# Understanding DNNs

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- Introduction
- Geometrical Study [with Modar]
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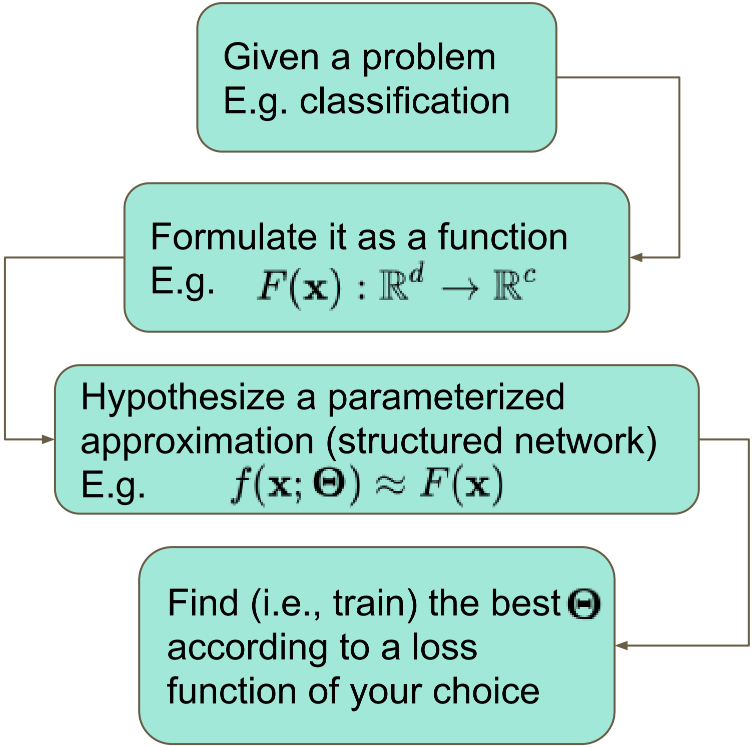
- References

# Introduction

- Standard Workflow Pipeline in Deep Learning
- Training DNNs Using Gradient Descent
- Universal Approximation Theorem
- Deeper vs. Wider Argument

# Standard Workflow Pipeline in Deep Learning




- The input has some distribution i.e., $\mathbf{x} \sim \mu$ (e.g., natural images)
- A **good enough** parameterized model should approximate the original function for most samples in the domain
- Most DNNs are constructed as a **hierarchy of layers**
- **Each layer** is a small parameterized function that might be followed by an activation function (e.g., ReLU or Sigmoid)

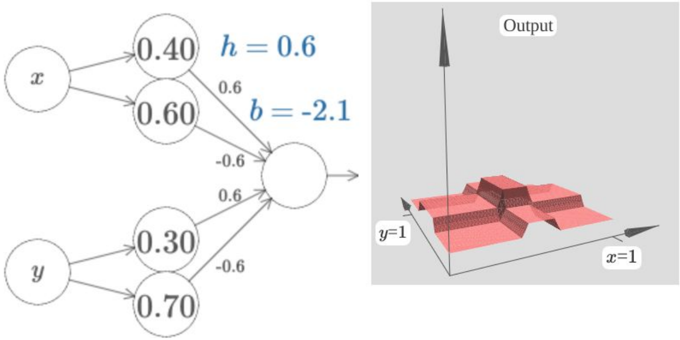
# Training DNNs Using Gradient Descent

1. Start with initial parameters $\mathbf{\Theta}_0$ and learning rate $\alpha$
2. Let $k \leftarrow 0$
3. Compute the loss of all the training data $\delta(\mathbf{X}, \mathbf{y}; \mathbf{\Theta}_k)$
4. Compute the partial subgradients of all the parameters $\frac{\partial}{\partial \mathbf{\Theta}_k} \delta(\mathbf{X}, \mathbf{y}; \mathbf{\Theta}_k)$
5. Backpropagate to all the parameters $\mathbf{\Theta}_{k+1} \leftarrow \mathbf{\Theta}_k - \alpha \frac{\partial}{\partial \mathbf{\Theta}_k} \delta(\mathbf{X}, \mathbf{y}; \mathbf{\Theta}_k)$
6. Let $k \leftarrow k + 1$
7. Change the learning rate if desired
8. Repeat steps 3-7 until some stopping criteria

**Linearization:** $f(\mathbf{x}) \approx f(\mathbf{a}) + \nabla f(\mathbf{a})^T (\mathbf{x} - \mathbf{a})$
Linearize the loss around the parameters $\delta(\mathbf{X}, \mathbf{y}; \mathbf{\Omega}_k) \approx \delta(\mathbf{X}, \mathbf{y}; \mathbf{\Theta}_k) + \frac{\partial}{\partial \mathbf{\Theta}_k} \delta(\mathbf{X}, \mathbf{y}; \mathbf{\Theta}_k)^T (\mathbf{\Omega}_k - \mathbf{\Theta}_k)$
Then, move opposite to the gradient to decrease the loss

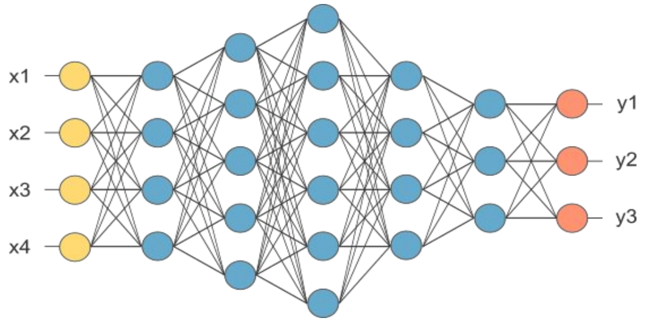
# Universal Approximation Theorem

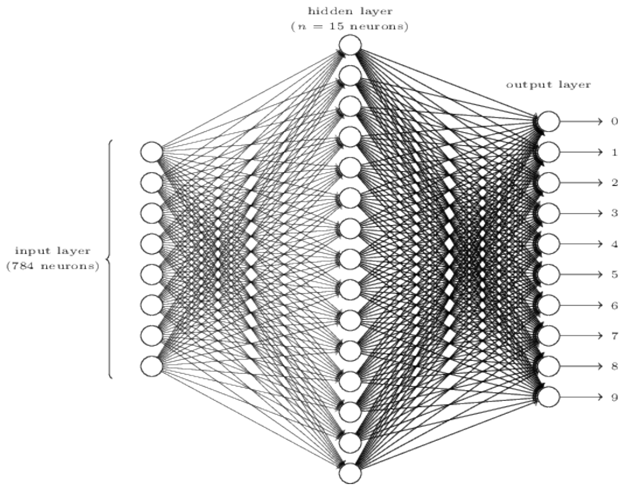
- Any arbitrary continuous function can be **approximated** effectively using a feed-forward neural network (i.e., a multilayer perceptron) with a single hidden layer, under mild assumptions on the activation function [1].
- A visual and interactive proof to this theorem is presented in [2,3].



# Deeper vs. Wider Argument

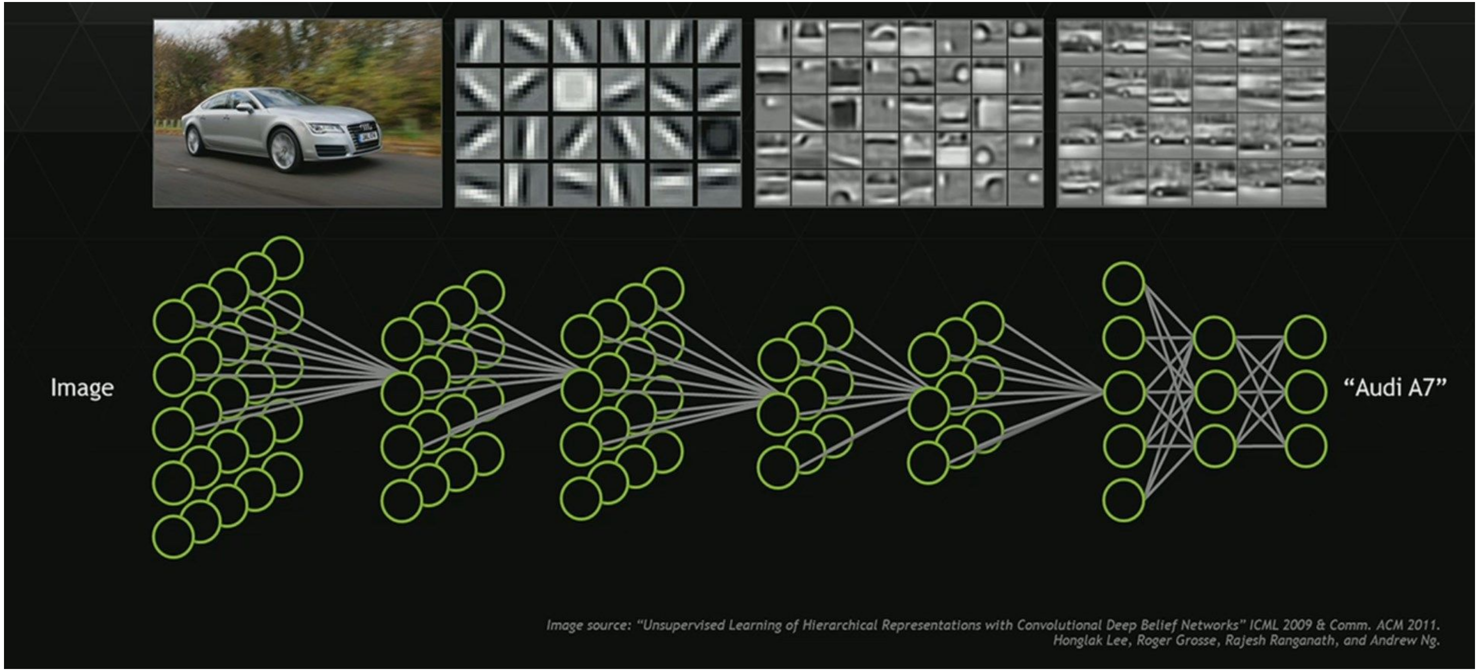
- Is it better to go deeper or wider? [4]
  - **Training difficulty** (e.g., vanishing gradients)
  - **Deployment restrictions** (e.g. high input dimensionality)
- Try different structures with Tensorflow Playground [here]



# Deeper vs. Wider Argument

Example of high dimensional input and proposed solution (CNNs)

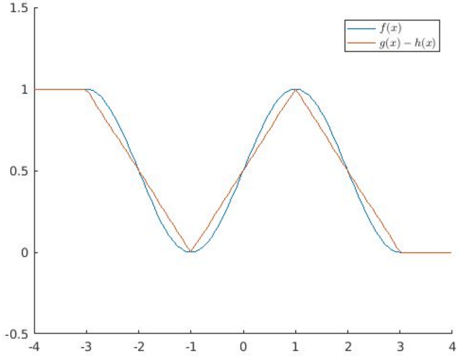


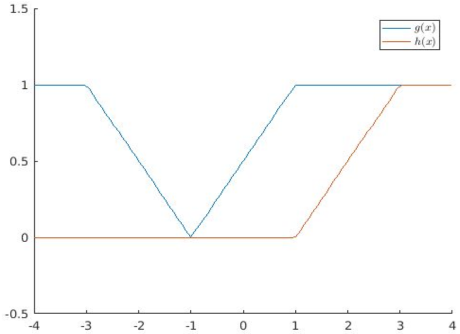
# Geometrical Study [with Modar]

- Continuous Piecewise Linear DNNs
- Gradient Images for PL-DNNs
- Sensitivity Analysis of PL-DNNs
- Adversarial Examples for PL-DNNs

# Continuous Piecewise Linear DNNs

Any Continuous PL function can be written as **a difference of only two** convex PL functions



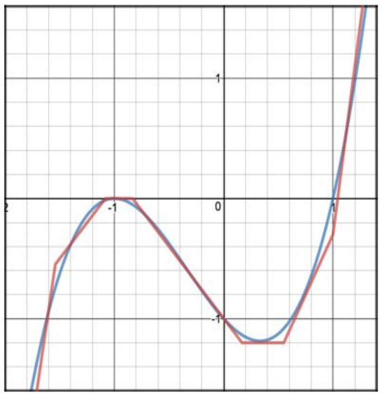

$$f(x) = \begin{cases} 1 & \text{if } x < -3 \\ \frac{1}{2}\sin(\frac{n}{2\pi}) + \frac{1}{2} & \text{if } -3 \le x < 3 \\ 0 & \text{if } 3 \le x \end{cases}$$

$$g(x) = \begin{cases} 1 & \text{if } x < -3 \\ \frac{2 - x - 3}{2} + 1 & \text{if } -3 \le x < -1 \\ \frac{x+1}{2} & \text{if } -1 \le x < 1 \\ 1 & \text{if } 1 \le x \end{cases}$$

$$h(x) = \begin{cases} 0 & \text{if } x < -1 \\ \frac{x+1}{2} & \text{if } -1 \le x < 1 \\ 1 & \text{if } 1 \le x \end{cases}$$

# Continuous Piecewise Linear DNNs

$$f(x) = x^3 + x^2 - x - 1$$



$$n_1(x) = Relu(-5x - 7.7)$$
$$n_2(x) = Relu(-1.2x - 1.3)$$
$$n_3(x) = Relu(1.2x + 1)$$
$$n_4(x) = Relu(1.2x - .2)$$
$$n_5(x) = Relu(2x - 1.1)$$
$$n_6(x) = Relu(5x - 5)$$

$$\begin{aligned} Z(x) = &-n_1(x) - n_2(x) - n_3(x) \\ &+ n_4(x) + n_5(x) + n_6(x) \end{aligned}$$

Example of a single hidden layer network

- Convex piecewise linear functions are defined as $f(\mathbf{x}) = \max_{i \in [1,m]} \{\mathbf{a}_i^T \mathbf{x}\}$
- Most **DNN layers** are piecewise linear [5] E.g., ReLU, MaxPool, Conv, FC
- The **composition** of two PL functions is PL
- Thus, Most DNNs are piecewise linear
- Note that, **Softmax is not PL**

# Continuous Piecewise Linear DNNs

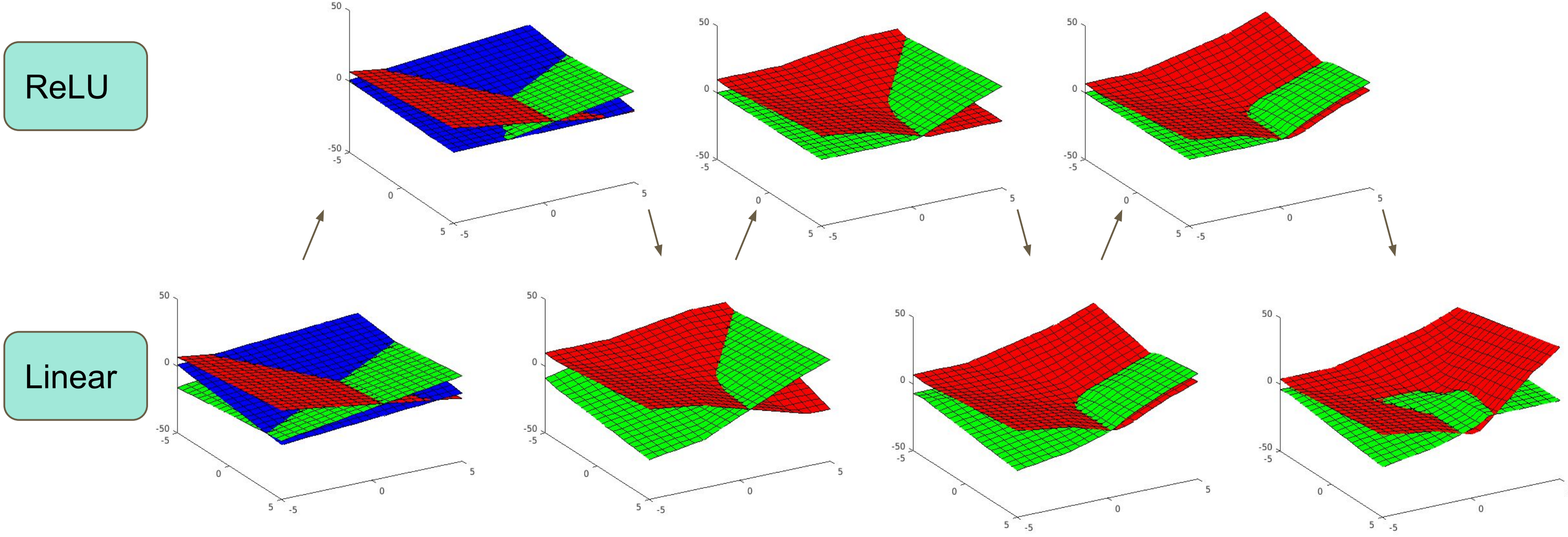
- For a classifier PL-DNN, let us recursively define $\forall i \in (0, L]$

| | |
|---|---|
| The network as a function | $f : \mathbb{R}^{m^0} \rightarrow \mathbb{R}^{m^L} \Rightarrow f(\mathbf{x}; \mathbf{\Theta}) = l^L(\mathbf{x})$ |
| Layer output: *activation(linear(input))* | $\Lambda^i(\mathbf{x}) = A^i(l^i(\mathbf{x}))$ |
| Linear layer | $l^i(\mathbf{x}) = \mathbf{W}^i \Lambda^{i-1}(\mathbf{x}) + \mathbf{b}^i$ |
| Base cases | $\mathbf{W}^0 = \mathbf{I}_{m_0}, \mathbf{b}^0 = \mathbf{1}_{m_0} \Rightarrow \Lambda^0(\mathbf{x}) = \mathbf{x}$ |
| Such that | $\Lambda^i : \mathbb{R}^{m^{i-1}} \rightarrow \mathbb{R}^{m^i}, \mathbf{W}^i \in \mathbb{R}^{m^i \times m^{i-1}}, \mathbf{b}^i \in \mathbb{R}^{m^i}$ |

- The parameters $\mathbf{\Theta}$ is the set $\{\mathbf{W}^i, \mathbf{b}^i | \forall i \in (0, L]\}$

# Continuous Piecewise Linear DNNs

- Example of three hidden-layers network on 2D input



# Continuous Piecewise Linear DNNs

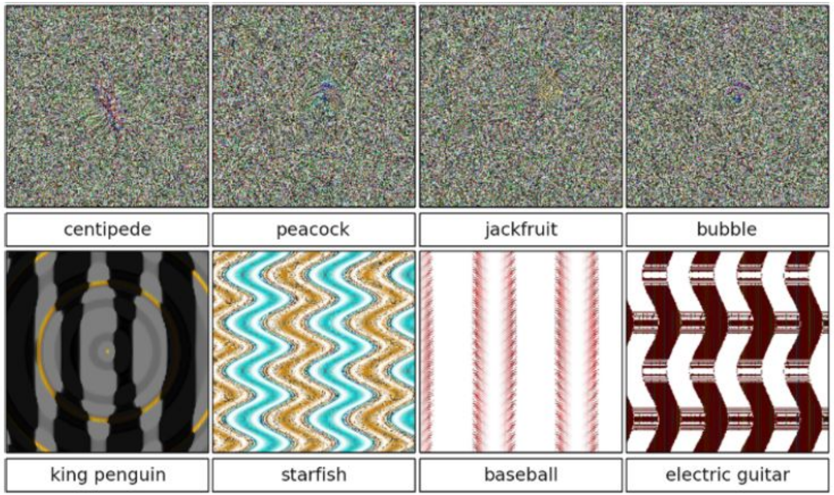
- PL-DNNs divides the input space into convex polyhedrons.
- There is a strong influence of the number of nonlinear layers and the number of wide layers on the complexity and expressivity of the network.
- A tight upper bound exists for number of knots neural networks that has input dimension of one and ReLU activations [15].

$$N \leq \sum_{i=1}^{L} m^i \prod_{j=i+1}^{L} (m^j + 1)$$

- The number of piecewise linear regions grows exponentially with the number of layers [16].

# Continuous Piecewise Linear DNNs

- It is possible to generate unnatural looking images that are classified with high confidence to be belonging to a certain class
- Using genetic algorithm with direct and indirect encoding [14]



# Gradient Images for PL-DNNs

- Gradients are the directions of the steepest change
- Let us define the gradient with respect to the input recursively

| | |
|---|---|
| Gradient of images of subnetwork | $\frac{\partial \Lambda^i}{\partial \mathbf{x}} = \frac{\partial A^i}{\partial l^i} \frac{\partial l^i}{\partial \mathbf{x}}$ (Chain Rule) |
| Gradient images of subnetwork | $\frac{\partial l^i}{\partial \mathbf{x}} = \frac{\partial l^i}{\partial \Lambda^{i-1}} \frac{\partial \Lambda^{i-1}}{\partial \mathbf{x}}$ (Chain Rule) |
| Gradient of linear layer | $\frac{\partial l^i}{\partial \Lambda^{i-1}} = \mathbf{W}^i$ |
| Base cases | $\frac{\partial \Lambda^0}{\partial \mathbf{x}} = \mathbf{I}_{m^0}$ |
| Such that | $\frac{\partial \Lambda^i}{\partial \mathbf{x}} \in \mathbb{R}^{m^i \times m^0}, \frac{\partial A^i}{\partial l^i} \in \mathbb{R}^{m^i \times m^i}, \frac{\partial l^i}{\partial \mathbf{x}} \in \mathbb{R}^{m^i \times m^0}$ |

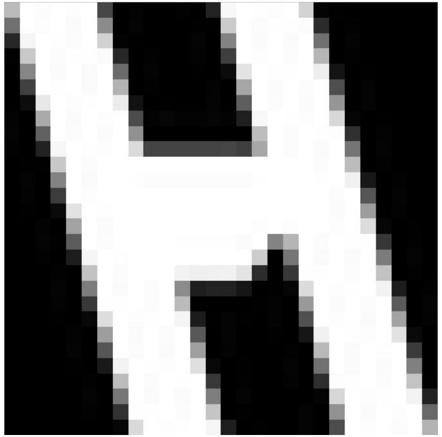
- Different activation functions have different gradients

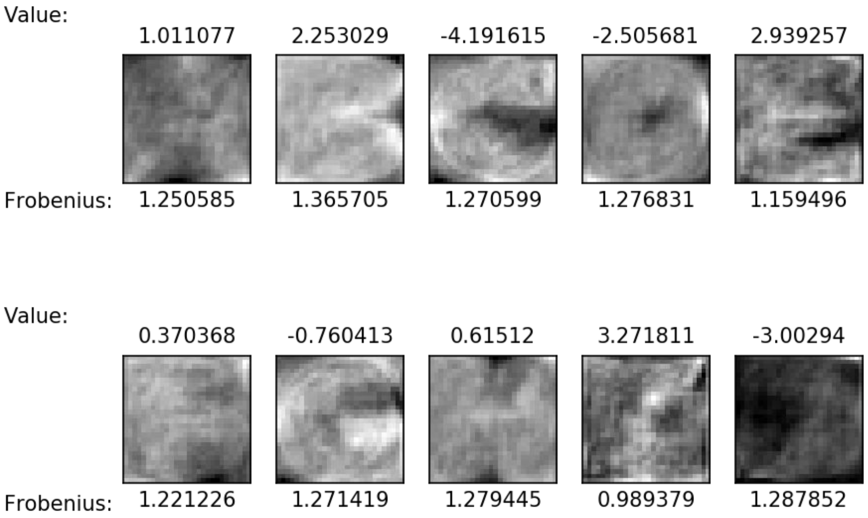
# Gradient Images for PL-CNNs

- Conv layers can be converted to FC layers (i.e., matrix-vector product)
- MaxPooling for a certain input can be converted as matrix-vector product
- We will consider the default activation for FC and Conv layers to be ReLU
- The default activation function for MaxPooling is the identity function
- For ReLU: $\frac{\partial A^i}{\partial l^i} = \mathbf{V}^i = diag(\mathbf{v}^i) \text{ s.t. } v^i_j = \begin{cases} 1 & \text{if } l^i_j(\mathbf{x}) > 0 \\ 0 & \text{otherwise} \end{cases}$
- Therefore, the gradient images are given by $\frac{\partial f}{\partial \mathbf{x}} = \mathbf{W}^L \mathbf{V}^{L-1} \mathbf{W}^{L-1} \ldots \mathbf{V}^1 \mathbf{W}^1$
- The Vs job is to select specific rows of the Ws and make them zeros
- The Vs are functions of the input image while the Ws are constants
- This product contains the gradients of the linearization around the input

# Gradient Images for PL-CNNs

- Example of gradient images with Not-MNIST [6] and a Single layer ANN
- The output is 10 classes





# Sensitivity Analysis of PL-DNNs

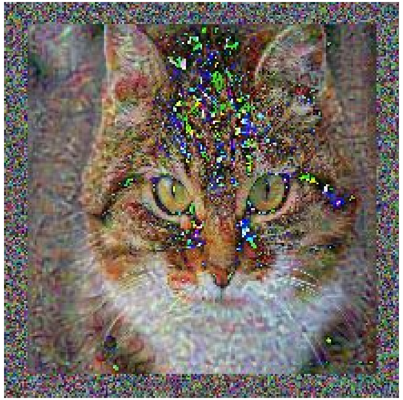
- How much can we change the input without changing the class label?
  - Move in a direction **orthogonal to all gradients** (i.e.,vector in the null space of $\frac{\partial}{\partial \mathbf{x}} f(\mathbf{x}, \boldsymbol{\Theta})$)
    - Any right singular vector that correspond to a zero singular value in the SVD
    - Minimum-energy solution $\mathbf{G} = \frac{\partial}{\partial \mathbf{x}} f(\mathbf{x}, \boldsymbol{\Theta}) \rightarrow \mathbf{G}^T(\mathbf{G}\mathbf{G}^T)^{-1}\mathbf{G}\mathbf{x}_0 - \mathbf{x}_0$ for any random $\mathbf{x}_0$
  - Move while keeping the **ordering** of final layer functions the same
    - Form this **convex polyhedral cone**
      Where $j_k = \begin{cases} k & \text{if } k < i \\ k+1 & \text{if } k > i \end{cases}$
      Find a point in this polyhedron

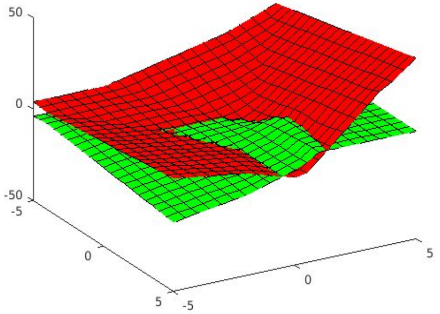
      $$\begin{bmatrix} (\nabla f_{j_1}(\mathbf{x}) - \nabla f_i(\mathbf{x}))^T \\ \vdots \\ \left(\nabla f_{j_{m^0-1}}(\mathbf{x}) - \nabla f_i(\mathbf{x})\right)^T \end{bmatrix} \mathbf{v} \leq \begin{bmatrix} f_i(\mathbf{x}) - f_{j_1}(\mathbf{x}) \\ \vdots \\ f_i(\mathbf{x}) - f_{j_{m^0-1}}(\mathbf{x}) \end{bmatrix} \Rightarrow \mathbf{A}\mathbf{v} \leq \mathbf{b}$$

      - Using Linear Programming (very expensive)
      - Start from the **intersection** then move inside $\mathbf{A}^T(\mathbf{A}\mathbf{A}^T)^{-1}(\mathbf{b} - \mathbf{c})$ s.t. $\mathbf{c} \geq \mathbf{0}$
    - With these techniques you have multiple points in a convex polyhedron
      Taking **any convex combination** of those points that is close enough to the original point will yield a point that has the same label as the original image

# Sensitivity Analysis of PL-DNNs

- Example of moving inside the convex polyhedral cone





# Sensitivity Analysis of PL-DNNs

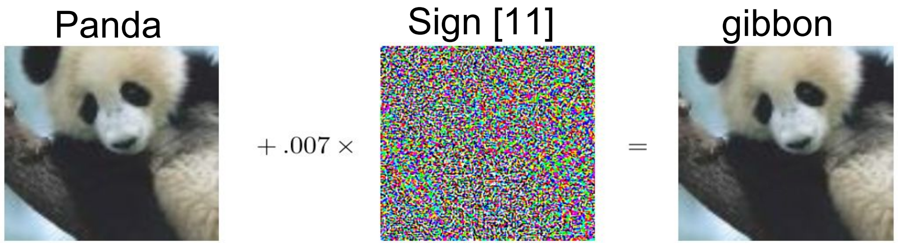
- **Lipschitz constant** tells us what is the effect of a small change in the input of a function to the output [7] $\forall \mathbf{x}, \mathbf{r} \| f(\mathbf{x}) - f(\mathbf{x} - \mathbf{r}) \|_2 \leq L \|\mathbf{r}\|_2$
- The smaller the constant the more smaller the change is going to be
- The Lipschitz constant of an FC layer bounded from above by the maximum singular value of the weights matrix
- The Lipschitz constant of a network is the product of its layers
- For a trained AlexNet [8] on imagenet dataset [9], Lipschitz constants are

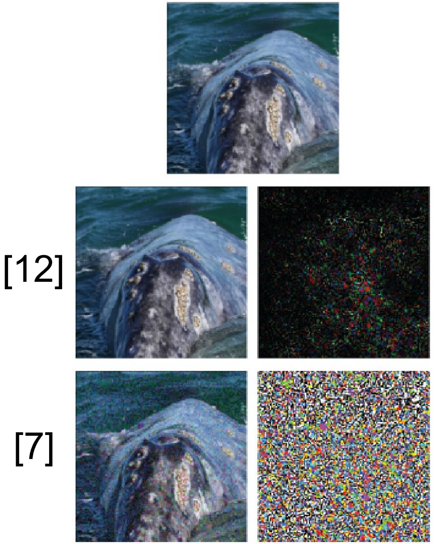
| Conv1 | Conv2 | Conv3 | Conv4 | Conv5 | FC6 | FC7 | FC8 |
|---|---|---|---|---|---|---|---|
| 2.75 | 10 | 7 | 7.5 | 11 | 3.12 | 4 | 4 |

- There is a way to train a network such that the Lipschitz constant is less than or equal to one for each layer to increase its robustness [10].

# Adversarial Examples for PL-DNNs

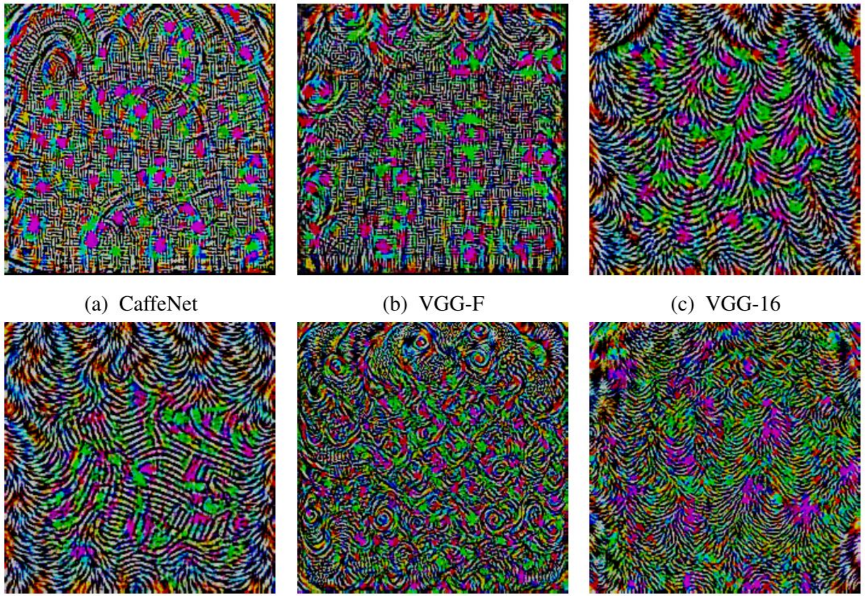
- Given an input image, add small perturbation to it to change its label.
  - Minimize the loss to a different label [7] (the minimization is done in very few steps)
  - Move along the sign of the gradient of the loss [11]
  - DeepFool: go outside the convex polyhedral cone [12]
  - Add an adversarial universal perturbation [13]



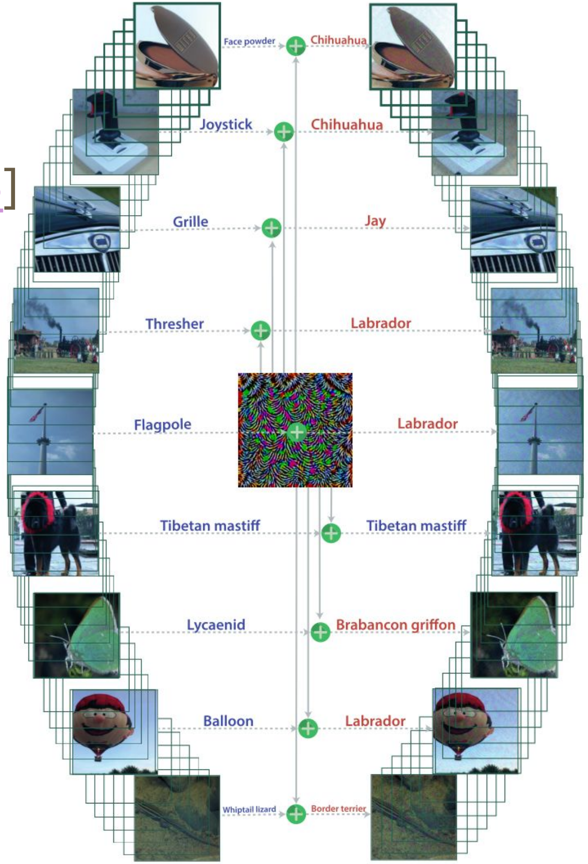
# Adversarial Examples for PL-DNNs

- More about universal adversarial perturbation [13]



(a) CaffeNet (b) VGG-F (c) VGG-16

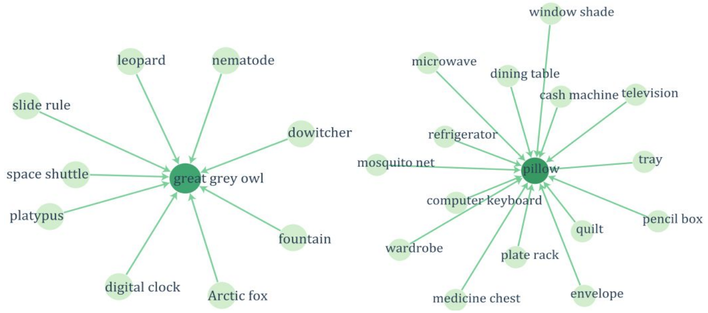
(d) VGG-19 (e) GoogLeNet (f) ResNet-152



# Adversarial Examples for PL-DNNs

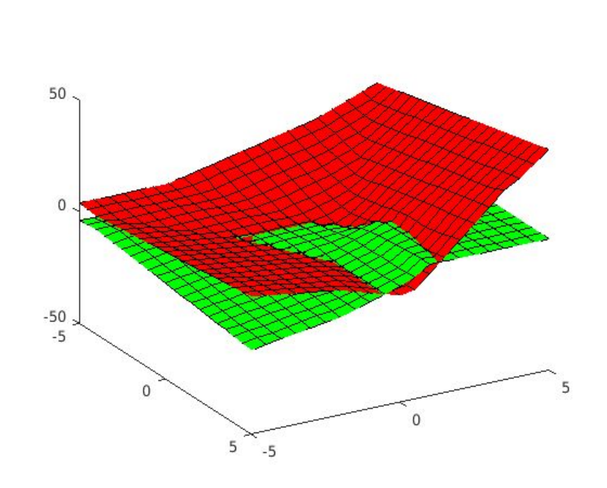
- These perturbation happen to be network-agnostic and there is even a high chance for an image to fool different networks by the same label
- Retraining with perturbed images doesn't help like filtering, JPEG compression and adversarial examples detector DNNs
- By studying the geometrical curvature of DNNs we can detect its adversarial examples [16].

| | VGG-F | CaffeNet | GoogLeNet | VGG-16 | VGG-19 | ResNet-152 |
|---|---|---|---|---|---|---|
| VGG-F | **93.7%** | 71.8% | 48.4% | 42.1% | 42.1% | 47.4 % |
| CaffeNet | 74.0% | **93.3%** | 47.7% | 39.9% | 39.9% | 48.0% |
| GoogLeNet | 46.2% | 43.8% | **78.9%** | 39.2% | 39.8% | 45.5% |
| VGG-16 | 63.4% | 55.8% | 56.5% | **78.3%** | 73.1% | 63.4% |
| VGG-19 | 64.0% | 57.2% | 53.6% | 73.5% | **77.8%** | 58.0% |
| ResNet-152 | 46.3% | 46.3% | 50.5% | 47.0% | 45.5% | **84.0%** |



# Suggested Reading

- Can neural networks solve any problem [2]?
- Universal adversarial perturbations [13].
- Classification regions of deep neural networks [16].



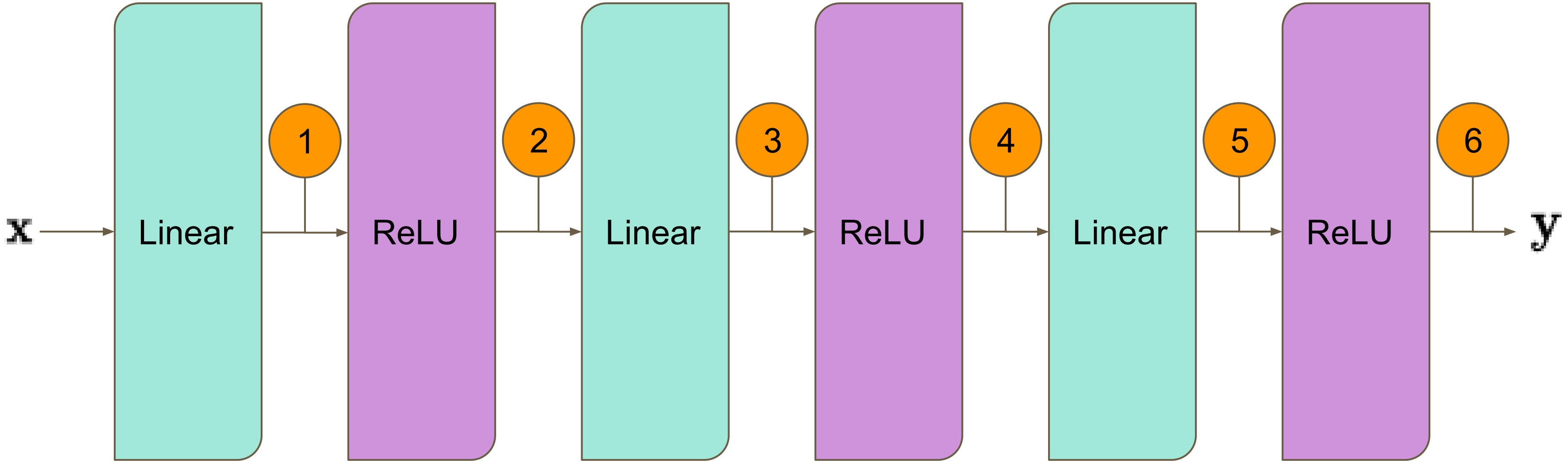
# Geometric Study ~ Conclusions

- DNNs are parametrized models that have high capacity to approximate continuous functions using different architectural choices (deep vs. wide).
- These models need to be trained with enough data from a certain distribution to be able to generalize well to new unseen examples.
- With the current training techniques there still appear blindspots to the model were adversarial examples live even after fine tuning on them.
- These adversarial samples appear to be universal with different DNNs.
- By studying the geometry of these constructions (i.e., PL-DNNs) we get insights on why these phenomenon occur and how to avoid them.
- We hope that we can use this knowledge to understand the capabilities and shortcoming of DNNs and how best to construct and train them.

# Probabilistic Study [with Adel]

- Statistical Analysis of Fully Connected Networks

# Statistical Analysis of Fully Connected Networks



# Thank You
# for
# Listening!

References list is on the next slide

# References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