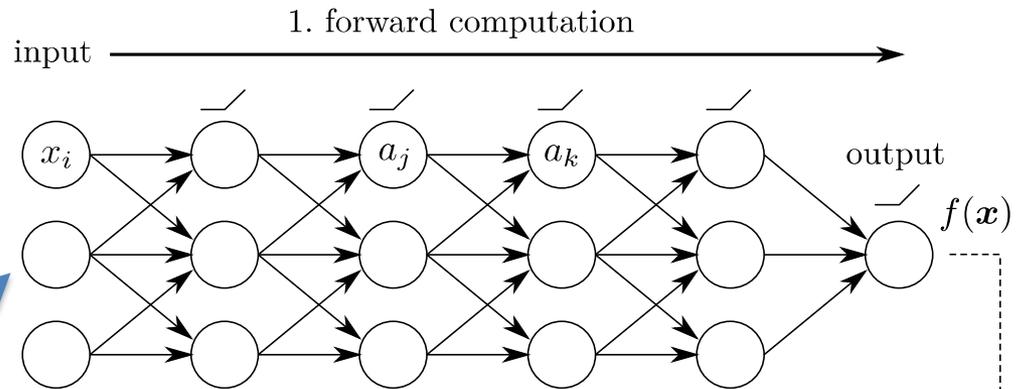
More toolboxes exist.

# Relevance propagation for LRP

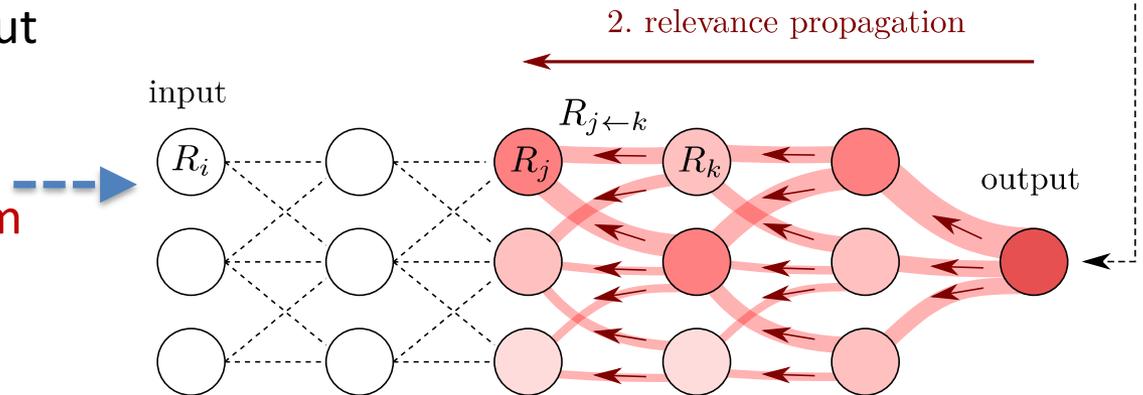
## LRP = Layer-wise Relevance Propagation

### How it works:

1. Feed in input sample.  
Regular forward pass of ANN  $\rightarrow$  calculates output



2. New backward pass to calculate relevance from layer to layer.



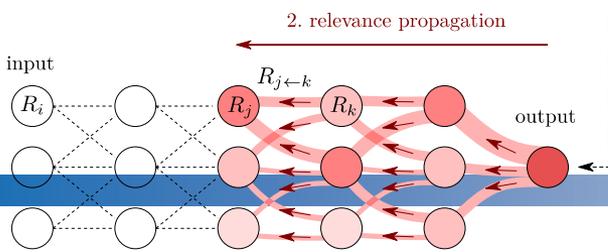
### Backward pass:

Need a new type of rule to distribute relevance.

This does *not* use the usual back propagation.

Rule: next slide – details in Montavon et al. (2018).

Image Source:  
Montavon et al. (2018)



# The $\alpha\beta$ –rule for LRP

Simplest formula for LRP backward relevance propagation (“**alpha-beta rule**”):

$$R_{i \leftarrow j}^{(l, l+1)} = R_j^{(l+1)} \cdot \left( \alpha \cdot \frac{z_{ij}^+}{z_j^+} + \beta \cdot \frac{z_{ij}^-}{z_j^-} \right)$$

$$z_{i,j} = w_{i,j} * \text{activ}_j$$

$z_{i,j}^+$  = positive part  
 $z_{i,j}^-$  = negative part  
 $z_j^+ = \sum_i z_{i,j}^+$   
 and  $\beta = 1 - \alpha$

$\alpha$  and  $\beta$  are tuning parameters:

$\alpha$  = how much positive attribution allowed

$\beta$  = how much negative attribution allowed

- $\alpha$  allows **manual control** of positive vs. negative attribution.
- Common choice:  $\alpha = 1, \beta = 0$  --> only positive attribution.
- **For details see Montavon et al. (2018).**

# Some comments on LRP

- We have found LRP to be extremely useful for many of our applications.
- How-to tips on LRP use: See Montavon et al. (2018)
- **Biggest limitation:**  
**LRP implementation only available for simple NN architectures so far, but extensions being developed as we speak.**

# Application 1

- Yoonjin Lee (ATS), Chris Kummerow (ATS) at CSU.
- Task: Detect convection from satellite images.

## Why is it important to detect convection?

- Convection releases heat.
- Determine locations of convection in satellite images → feed that info into numerical weather prediction (NWP) model in real time to improve forecast.
- This is a Data Assimilation task:  
Use current observations to adjust *weather model* in real time.
- Potentially high impact area for ML.



**Yoonjin Lee**  
Ph.D. student  
(Kummerow group)

Lee et al., 2020.



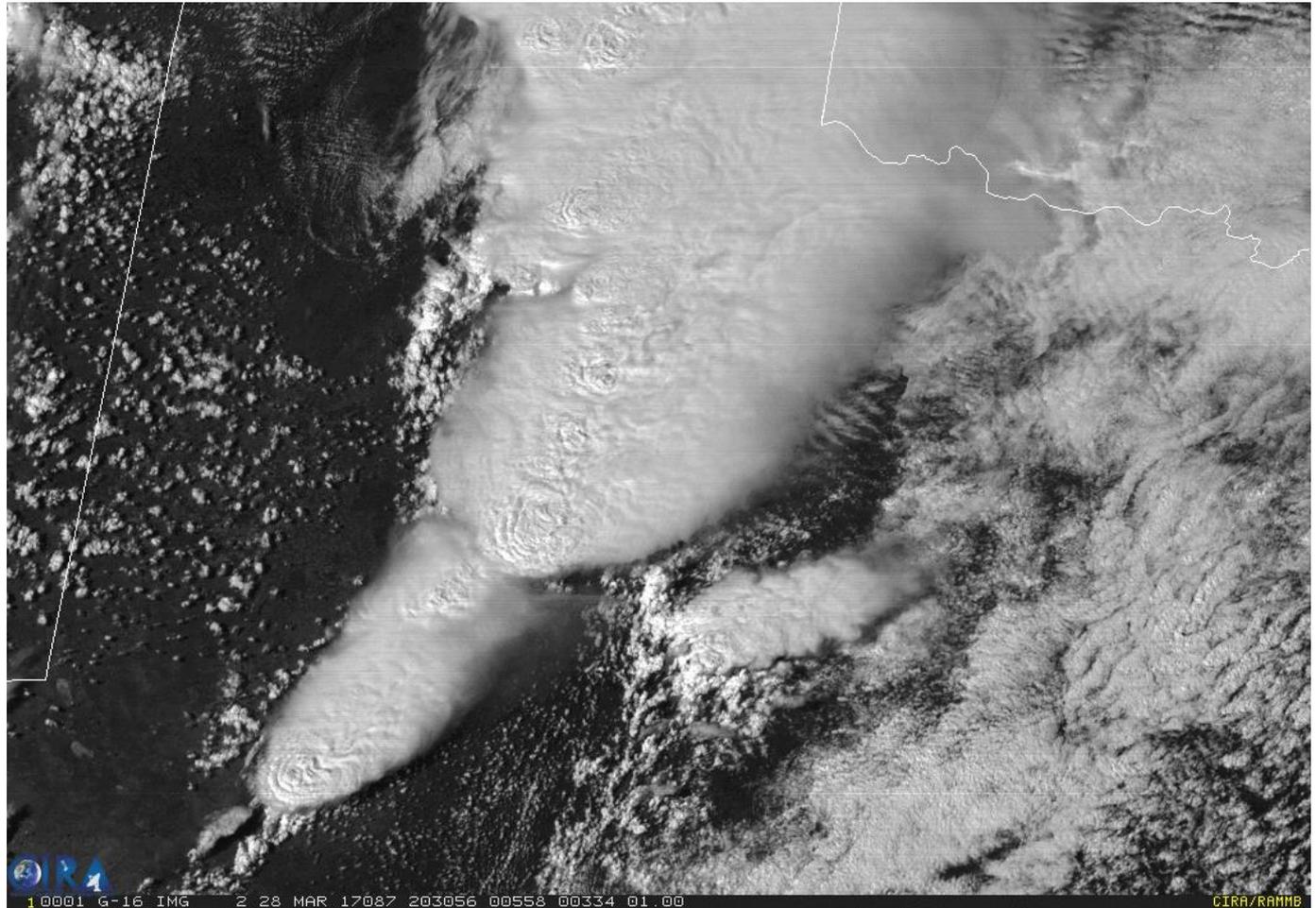
# GOES-16 band 2 imagery (30-Second, 0.5 km) West Texas – 28 Mar. 2017

Video – Courtesy  
of CIRA

Look for  
convection:  
Wherever clouds  
have high  
brightness and are  
“bubbling”.

Easy to see with  
our eyes from  
animation!

Best way to detect  
with ML?



(Animation)

# Detecting convection

## Q1: How do humans detect convection?

Look for clouds with combination of

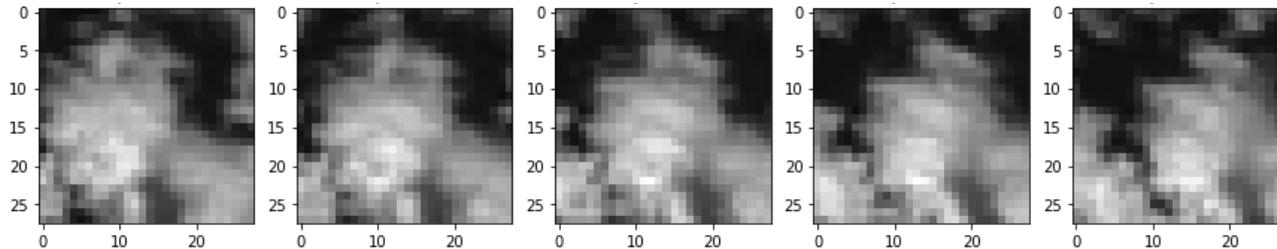
1. High brightness;
2. Texture: “bubbling”. *Especially apparent in videos.*

Next: Trained an ANN to detect convection.

## Q2: How does the ANN detect convection?

First, discuss set-up for ANN:

- **Input:** Sequence of five image patches, 2 minutes apart



- **Architecture:** CNN - Typical image classification network
- **Output:** Two output neurons representing two classes:
  - i) There is convection in image sequence
  - ii) There is no convection in image sequence.

# Q: How is ANN detecting convection?

**We hope to answer the following questions:**

1. Is our ANN paying attention to all the clues we know are important? If not, there's probably room for improvement.
2. Is our ANN using faulty reasoning? Example: using correlation present in data, but not representative of real world.
3. In short, **do we agree with the strategies used by the ANN?**

**Method used: Layer-wise relevance propagation (LRP)**

Step 1: Train the ANN.

Step 2: Freeze the ANN → Weights and biases are now fixed.

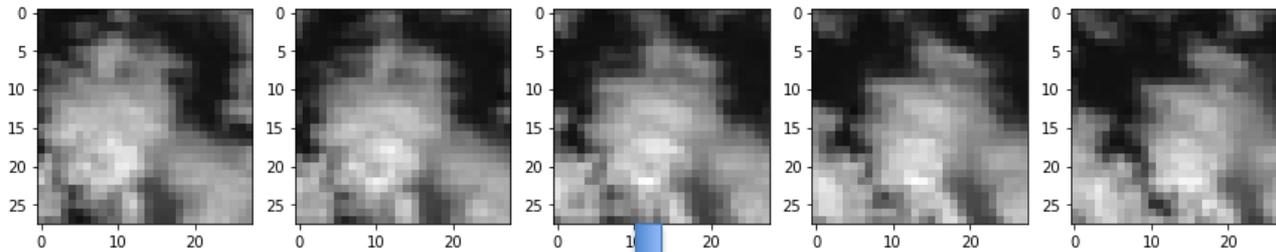
Step 3: Feed specific input sample into ANN to get ANN output.

Step 4: Apply LRP analysis for this specific sample.

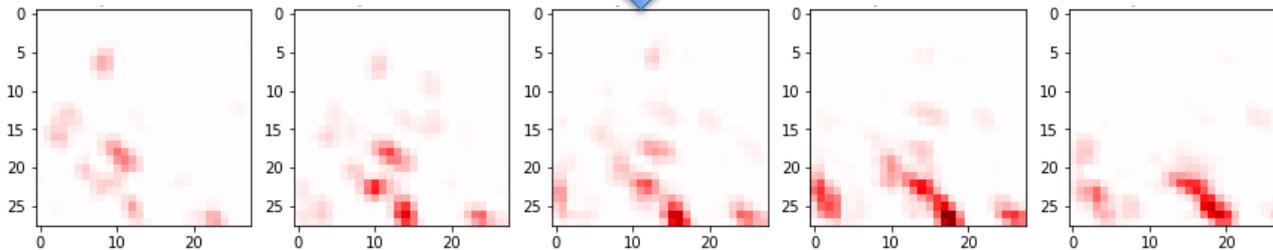
→ tells us **which part/area** of input sample is important for this ANN output.

# LRP result for our “convection ANN”

Input:  
Sequence of  
five images



Apply LRP → Where is ANN looking?



Visual analysis of heatmaps by domain expert tells us:

This ANN looks primarily for high brightness, does *not* focus on texture!

→ Lesson: ANN not using all information, missing texture signal. Sub-optimal.

→ Explore methods that force ANN to focus on texture, too.

→ Ex.: Pre-train on samples that mainly have texture signal;

reformulate as segmentation task - to give ANN *feedback* on where to look.

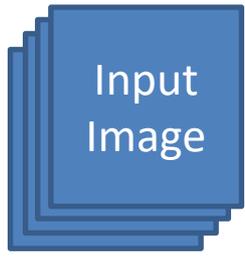
Key point: Visualization tools → We can “see” better what’s working well / badly.

→ Brings ANN reasoning back to space of physics and expert knowledge!

# Application 2: Generating synthetic radar images from GOES imagery

Input: GOES Channels C07, C09, C13, GLM. Output: MRMS (radar).

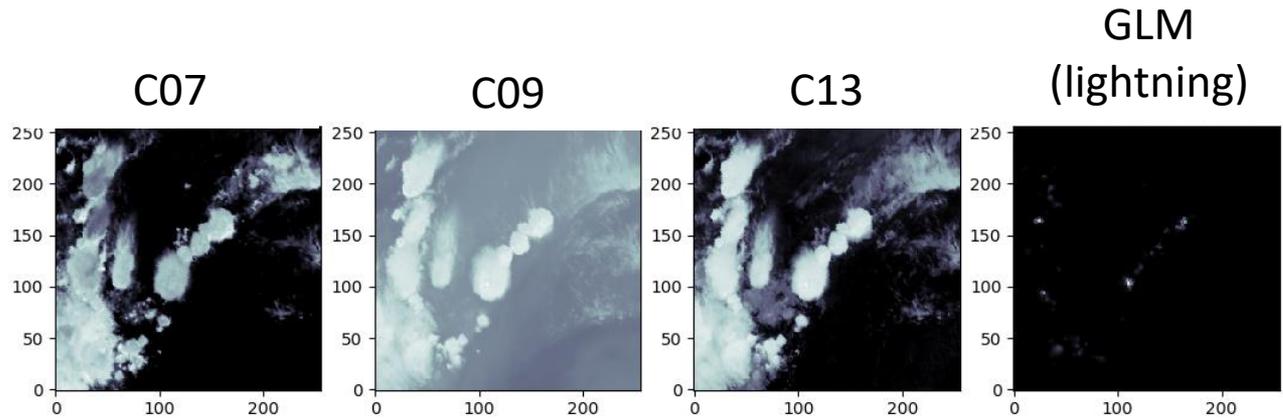
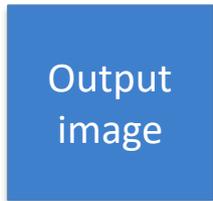
Input:



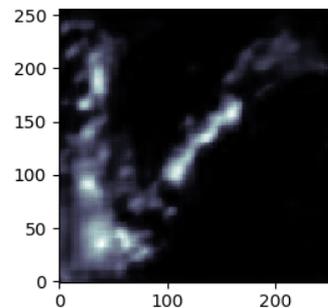
4 channels

NN

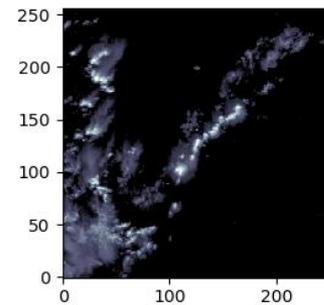
Output:



MRMS - estimate



MRMS - observed



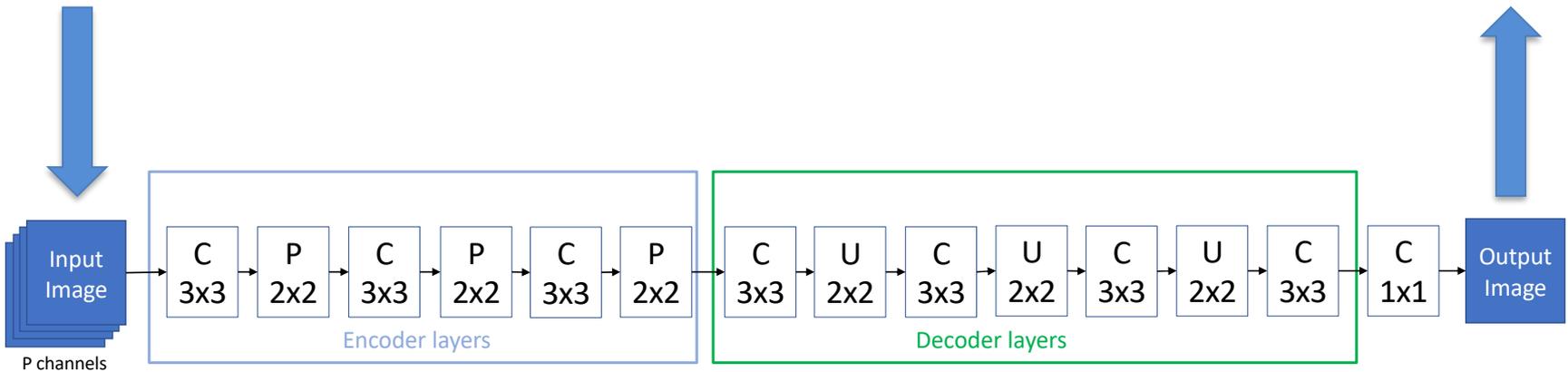
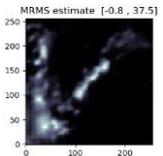
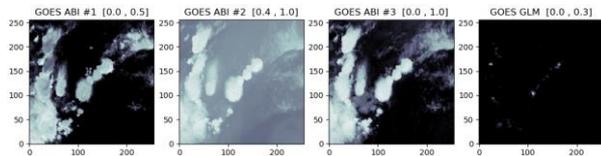
Kyle Hilburn

*Motivation: GOES imagery is available in all of CONUS, but MRMS is not.*

# Application 2 – NN architecture

Input: GOES channels

Output: MRMS estimate



C = convolution layer

P = pooling layer (downsampling)

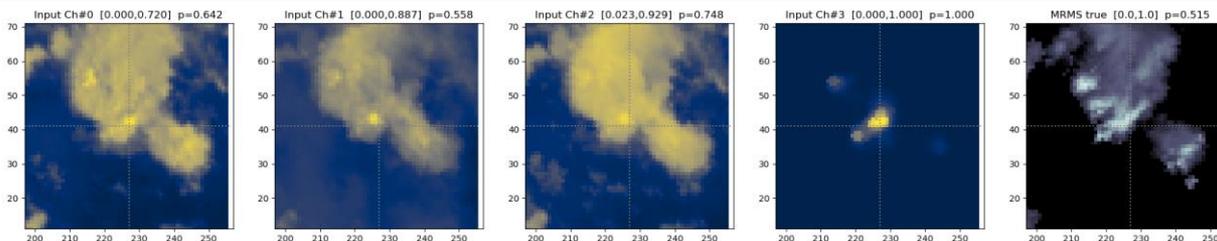
U = upsampling

Numbers: size of filters/masks

Question: How does NN know when to create large MRMS estimates?

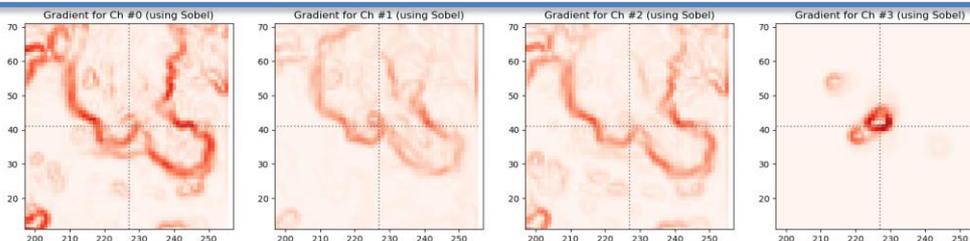
Method: Select examples where MRMS estimate is high. Where is NN looking (LRP)?

Inputs:

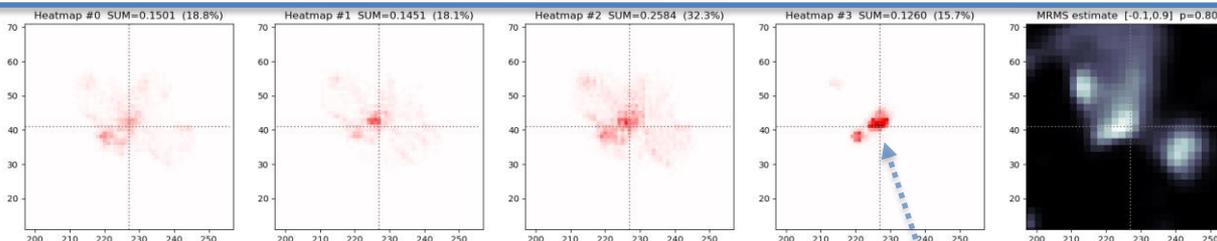


MRMS truth

Gradient of inputs:

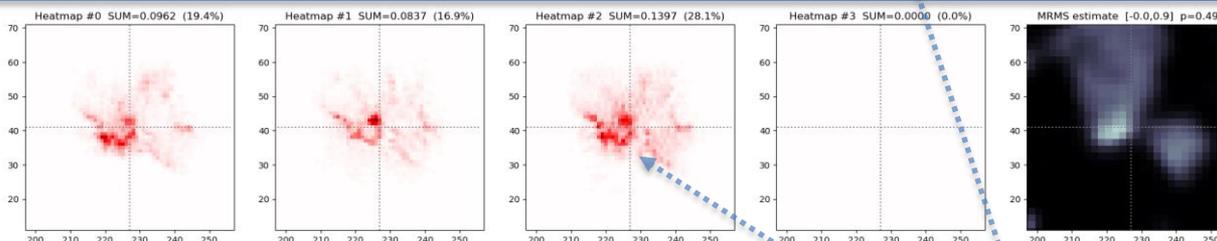


LRP for one output pixel



MRMS est.

LRP if GLM signal erased



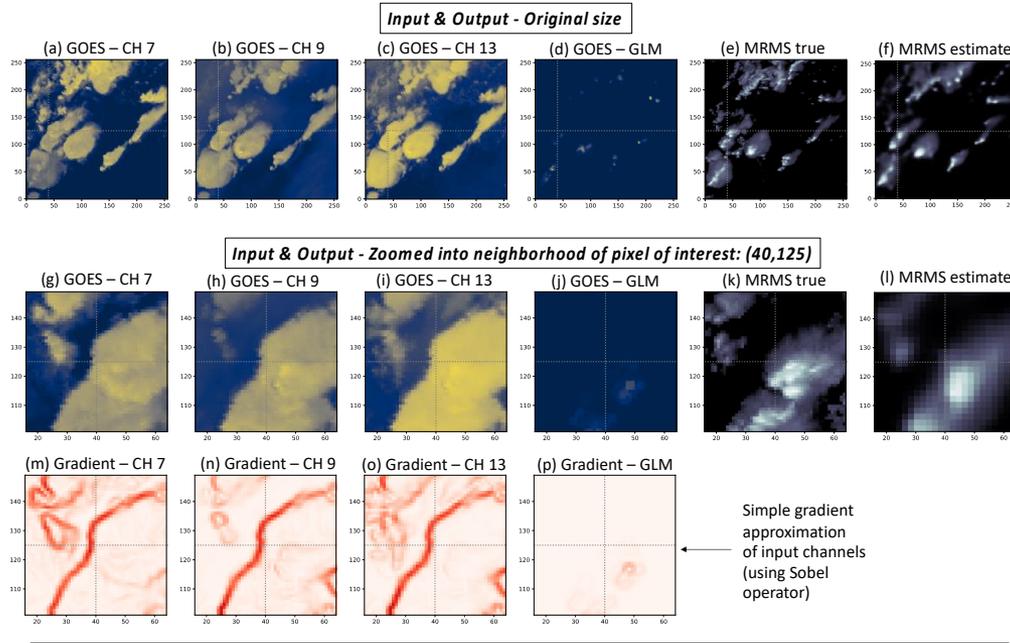
MRMS est.

LRP yields 2 strategies for creating large MRMS estimates:

Strategy 1: Presence of lightning triggers high MRMS values. **Lightning** = strongest trigger.

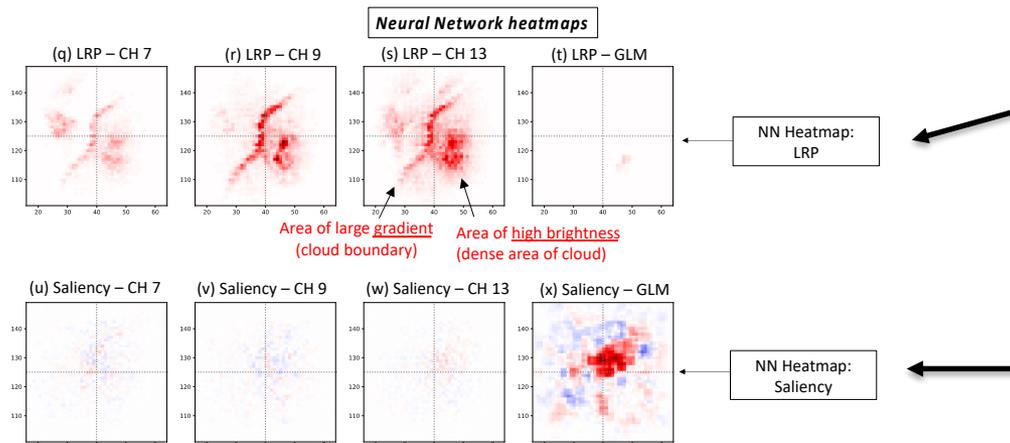
Strategy 2: In no lightning NN focuses on locations with strong gradients: **cloud boundaries**.

# LRP vs. Saliency heatmaps



REFs:

- Hilburn et al. (2020)
- Ebert-Uphoff and Hilburn (2020)



**LRP found 3<sup>rd</sup> strategy:**  
**Strategy #3: Extremely dense areas of clouds trigger high MRMS values.**

**Saliency method:**  
 Only identified one strategy (lightning) – and not even concisely.

# Application 3: XAI for Science Discovery

Use LRP and other tools to *discover new science*.

## Example:

**Find indicator patterns of climate change:**

What are the **spatial patterns** (in temp or precip) most indicative of climate change?

**Why use AI for this purpose?**

- 1) Great at picking up and utilizing spatial patterns.
- 2) Can use visualization tools to look at those patterns.

## References (XAI for science discovery):

Toms, B. A., Barnes, E. A., & Ebert-Uphoff, I. Physically Interpretable Neural Networks for the Geosciences: Applications to Earth System Variability, 2020 ([preprint](#)).

Barnes, E. A., Hurrell, J. W., Ebert-Uphoff, I., Anderson, C., & Anderson, D., [Viewing forced climate patterns through an AI Lens](#). Geophysical Research Letters, 2019.

Barnes, E. A., Toms, B., Hurrell, J. W., Ebert-Uphoff, I., Anderson, C., & Anderson, D. **Indicator patterns of forced change learned by an artificial neural network**, 2020 ([preprint](#)).



Ben Toms



Elizabeth Barnes

# Last topic: Receptive Fields in CNNs

We know that layers in a CNN represent increasingly complex spatial patterns, in increasing size.

For many earth science applications it's hard to identify such specific patterns (b/c of fuzzy boundaries, no ears/eyes/etc.).

- But what about size of features?
- Can we say something about the **size of meteorological features that each layer can recognize?**
- Yes!
- That's called the receptive field!

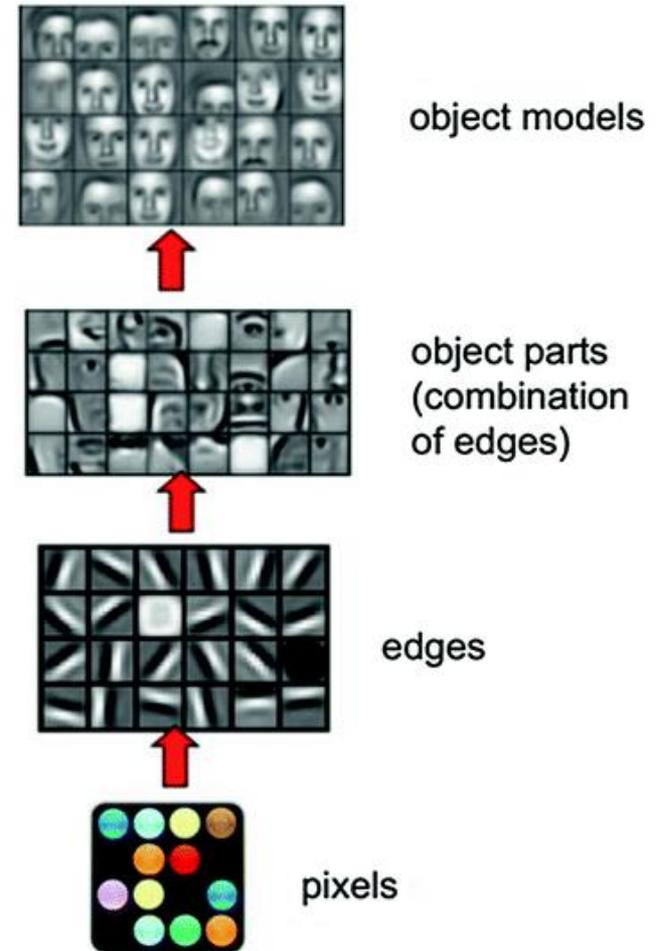
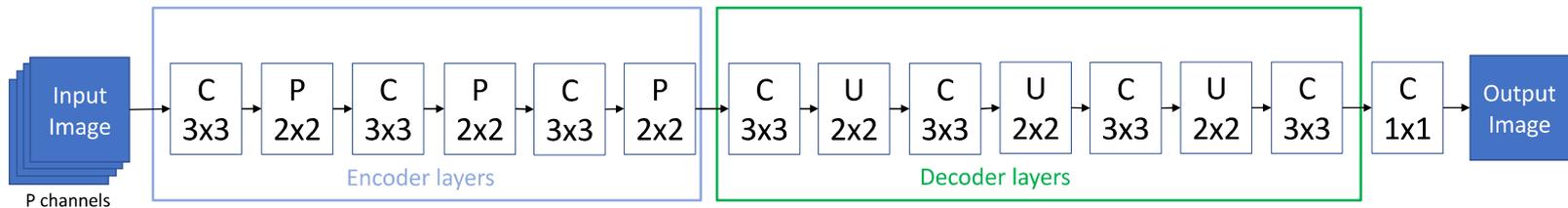


Image source: Garg, D., & Kotecha, K. (2018). Object Detection from Video Sequences Using Deep Learning: An Overview. In *Advanced Computing and Communication Technologies* (pp. 137-148).

# Last topic: Receptive Fields in CNNs

Consider a “purely convolutional” NN:

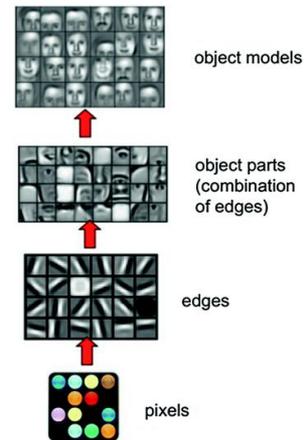
- Layer types: convolution, pooling, upsampling
- No fully-connected (dense) layers allowed.



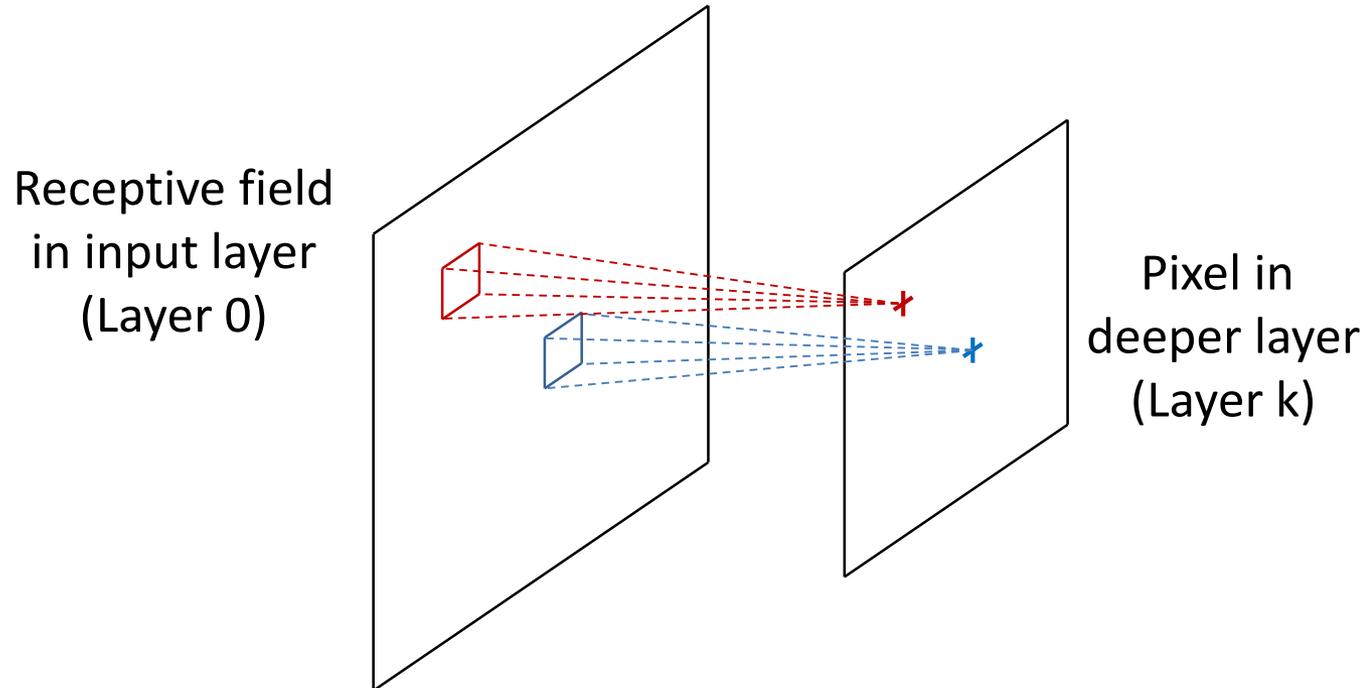
**Question: How big exactly is spatial context at each layer of this NN?**

**Answer: Determine “receptive field (RF)” of each layer.**

**Then: Can roughly match those RF sizes to size of meteorological phenomena we want to detect → architecture starting point.**



# Receptive Field (RF)



## Receptive field of Layer k:

1. Consider a single pixel in Layer k (**red cross**).
2. Determine the **smallest box size in input layer (red box)** that **contains all pixels connected in the NN to that pixel in Layer k**.

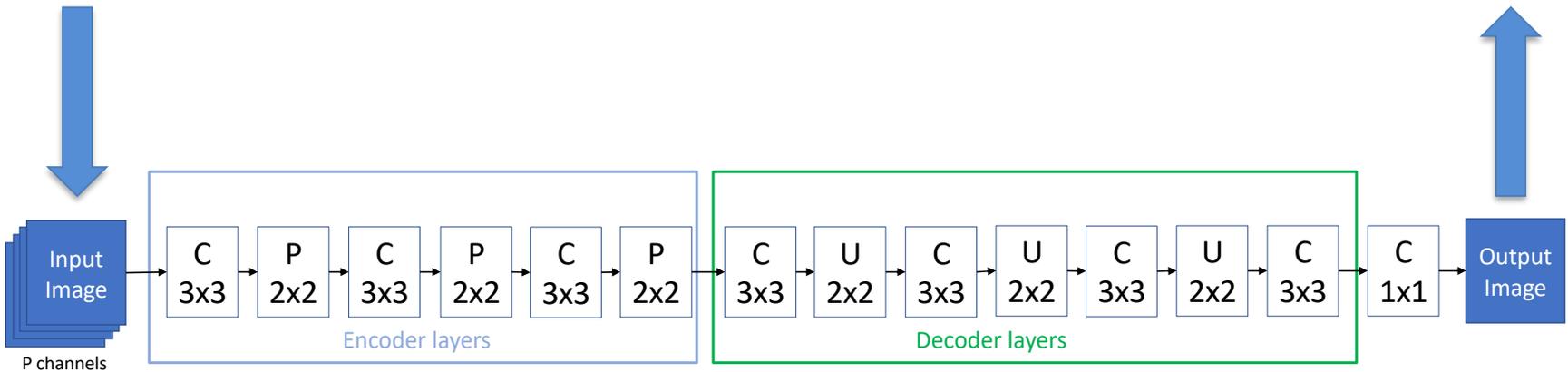
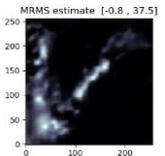
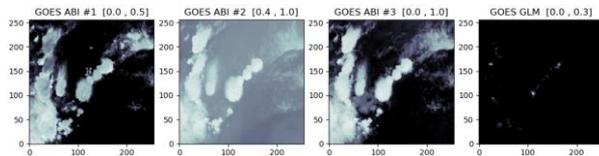
→ RF = Which pixels in input image can affect the pixel (**red cross**) in Layer k?

→ RF = Max size of any spatial pattern in original input that Layer k can recognize.

# RF for Application 2

Input: GOES channels

Output: MRMS estimate



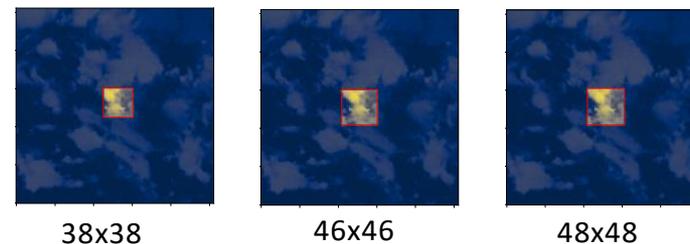
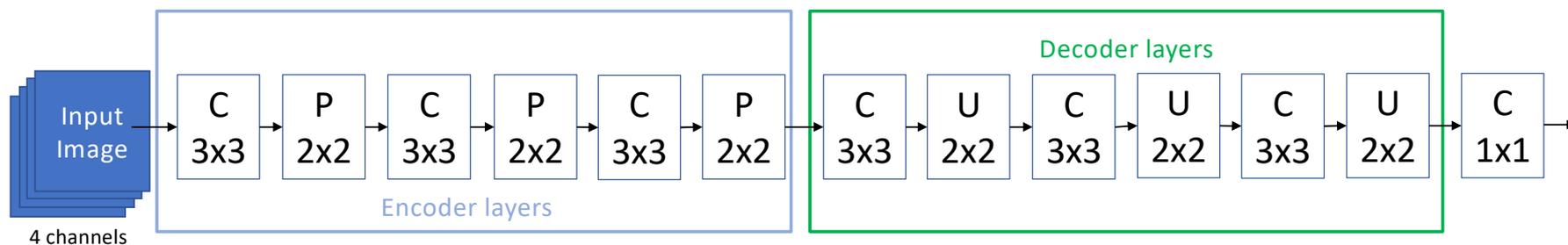
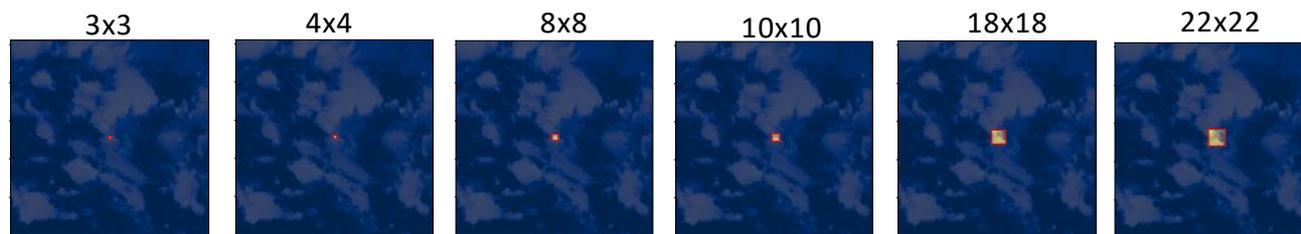
C = convolution layer

P = pooling layer (downsampling)

U = upsampling

Numbers = size of filters/masks

# Visualization of Theoretical Receptive Field (TRF)

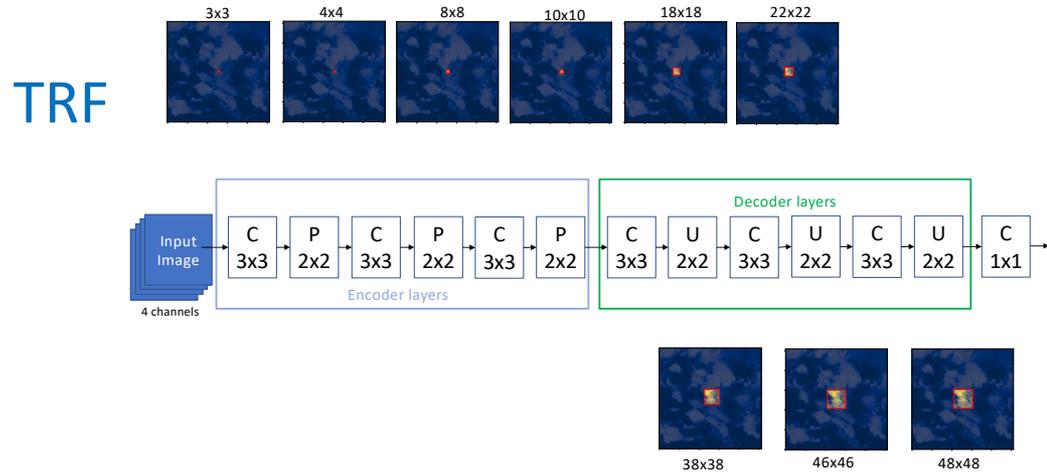


- Input image: 256x256 pixels
- Red box = size of spatial context at each layer
- TRF grows to 48x48 pixels.
- TRF = max spatial context of layer.

# Effective Receptive Field (ERF)

## Theoretical receptive field (TRF):

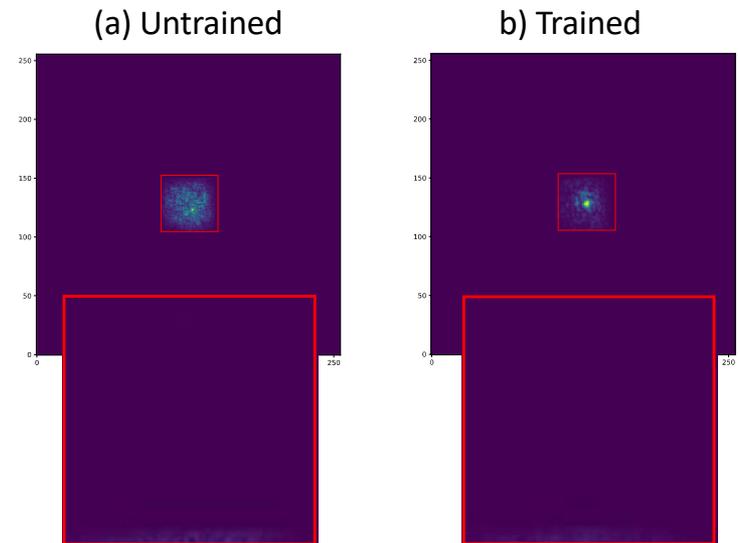
- Provides max bounding box
- But impact is not uniform within box.



## → Effective receptive field (ERF)

- Roughly Gaussian distribution
- Changes during training (see image on right).
- Here: getting more focused.

## ERF

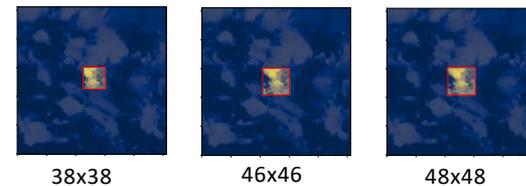
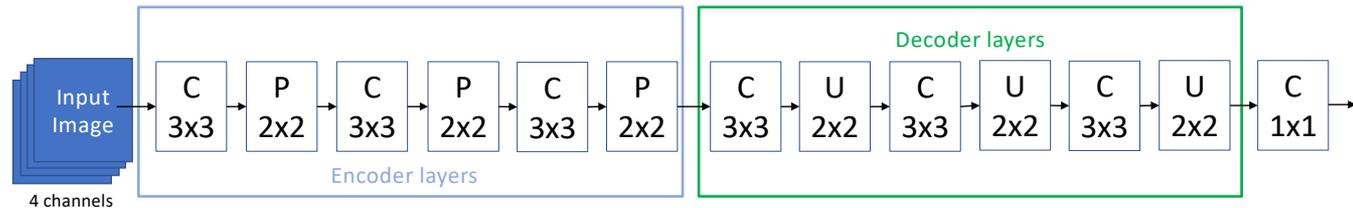
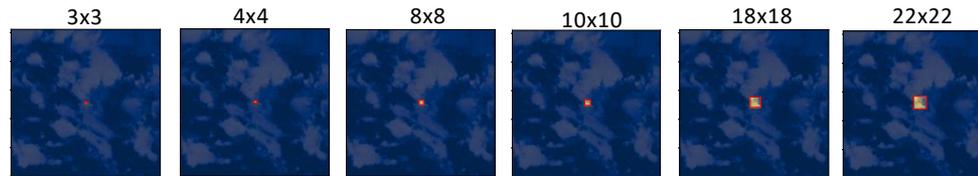


# Effective Receptive Field (ERF)

Theoretical receptive field (TRF):

- Provides max bounding box
- Impact is not uniform within box.

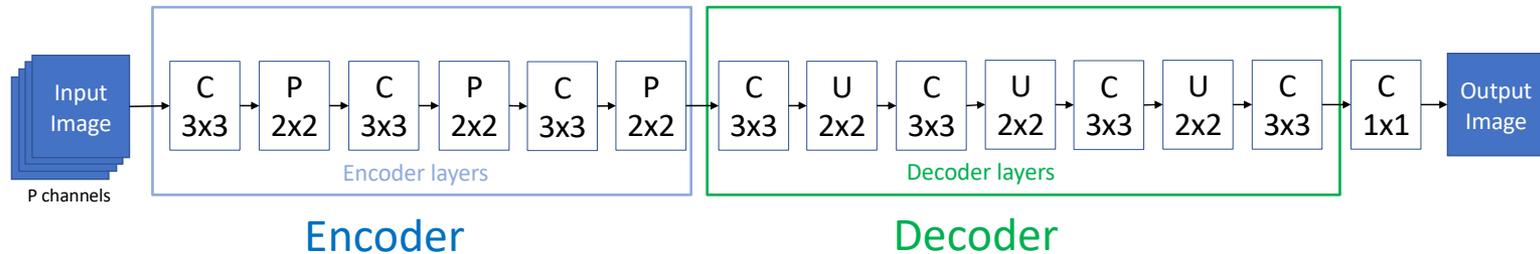
TRF



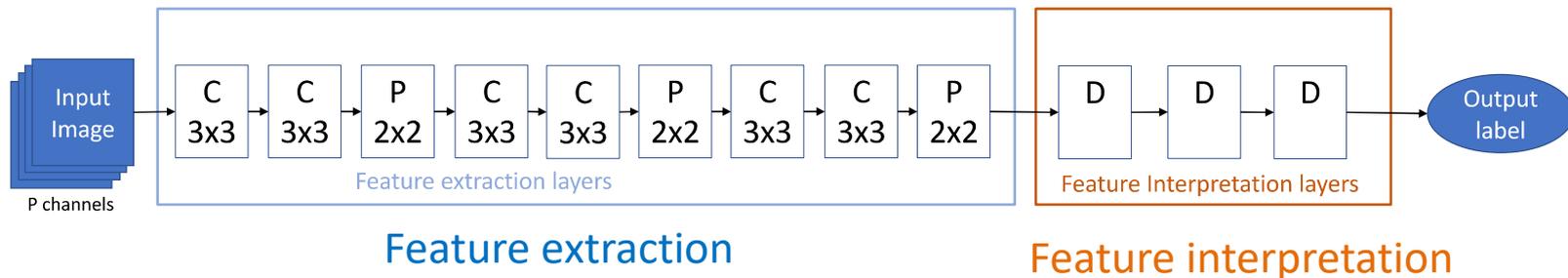
**Key lesson:** Always makes sure your theoretical receptive field (TRF) is big enough to capture meteorological features.

# Receptive field when there are dense layers

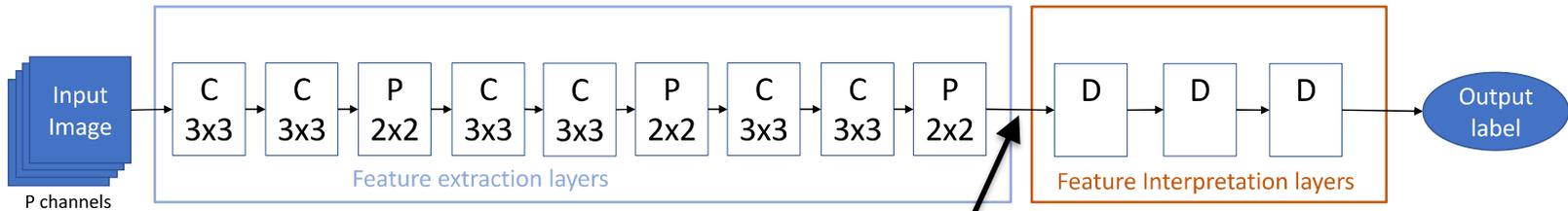
Architecture we just looked at (no dense layer):



Typical architecture for image classification (dense layers at end):



# Architecture for classification



## Function:

- This block has same function as encoder layer in image translation!
- Extract features from image.

## Function:

- Interpret presence of detected features.
- Assign corresponding output label.

What about receptive field?

- **Apply at output layer of blue block:**  
**Provides size of features that can be detected in input space.**  
Rest of the network just *interprets* those features.

Once you reach a dense layer:

- Receptive field = entire input space.
- So analyze feature size before first dense layer instead (as indicated above).

# NN Interpretation – Final Thoughts

## Gaining insights into an NN is

- An **iterative, scientist-driven discovery process**,
- Driven by old fashioned methods of experimental design, and hypothesis generation and testing,
- **NN visualization tools simply provide additional tools to *assist* this process** (but they are not driving this process).

So far there is no such thing as an automated, one-size fits-all visualization method. And there *might* never be.

→ Earth scientist always remains crucial in the entire process.

# ANNs are not a black box anymore

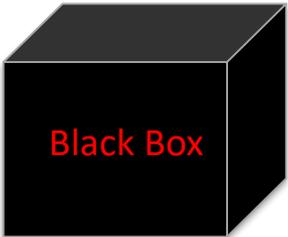
## How much can visualization help?



Put backpack into  
X ray scanner



Inside  
view



Put box  
into tool

Tools for visualization +  
interpretation of ML methods

Inside  
view

Box getting  
more  
transparent

Not perfect, but better  
than a black box.

# Thank you!

Remaining slides contain links to toolboxes and lots of REFs sorted by topic.

## Questions?



# Some Available software

- **“Keras explanation toolbox” - aka “iNNvestigate neural networks”**
  - What: LRP and other methods
  - For: Keras with Tensorflow backend
  - Level of development support: high
  - Where: [www.Heatmapping.org](http://www.Heatmapping.org)
- **“LRP toolbox”**
  - What: LRP only
  - For: Tensorflow
  - Level of development support: decreasing
  - Where: [www.Heatmapping.org](http://www.Heatmapping.org)
- **“LUCID”**
  - What: Lots of feature visualization methods. Implements method discussed by Olah et al. (2017)
  - For: Tensorflow
  - Where: <https://github.com/tensorflow/lucid>

Some additional REFs  
are in presentation.

# References

**Seminal article** - written for climate/weather community:

McGovern A, Lagerquist R, Gagne DJ, Jergensen GE, Elmore KL, Homeyer CR, Smith T. , **Making the black box more transparent: Understanding the physical implications of machine learning.** *Bulletin of the American Meteorological Society.* **Aug 22, 2019.**

<https://journals.ametsoc.org/doi/abs/10.1175/BAMS-D-18-0195.1>

**Provides:**

**Overview of general ML interpretation/visualization methods.**

**Specifically for ANNs:**

- Saliency maps (discussed below)
- Backwards Optimization (discussed below)
- Gradient-weighted Class-activation Maps
- Novelty Detection

**Demonstration for applications:**

- Storm-mode, precipitation type, tornado prediction, and hail prediction.

# References

## **Description of LRP and its use for Application #2 of this presentation:**

Ebert-Uphoff, I., & Hilburn, K. A. Evaluation, **Tuning and Interpretation of Neural Networks for Meteorological Applications**. Submitted to BAMS (in review), 2020. (arXiv preprint [here](#)).

Hilburn, K. A., Ebert-Uphoff, I., and Miller, S. D., **Development and Interpretation of a Neural Network-Based Synthetic Radar Reflectivity Estimator Using GOES-R Satellite Observations**.

Submitted to Journal of Applied Meteorology and Climatology (in review), 2020. (arXiv preprint: [here](#))

## **Application #1 of this presentation (with a bit of LRP):**

Lee, Y., Kummerow, C.D, Ebert-Uphoff, I., **Applying Machine Learning Methods to Detect Convection Using GOES-16 ABI Data** (in preparation), 2020.

# References

## Using visualization for Science Discovery in earth science (Application #3):

Toms, B. A., Barnes, E. A., & Ebert-Uphoff, I. **Physically Interpretable Neural Networks for the Geosciences: Applications to Earth System Variability.** Submitted to Journal of Advances in Modeling Earth Systems (JAMES) (in review). (arXiv preprint: [here](#))

Barnes, E. A., Hurrell, J. W., Ebert-Uphoff, I., Anderson, C., & Anderson, D., [Viewing forced climate patterns through an AI Lens](#). Geophysical Research Letters, 46(22), 13389-13398, <https://doi.org/10.1029/2019GL084944>, Nov 2019.

Barnes, E. A., Toms, B., Hurrell, J. W., Ebert-Uphoff, I., Anderson, C., & Anderson, D. **Indicator patterns of forced change learned by an artificial neural network.** Submitted to Journal of Advances in Modeling Earth Systems (JAMES), in review. (arXiv preprint [here](#)).

# References

## **Recent tutorial on XAI** - *not* specific to climate/weather:

Interpretable Machine Learning for Computer Vision

½ day tutorial at CVPR 2020, June 15, 2020.

All four lectures available as videos: <https://interpretablevision.github.io/>

## **Recent book on Explainable AI (XAI)** - *not* specific to climate/weather:

Samek, W., Montavon, G., Vedaldi, A., Hansen, L.K., Muller, K.-R.,

**Explainable AI: Interpreting, Explaining and Visualizing Deep Learning.**

Springer Nature, **Aug 30, 2019.**

[https://www.springer.com/gp/book/9783030289539.](https://www.springer.com/gp/book/9783030289539)

### **Provides:**

- General overview of interpretation and visualization methods.
- Primarily for ANNs.
- 439 pages.

# References

## Feature visualization (Type A):

### Olah et al. (2017)

Olah, C., et al. “Feature Visualization.” *Distill*, distill.pub, 2017, <https://distill.pub/2017/feature-visualization/>.

### Olah et al. (2018)

Olah, C., et al. “The Building Blocks of Interpretability.” *Distill*, distill.pub, 2018, <https://distill.pub/2018/building-blocks/>.

Tutorial by C. Olah (video lecture):

CVPR 2020 Tutorial on Interpretable Machine Learning for Computer Vision  
June 15, 2020. See <https://interpretablevision.github.io/>

See Lecture #4: Christopher Olah, **Introduction to Circuits in CNNs.**

# References

## Deep Taylor / LRP:

### **Montavon et al. (2015)**

Montavon, Grégoire, et al. “Explaining NonLinear Classification Decisions with Deep Taylor Decomposition.” *arXiv [cs.LG]*, 8 Dec. 2015, <http://arxiv.org/abs/1512.02479>. arXiv. **(Earlier version of 2017 paper. Supplement has proves of Deep Taylor statements.)**

### **Montavon et al. (2017)**

Montavon, Grégoire, et al. “Explaining Nonlinear Classification Decisions with Deep Taylor Decomposition.” *Pattern Recognition*, vol. 65, May 2017, pp. 211–22, doi:10.1016/j.patcog.2016.11.008.

**(Emphasis on Deep Taylor)**

### **Montavon et al. (2018)**

Montavon, Grégoire, et al. “Methods for Interpreting and Understanding Deep Neural Networks.” *Digital Signal Processing*, vol. 73, Feb. 2018, pp. 1–15, doi:10.1016/j.dsp.2017.10.011.

**(Deep Taylor + LRP)**

# References

## LRP original:

### **Bach et al. (2015)**

Bach, Sebastian, et al. "On Pixel-Wise Explanations for Non-Linear Classifier Decisions by Layer-Wise Relevance Propagation." *PLoS One*, vol. 10, no. 7, July 2015, p. e0130140, doi:10.1371/journal.pone.0130140.

**(LRP original paper. Main LRP formula is Eq. (60).)**

## LRP + t-SNE:

### **Lapuschkin et al. (2019)**

Lapuschkin, S., Wäldchen, S., Binder, A., Montavon, G., Samek, W., & Müller, K. R. (2019). Unmasking Clever Hans predictors and assessing what machines really learn. *Nature communications*, 10(1), 1096.