Understanding DNNs

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Outline

- Introduction
- Geometrical Study [with Modar]
- Probabilistic Study [with Adel]
- References

Prerequisites

Basic level grasping and understanding of:

- Deep Learning
- Deep Neural Networks
- Multivariable Calculus
- Linear Algebra
- Statistics [for Part 2]

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

Given a problem
E.g. classification

Formulate it as a function
E.g. $F(\mathbf{x}) : \mathbb{R}^d \rightarrow \mathbb{R}^c$

Hypothesize a parameterized approximation (structured network)
E.g. $f(\mathbf{x}; \mathbf{\Theta}) \approx F(\mathbf{x})$

Find (i.e., train) the best $\mathbf{\Theta}$ according to a loss function of your choice

- 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)

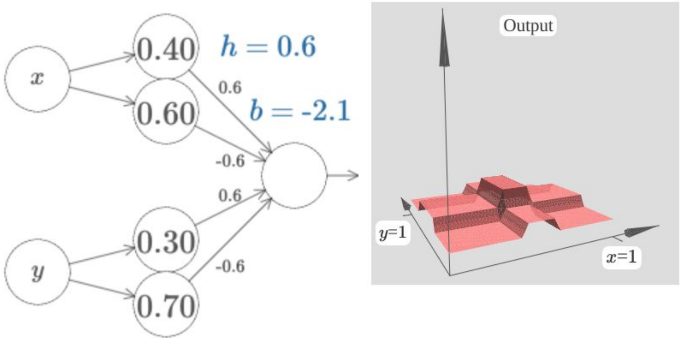
Training DNNs Using Gradient Descent

1. Start with initial parameters $\mathbf{\Theta}_0$ and learning rate α
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

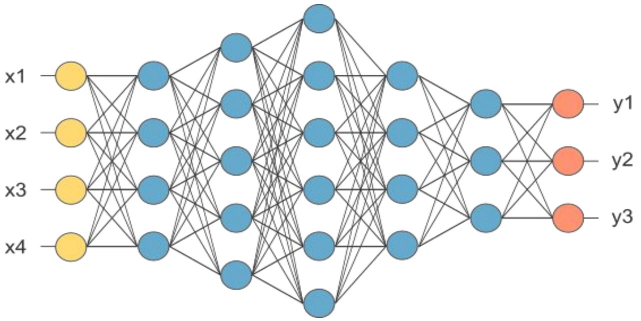
Universal Approximation Theorem

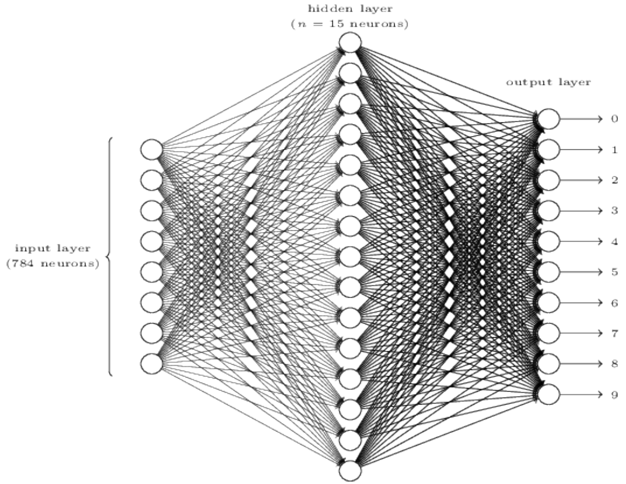
- Any arbitrary continuous function can be **approximated** effectively using a feed-forward neural network (i.e., a multilayer perceptron) with a single hidden layer, under mild assumptions on the activation function [1].
- A visual and interactive proof to this theorem is presented in [2,3].



Deeper vs. Wider Argument

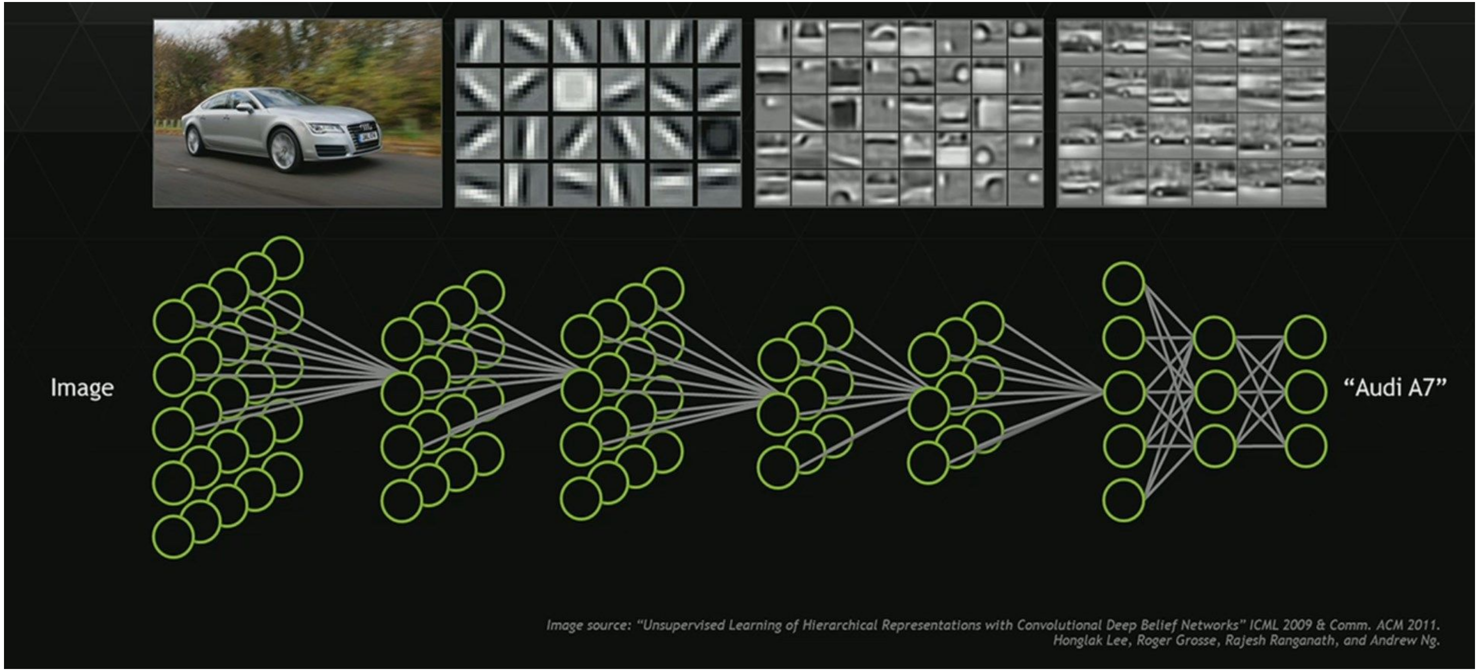
- Is it better to go deeper or wider? [4]
  - **Training difficulty** (e.g., vanishing gradients)
  - **Deployment restrictions** (e.g. high input dimensionality)
- Try different structures with Tensorflow Playground [here]





Deeper vs. Wider Argument

Example of high dimensional input and proposed solution (CNNs)



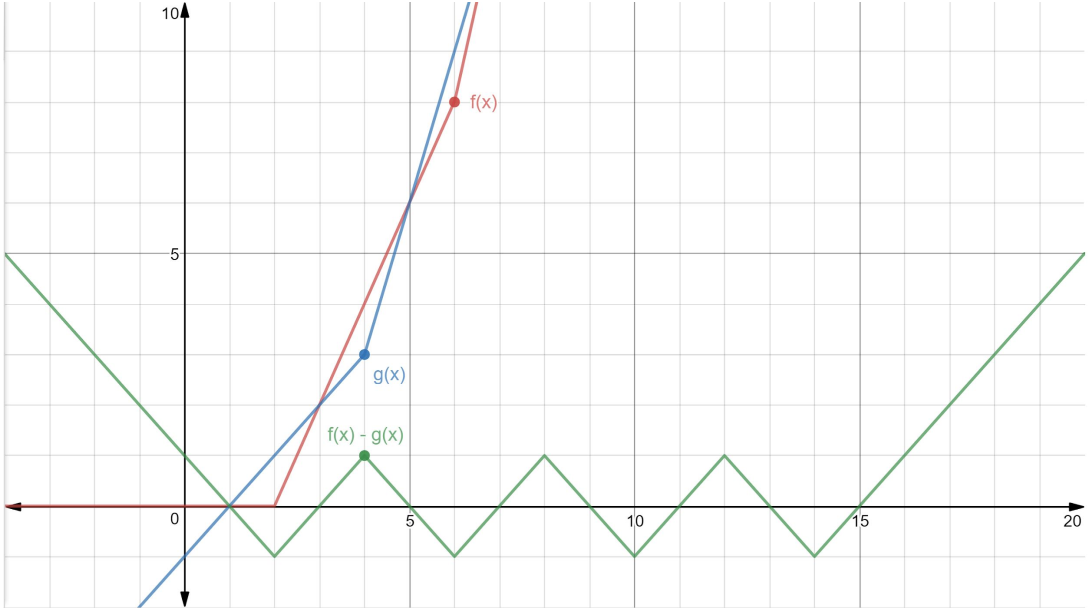
Geometrical Study [with Modar]

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

Continuous Piecewise Linear DNNs

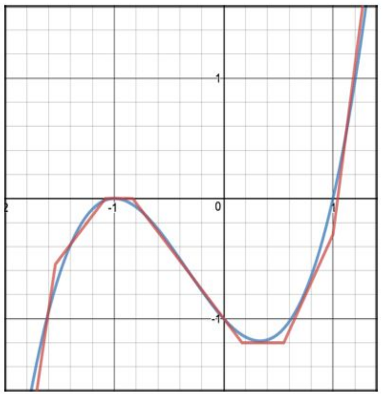
Any Continuous PL function can be written as **a difference of only two** convex PL functions

$$f(x) = \max\{0, 2(x-2), 4(x-4), 6(x-6), 8(x-8)\}$$
$$g(x) = \max\{(x-1), 3(x-3), 5(x-5), 7(x-7)\}$$



Continuous Piecewise Linear DNNs

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



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

$$Z(x) = -n_1(x) - n_2(x) - n_3(x) + n_4(x) + n_5(x) + n_6(x)$$

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

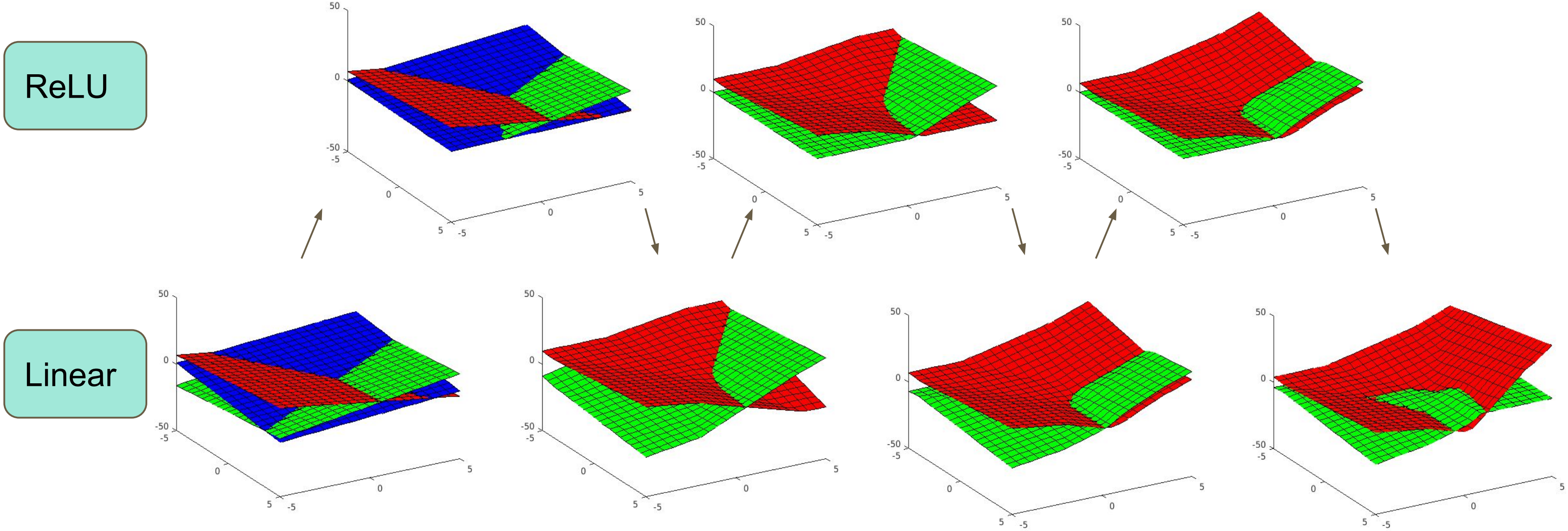
- For a classifier PL-DNN, let us recursively define $\forall i \in (0, L]$

The network as a function	$f : \mathbb{R}^{m^0} \rightarrow \mathbb{R}^{m^L} \Rightarrow f(\mathbf{x}; \boldsymbol{\Theta}) = l^L(\mathbf{x})$
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	$\Lambda^i : \mathbb{R}^{m^{i-1}} \rightarrow \mathbb{R}^{m^i}, \mathbf{W}^\mathbf{i} \in \mathbb{R}^{m^i \times m^{i-1}}, \mathbf{b}^i \in \mathbb{R}^{m^i}$

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

Continuous Piecewise Linear DNNs

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



Continuous Piecewise Linear DNNs

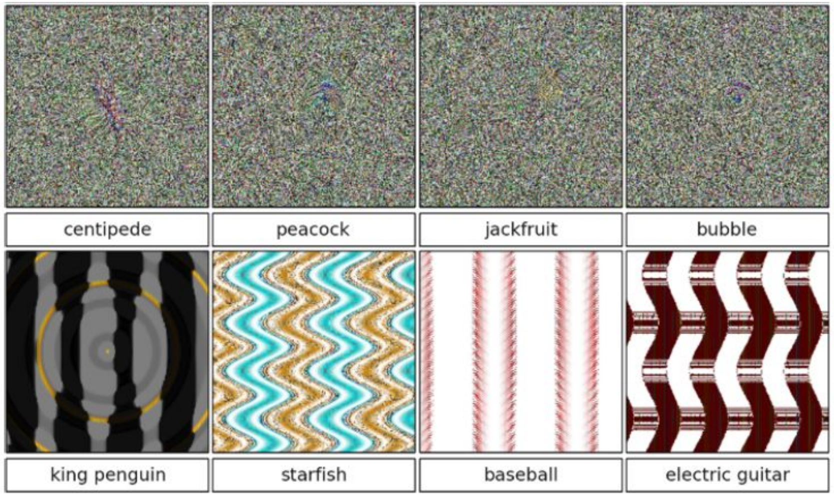
- PL-DNNs divides the input space into polyhedrons.
- There is a strong influence of the number of nonlinear layers and the number of wide layers on the complexity and expressivity of the network.
- A tight upper bound exists for number of knots neural networks that has input dimension of one and ReLU 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	$\frac{\partial \Lambda^i}{\partial \mathbf{x}} \in \mathbb{R}^{m^i \times m^0}, \frac{\partial A^i}{\partial l^i} \in \mathbb{R}^{m^i \times m^i}, \frac{\partial l^i}{\partial \mathbf{x}} \in \mathbb{R}^{m^i \times m^0}$

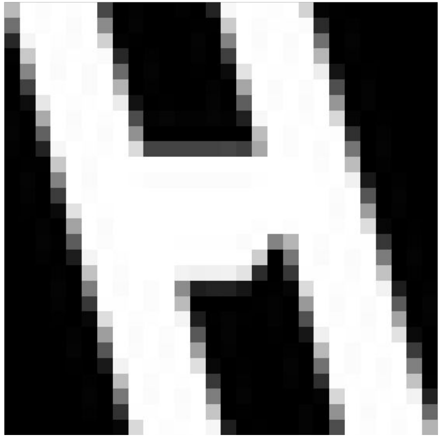
- Different activation functions have different gradients

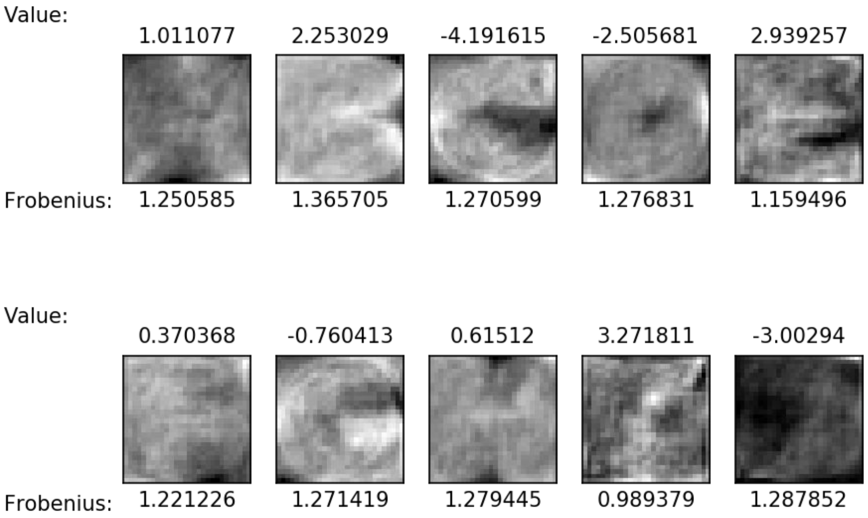
Gradient Images for PL-CNNs

- 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 $\boxed{\frac{\partial f}{\partial \mathbf{x}} = \mathbf{W}^L \mathbf{V}^{L-1} \mathbf{W}^{L-1} \ldots \mathbf{V}^1 \mathbf{W}^1}$
- 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 $\frac{\partial}{\partial \mathbf{x}} f(\mathbf{x}, \mathbf{\Theta})$)
    - Any right singular vector that correspond to a zero singular value in the SVD
    - Minimum-energy solution $\mathbf{G} = \frac{\partial}{\partial \mathbf{x}} f(\mathbf{x}, \mathbf{\Theta}) \rightarrow \mathbf{G}^T(\mathbf{G}\mathbf{G}^T)^{-1}\mathbf{G}\mathbf{x}_0 - \mathbf{x}_0$ for any random $\mathbf{x}_0$
  - Move while keeping the **ordering** of final layer functions the same
    - Form this **convex polyhedral cone** $\begin{bmatrix} (\nabla f_{j_1}(\mathbf{x}) - \nabla f_i(\mathbf{x}))^T \\ \vdots \\ \left(\nabla f_{j_{m0-1}}(\mathbf{x}) - \nabla f_i(\mathbf{x})\right)^T \end{bmatrix} \mathbf{v} \leq \begin{bmatrix} f_i(\mathbf{x}) - f_{j_1}(\mathbf{x}) \\ \vdots \\ f_i(\mathbf{x}) - f_{j_{m0-1}}(\mathbf{x}) \end{bmatrix} \Rightarrow \mathbf{A}\mathbf{v} \leq \mathbf{b}$

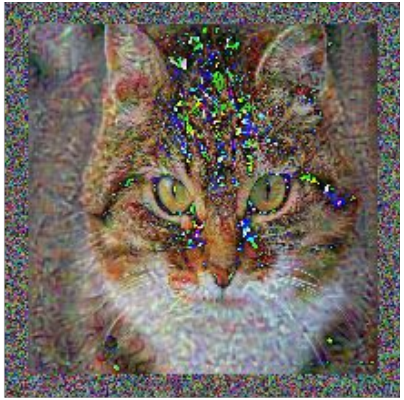
      Where $j_k = \begin{cases} k & \text{if } k < i \\ k+1 & \text{if } k > i \end{cases}$

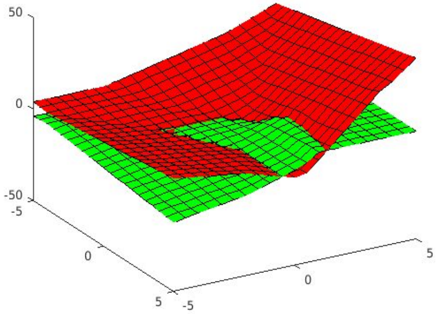
      Find a point in this polyhedron
      - Using Linear Programming (very expensive)
      - Start from the **intersection** then move inside $\mathbf{A}^T(\mathbf{A}\mathbf{A}^T)^{-1}(\mathbf{b} - \mathbf{c})$ s.t. $\mathbf{c} \geq \mathbf{0}$
    - With these techniques you have multiple points in a convex 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

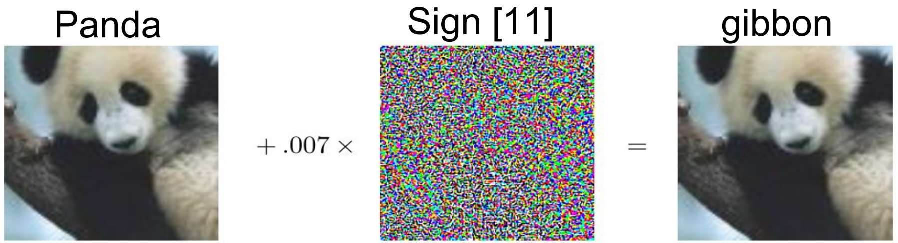
- **Lipschitz constant** tells us what is the effect of a small change in the input of a function to the output [7] $\forall \mathbf{x}, \mathbf{r} \| f(\mathbf{x}) - f(\mathbf{x} - \mathbf{r}) \|_2 \leq L \|\mathbf{r}\|_2$
- The smaller the constant the more smaller the change is going to be
- The Lipschitz 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

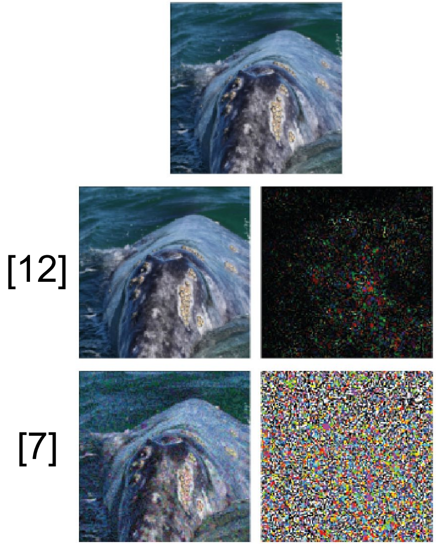
Conv1	Conv2	Conv3	Conv4	Conv5	FC6	FC7	FC8
2.75	10	7	7.5	11	3.12	4	4

- 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

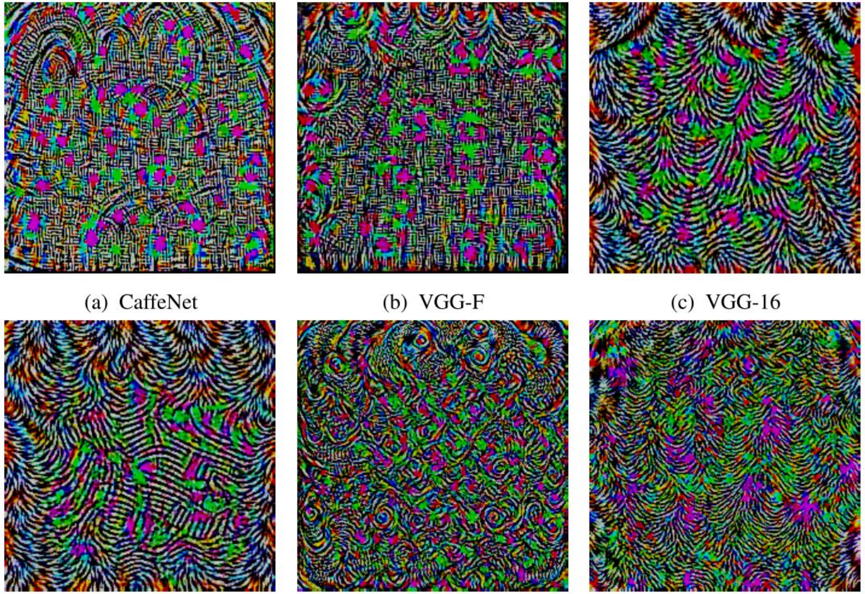
- Given an input image, add small perturbation to it to change its label.
  - Minimize the loss to a different label [7] (the minimization is done in very few steps)
  - Move along the sign of the gradient of the loss [11]
  - DeepFool: go outside the convex polyhedral cone [12]
  - Add an adversarial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





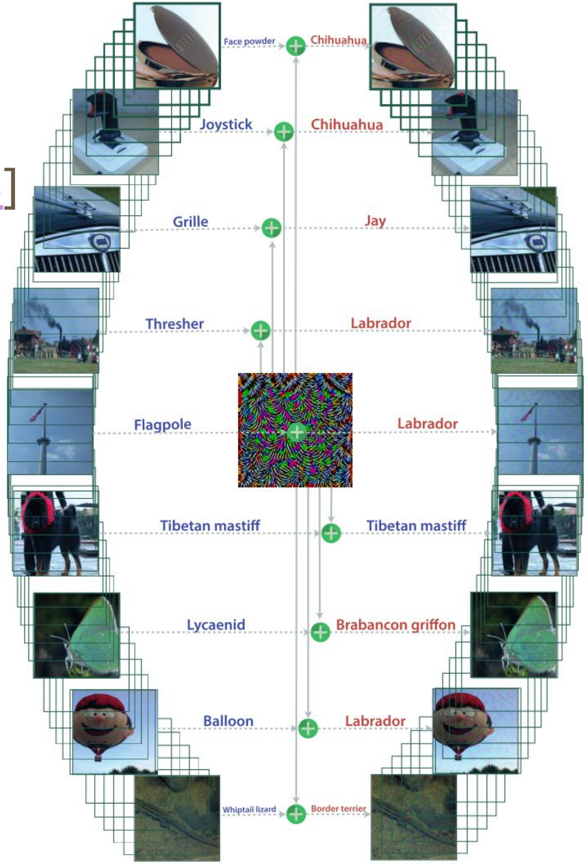
Adversarial Examples for PL-DNNs

- More about universal adversarial perturbation [13]



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

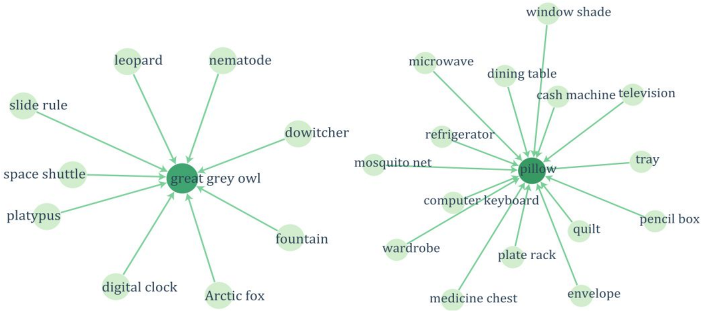
(d) VGG-19 (e) GoogLeNet (f) ResNet-152



Adversarial Examples for PL-DNNs

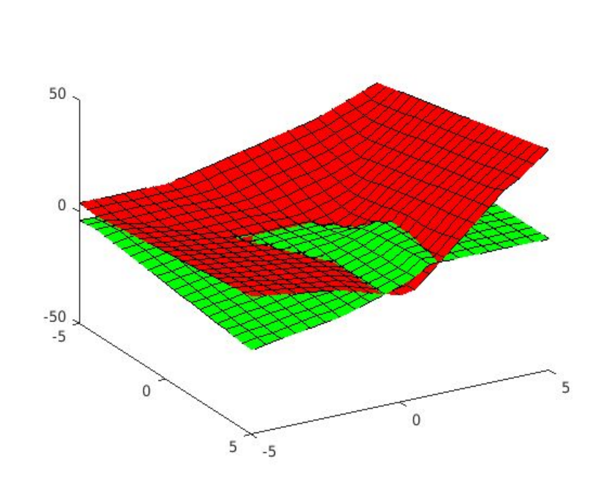
- These perturbation happen to be network-agnostic and there is even a high chance for an image to fool different networks by the same label
- Retraining with perturbed images doesn't help like filtering, JPEG compression and adversarial examples detector DNNs
- By studying the geometrical curvature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

- Understanding NNs with TensorFlow Playground [17].
- Can neural networks solve any problem [2]?
- Universal adversarial perturbations [13].
- Classification regions of deep neural networks [16].



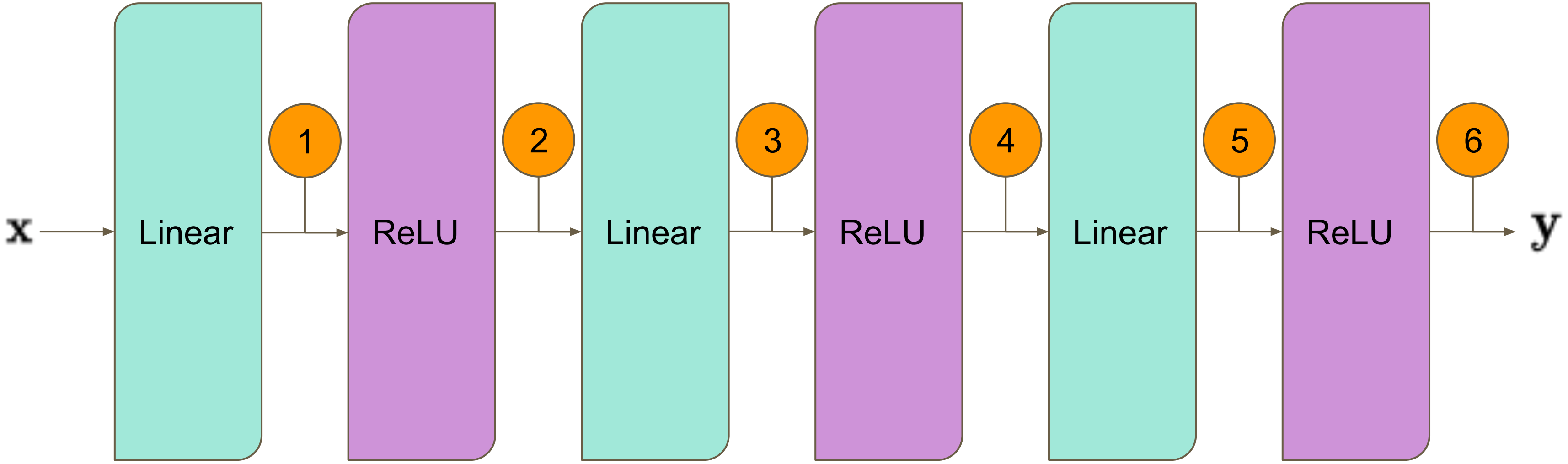
Geometric Study ~ Conclusions

- 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
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Listening!

References list is on the next slide

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