



# Topics on CNN: Transfer Learning, Visualization, Neural Style, and Adversarial Examples

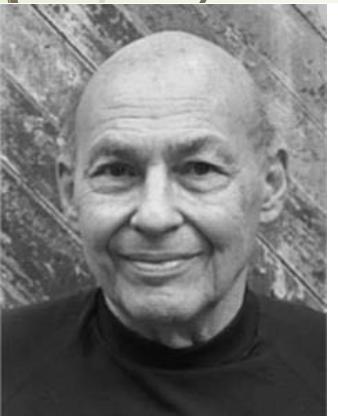
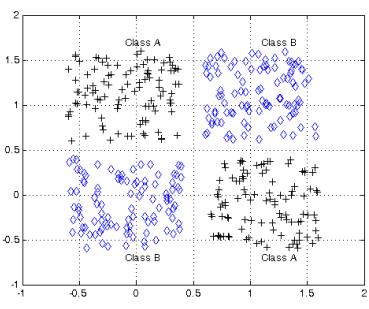
Yuan YAO  
HKUST

# Locality or Sparsity of Computation

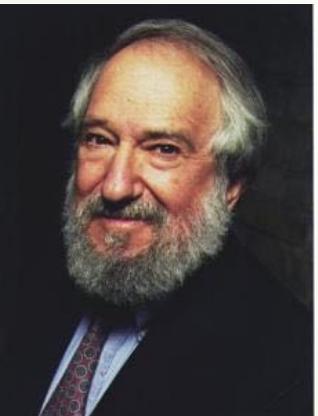
Minsky and Papert, 1969

Perceptron can't do **XOR** classification

Perceptron needs infinite global  
information to compute **connectivity**



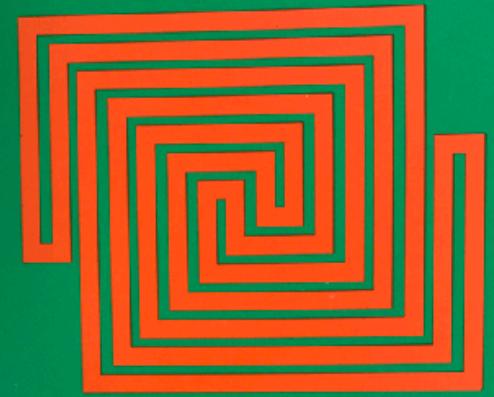
Marvin Minsky



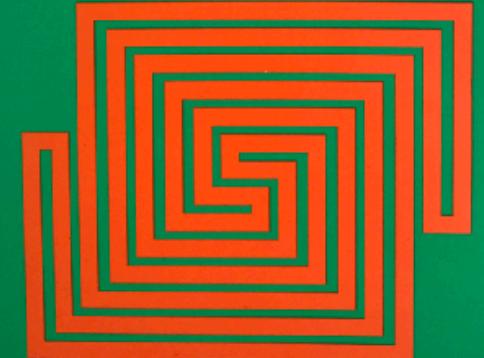
Seymour Papert

**Locality** or **Sparsity** is important:  
Locality in time?  
Locality in space?

Expanded Edition



Perceptrons



Marvin L. Minsky  
Seymour A. Papert

# Connectivity is of infinite order

- Which one of these two figures is connected?

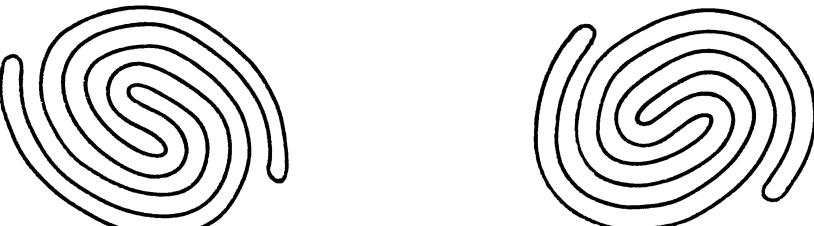


Figure 5.1

Theorem (Minsky-Papert'1969)

*The decision function that  $f(X) = [X \text{ is connected}]$  for  $X \subseteq \mathbb{R}^p$  is **not of any finite order**, i.e. for any  $k < \infty$ , there does not exist a (possibly of infinite members) family of  $\{\phi_\alpha(X) : \text{supp}(\phi_\alpha) \leq k\}$  whose supports are at most  $k$ , such that*

$$f(X) = \left[ \sum_{\alpha} \phi_{\alpha}(X) \geq 0 \right] \quad (21)$$

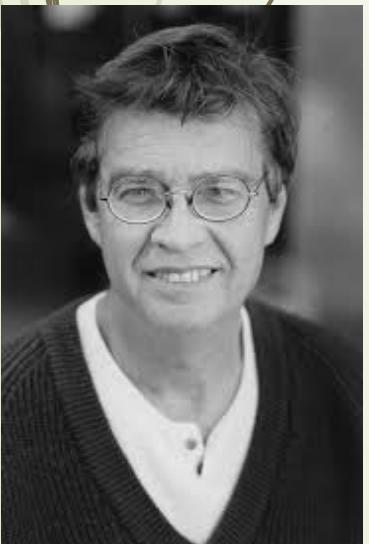
# Multilayer Perceptrons (MLP) and Back-Propagation (BP) Algorithms

Rumelhart, Hinton, Williams (1986)

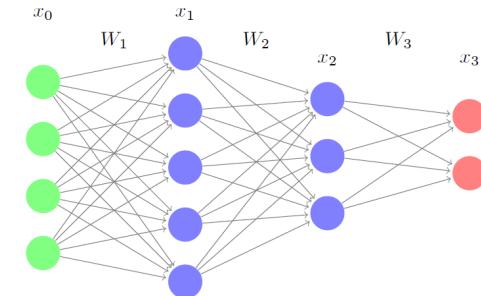
Learning representations by back-propagating errors, Nature, 323(9): 533-536

BP algorithms as **stochastic gradient descent** algorithms (**Robbins–Monro 1950; Kiefer–Wolfowitz 1951**) with Chain rules of Gradient maps

MLP classifies **XOR**, but the global hurdle on topology (connectivity) computation still exists



NATURE VOL. 323 9 OCTOBER 1986 LETTERS TO NATURE 533



## Learning representations by back-propagating errors

David E. Rumelhart\*, Geoffrey E. Hinton† & Ronald J. Williams\*

\* Institute for Cognitive Science, C-015, University of California, San Diego, La Jolla, California 92093, USA  
† Department of Computer Science, Carnegie-Mellon University, Pittsburgh, Philadelphia 15213, USA

We describe a new learning procedure, back-propagation, for networks of neuron-like units. The procedure repeatedly adjusts the weights of the connections in the network so as to minimize a measure of the difference between the actual output vector of the net and the desired output vector. As a result of the weight adjustments, internal 'hidden' units which are not part of the input or output code to represent important features of the task domain, and the regularities in the task are captured by the interactions of these units. The ability to create useful new features distinguishes back-propagation from earlier, simpler methods such as the perceptron, counter-propagation, and others.

There have been many attempts to design self-organizing neural networks. The aim is to find a powerful synaptic modification rule that will allow an arbitrarily connected neural network to develop an internal structure that is appropriate for a particular task domain. The task is specified by giving the desired state vector of the output units for each state vector of the input units. If the input units are directly connected to the output units it is relatively easy to find learning rules that iteratively adjust the relative strengths of the connections so as to progressively reduce the difference between the actual and desired output vectors\*. Learning becomes more interesting but

more difficult when we introduce hidden units whose actual or desired states are not specified by the task. (In perceptrons, there are 'feature analysers' between the input and output that are not true hidden units because their input connections are fixed by hand, so their states are completely determined by the input vector: they do not learn representations.) The learning procedure must decide under what circumstances the hidden units should be active in order to help achieve the desired input-output behaviour. This amounts to deciding what these units should represent. We demonstrate that a general purpose and relatively simple procedure is powerful enough to construct appropriate learned representations.

The simplest form of the learning procedure is for layered networks which have a layer of input units at the bottom, any number of intermediate layers, and a layer of output units at the top. Connections within a layer or from higher to lower layers are forbidden, but connections can skip intermediate layers. An input vector is presented to the network by setting the states of the input units. Then the states of the units in each layer are determined by applying equations (1) and (2) to the connections coming from lower layers. All units within a layer have their states set in parallel, but different layers have their states set sequentially, starting at the bottom and working upwards until the states of the output units are determined.

The total input,  $x_j$ , to unit  $j$  is a linear function of the outputs,  $y_i$ , of the units that are connected to  $j$  and of the weights,  $w_{ij}$ , on these connections

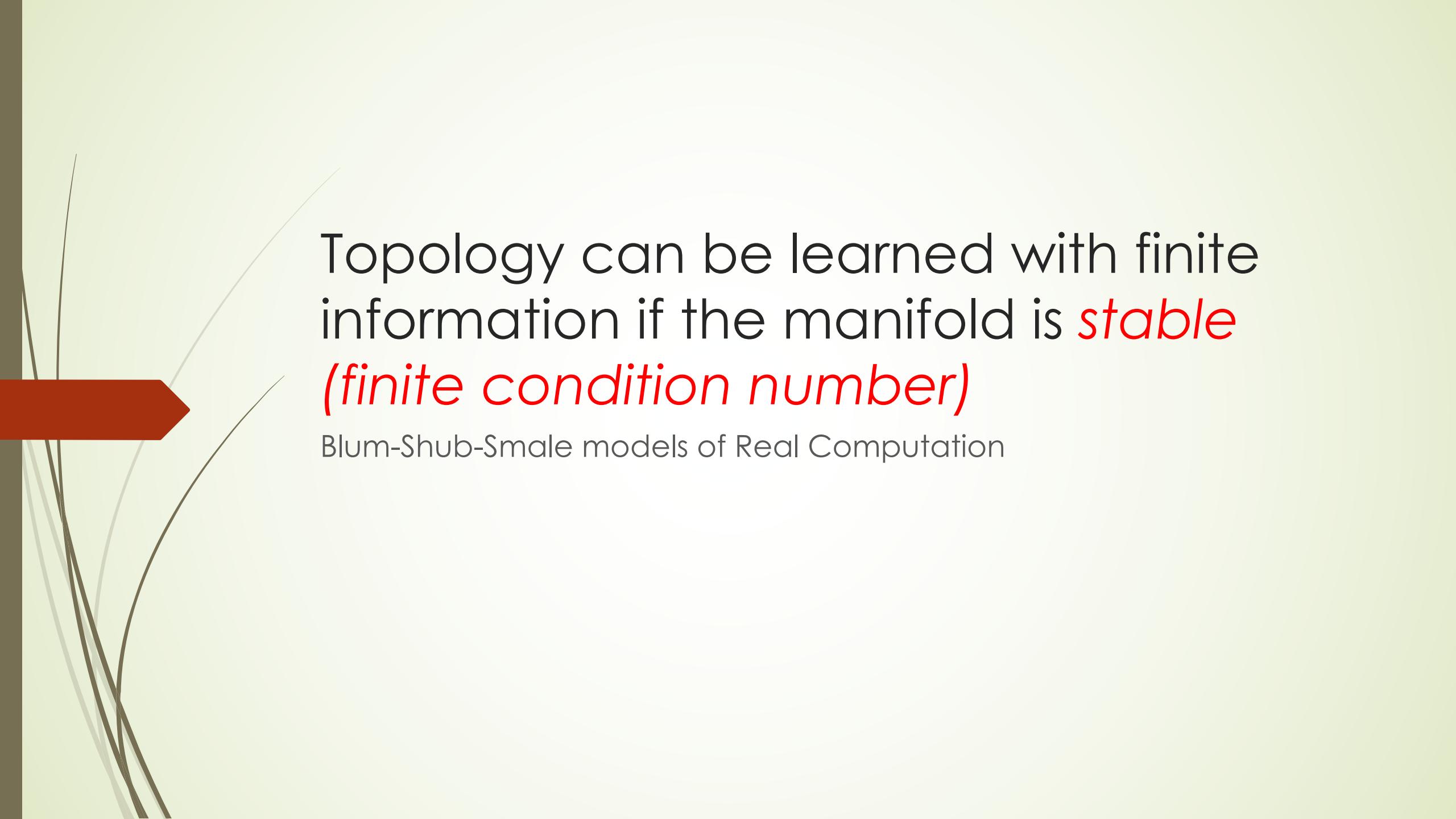
$$x_j = \sum_i y_i w_{ij} \quad (1)$$

Units can be given biases by introducing an extra input to each unit which always has a value of 1. The weight on this extra input is called the bias and is equivalent to a threshold of the opposite sign. It can be treated just like the other weights.

A unit has a real-valued output,  $y_j$ , which is a non-linear function of its total input

$$y_j = \frac{1}{1 + e^{-x_j}} \quad (2)$$

\* To whom correspondence should be addressed



Topology can be learned with finite information if the manifold is *stable*  
*(finite condition number)*

Blum-Shub-Smale models of Real Computation

# A Model of Real Computation



- ▶ Starting from **Blum, Shub, Smale** (1989)
- ▶ It admits inputs and operations (addition, subtraction, multiplication, and (in the case of fields) division) of **real (complex) numbers** with *infinite precision*
- ▶ “The key importance of the **condition number**, which measures the closeness of a problem instance to the manifold of ill-posed instances, is clearly developed.” – **Richard Karp**



# The Condition Number of a Manifold

Throughout our discussion, we associate to  $\mathcal{M}$  a condition number ( $1/\tau$ ) where  $\tau$  is defined as the largest number having the property: The open normal bundle about  $\mathcal{M}$  of radius  $r$  is embedded in  $\mathbb{R}^N$  for every  $r < \tau$ . Its image  $\text{Tub}_\tau$  is a tubular neighborhood of  $\mathcal{M}$  with its canonical projection map

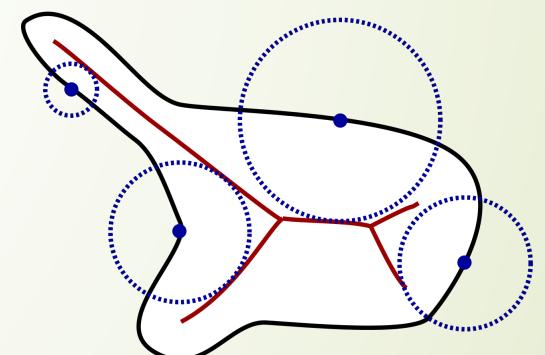
$$\pi_0 : \text{Tub}_\tau \rightarrow \mathcal{M}.$$

## Smallest Local Feature Size

$$G = \{x \in \mathbb{R}^N \text{ such that } \exists \text{ distinct } p, q \in \mathcal{M} \text{ where } d(x, \mathcal{M}) = \|x - p\| = \|x - q\|\},$$

where  $d(x, \mathcal{M}) = \inf_{y \in \mathcal{M}} \|x - y\|$  is the distance of  $x$  to  $\mathcal{M}$ . The closure of  $G$  is called the medial axis and for any point  $p \in \mathcal{M}$  the local feature size  $\sigma(p)$  is the distance of  $p$  to the medial axis. Then it is easy to check that

$$\tau = \inf_{p \in \mathcal{M}} \sigma(p).$$



# Find Homology with Finite Samples

[Niyogi, Smale, Weinberger (2008)]

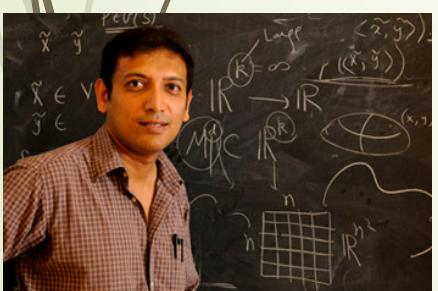
**Theorem 3.1** Let  $\mathcal{M}$  be a compact submanifold of  $\mathbb{R}^N$  with condition number  $\tau$ . Let  $\bar{x} = \{x_1, \dots, x_n\}$  be a set of  $n$  points drawn in i.i.d. fashion according to the uniform probability measure on  $\mathcal{M}$ . Let  $0 < \epsilon < \tau/2$ . Let  $U = \bigcup_{x \in \bar{x}} B_\epsilon(x)$  be a correspondingly random open subset of  $\mathbb{R}^N$ . Then for all

$$n > \beta_1 \left( \log(\beta_2) + \log\left(\frac{1}{\delta}\right) \right),$$

the homology of  $U$  equals the homology of  $\mathcal{M}$  with high confidence (probability  $> 1 - \delta$ ).

$$\beta_1 = \frac{\text{vol}(\mathcal{M})}{(\cos^k(\theta_1))\text{vol}(B_{\epsilon/4}^k)} \quad \text{and} \quad \beta_2 = \frac{\text{vol}(\mathcal{M})}{(\cos^k(\theta_2))\text{vol}(B_{\epsilon/8}^k)}.$$

Here  $k$  is the dimension of the manifold  $\mathcal{M}$  and  $\text{vol}(B_\epsilon^k)$  denotes the  $k$ -dimensional volume of the standard  $k$ -dimensional ball of radius  $\epsilon$ . Finally,  $\theta_1 = \arcsin(\epsilon/8\tau)$  and  $\theta_2 = \arcsin(\epsilon/16\tau)$ .



# Curse of Dimensionality and “Quantum Algorithms”

To construct a Rips-complex of dimension of  $n$  points:  $O(2^n)$  number of simplices is needed in the worst case =>  $O(\text{poly}(n))$  in Quantum Algorithms



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Quantum algorithms for topological and geometric analysis of data

Seth Lloyd<sup>1</sup>, Silvano Garnerone<sup>2</sup> & Paolo Zanardi<sup>3</sup>

# A Proof of Concept Demonstration by 6-photon Quantum Computer [Huang et al. 2018, arXiv:1801.06316]

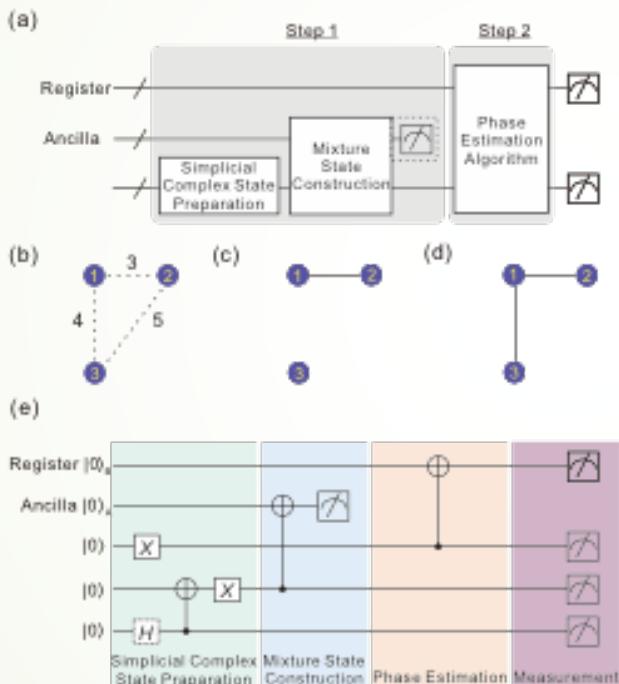


FIG. 2. Quantum circuit for quantum TDA. (a) Outline of the original quantum circuit. (b) A scatterplot including three data points. (c) Graph representation of the 1-simplices state  $|\varphi\rangle_1^{e_1} = |110\rangle$  for  $3 < \epsilon_1 < 4$ . The first and second data points are connected by an edge. (d) Graph representation of 1-simplices state  $|\varphi\rangle_1^{e_2} = (|110\rangle + |101\rangle)/\sqrt{2}$  for  $4 < \epsilon_2 < 5$ . The first data point is connected to the second and third points by two edges. (e) Optimized circuit with 5 qubits. The blocks with different colors represent the four basic stages.

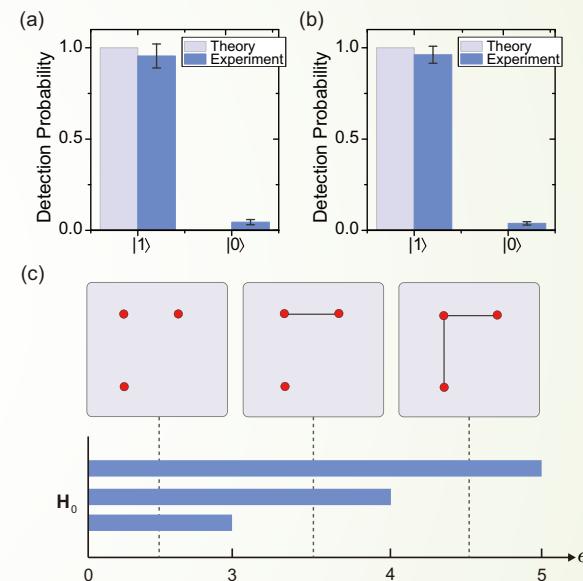
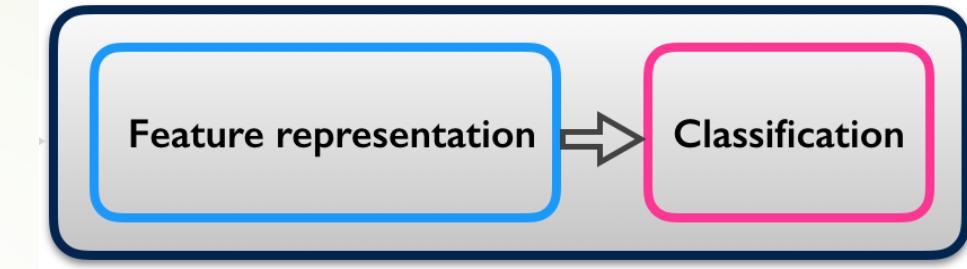


FIG. 4. Final experimental results. The output is determined by measuring the eigenvalue register in the Pauli-Z basis. Measured expectation values (blue bars) and theoretically predicted values (gray bars) are shown for two different 1-simplices state inputs: (a)  $|\varphi\rangle_1^{e_1} = |110\rangle$ , (b)  $|\varphi\rangle_1^{e_2} = (|110\rangle + |101\rangle)/\sqrt{2}$ . Error bars represent one standard deviation, deduced from propagated Poissonian counting statistics of the raw detection events. (c) The barcode for  $0 < \epsilon < 5$ . Since no  $k$ -dimensional holes for  $k \geq 1$  exist at these scales, only the 0-th Betti barcode is given here. For  $0 < \epsilon < 3$ , there is no connection between each point, so the 0-th Betti number is equal to the number of points. That is, there are three bars at  $0 < \epsilon < 3$ . At scales of  $3 < \epsilon_1 < 4$  and  $4 < \epsilon_2 < 5$ , the 0-th Betti number are 2 and 1.



# Transfer Learning: Fine Tuning

# Transfer Learning?

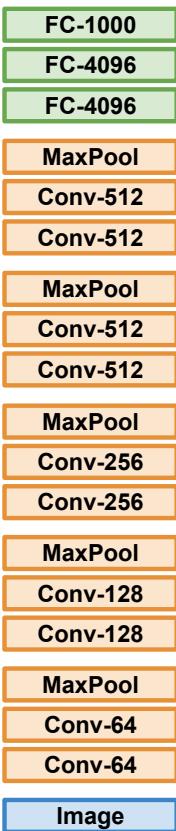


- Filters learned in first layers of a network are transferable from one task to another
- When solving another problem, no need to retrain the lower layers, just fine tune upper ones
- Is this simply due to the large amount of images in ImageNet?
- Does solving many classification problems simultaneously result in features that are more easily transferable?
- Does this imply filters can be learned in unsupervised manner?
- Can we characterize filters mathematically?

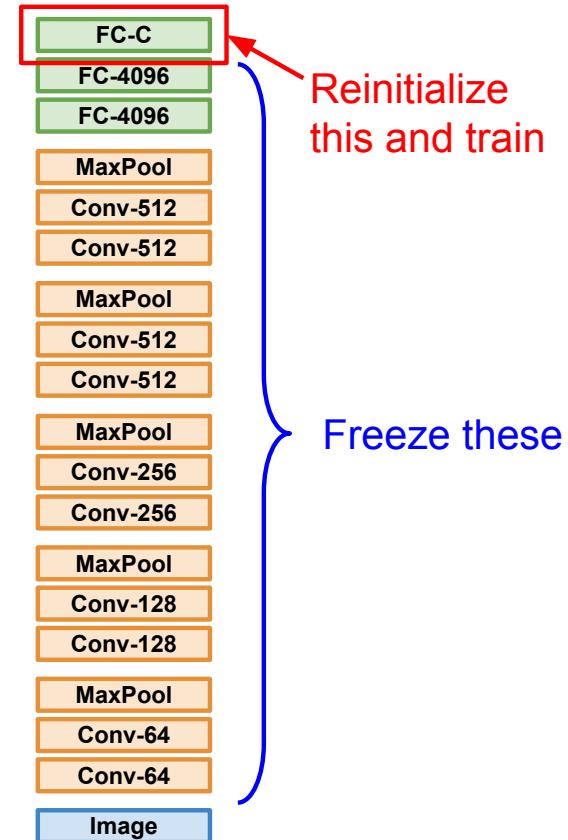
Donahue et al, "DeCAF: A Deep Convolutional Activation Feature for Generic Visual Recognition", ICML 2014  
Razavian et al, "CNN Features Off-the-Shelf: An Astounding Baseline for Recognition", CVPR Workshops 2014

# Transfer Learning with CNNs

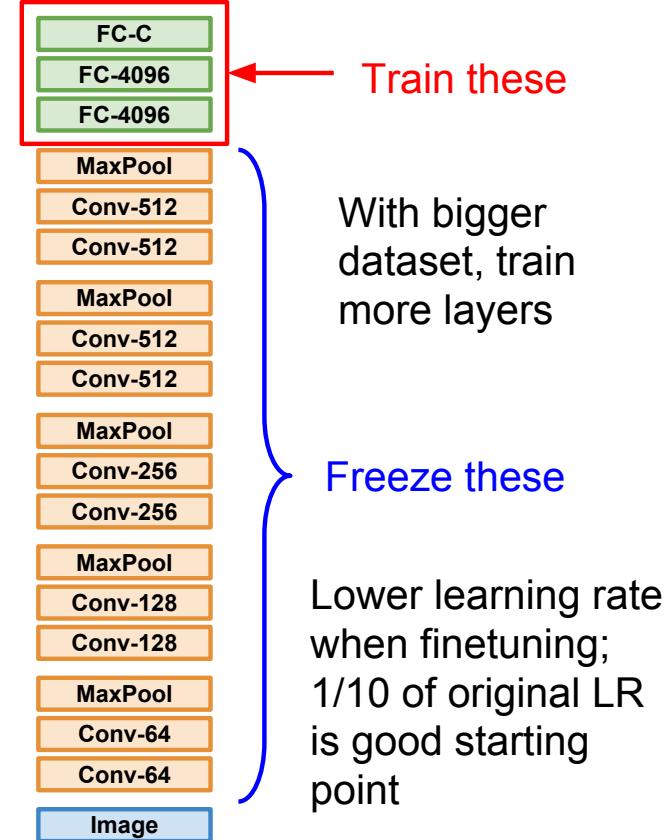
## 1. Train on Imagenet



## 2. Small Dataset (C classes)



## 3. Bigger dataset





More specific

More generic

	<b>very similar dataset</b>	<b>very different dataset</b>
<b>very little data</b>	Use Linear Classifier on top layer	You're in trouble... Try linear classifier from different stages
<b>quite a lot of data</b>	Finetune a few layers	Finetune a larger number of layers

# Example Demo

- ▶ Jupyter notebook with pytorch

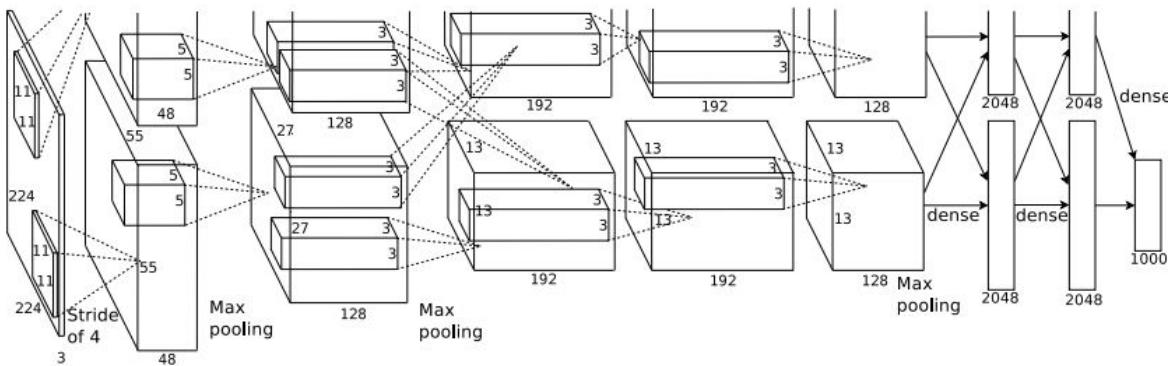


# Visualizing Convolutional Networks

# Understanding intermediate neurons?



Input Image:  
3 x 224 x 224



What are the intermediate features looking for?

Class Scores:  
1000 numbers

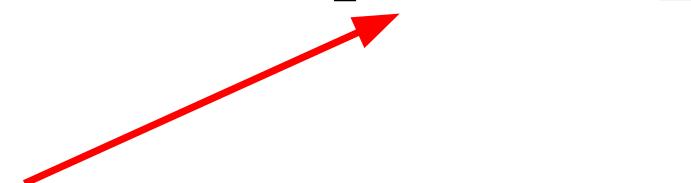
# Visualizing CNN Features: Gradient Ascent

- **Gradient ascent:** Generate a synthetic image that maximally activates a neuron

$$I^* = \arg \max_I f(I) + R(I)$$

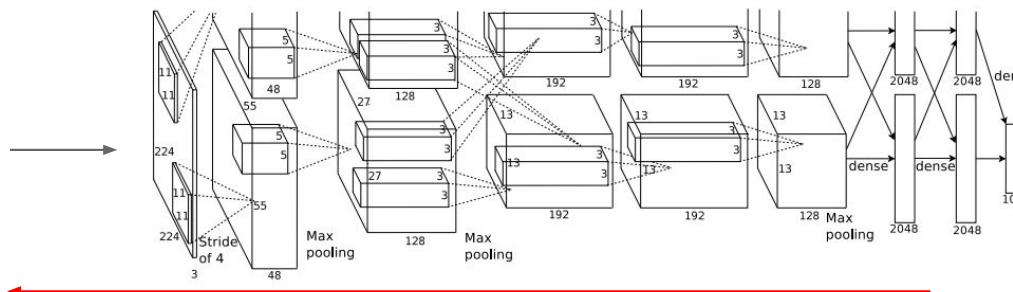
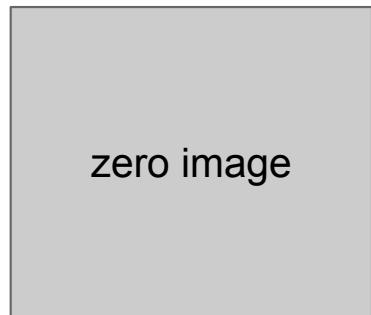
Neuron value

Natural image regularizer



# Visualizing CNN Features: Gradient Ascent

1. Initialize image to zeros



Repeat:

2. Forward image to compute current scores
3. Backprop to get gradient of neuron value with respect to image pixels
4. Make a small update to the image

$$\arg \max_I S_c(I) - \lambda \|I\|_2^2$$

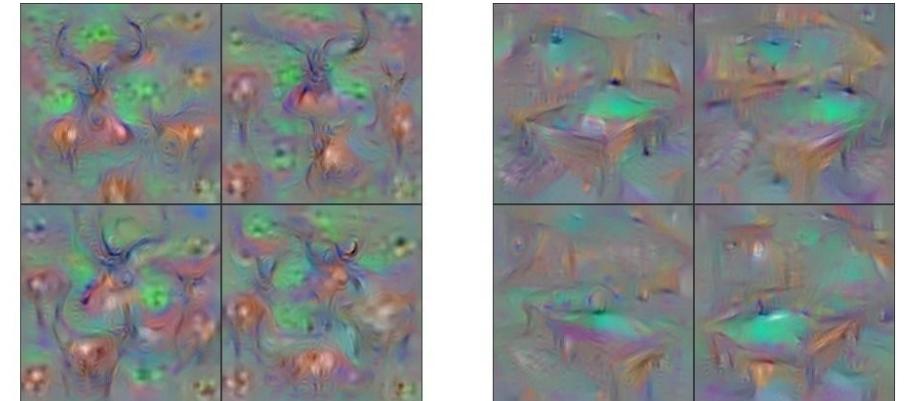
score for class c (before Softmax)

# Visualizing CNN Features: Gradient Ascent

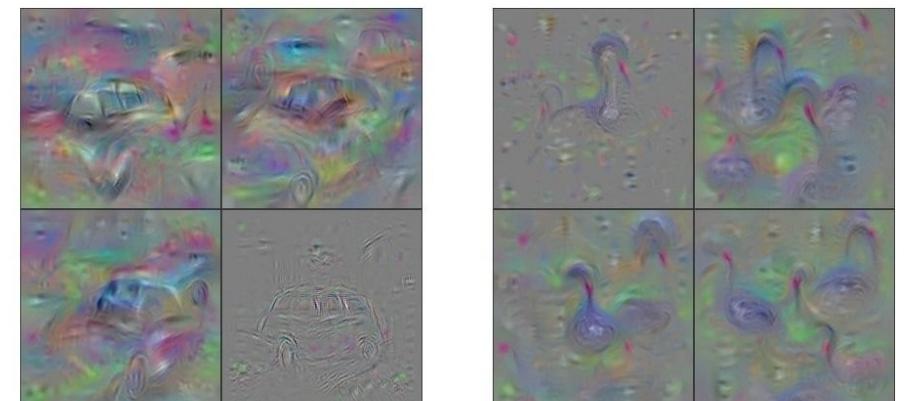
$$\arg \max_I S_c(I) - \lambda \|I\|_2^2$$

Better regularizer: Penalize L2 norm of image; also during optimization periodically

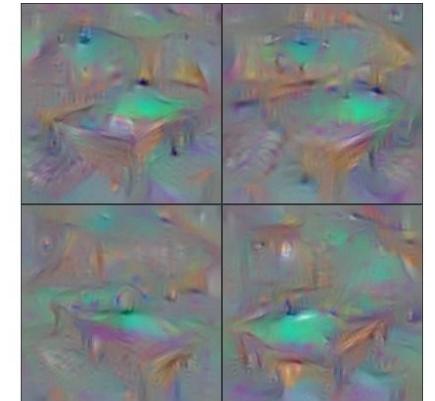
- (1) Gaussian blur image
- (2) Clip pixels with small values to 0
- (3) Clip pixels with small gradients to 0



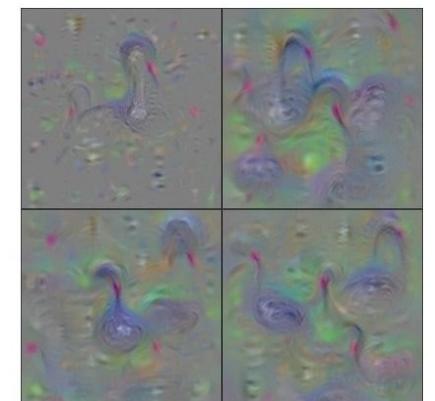
Hartebeest



Station Wagon



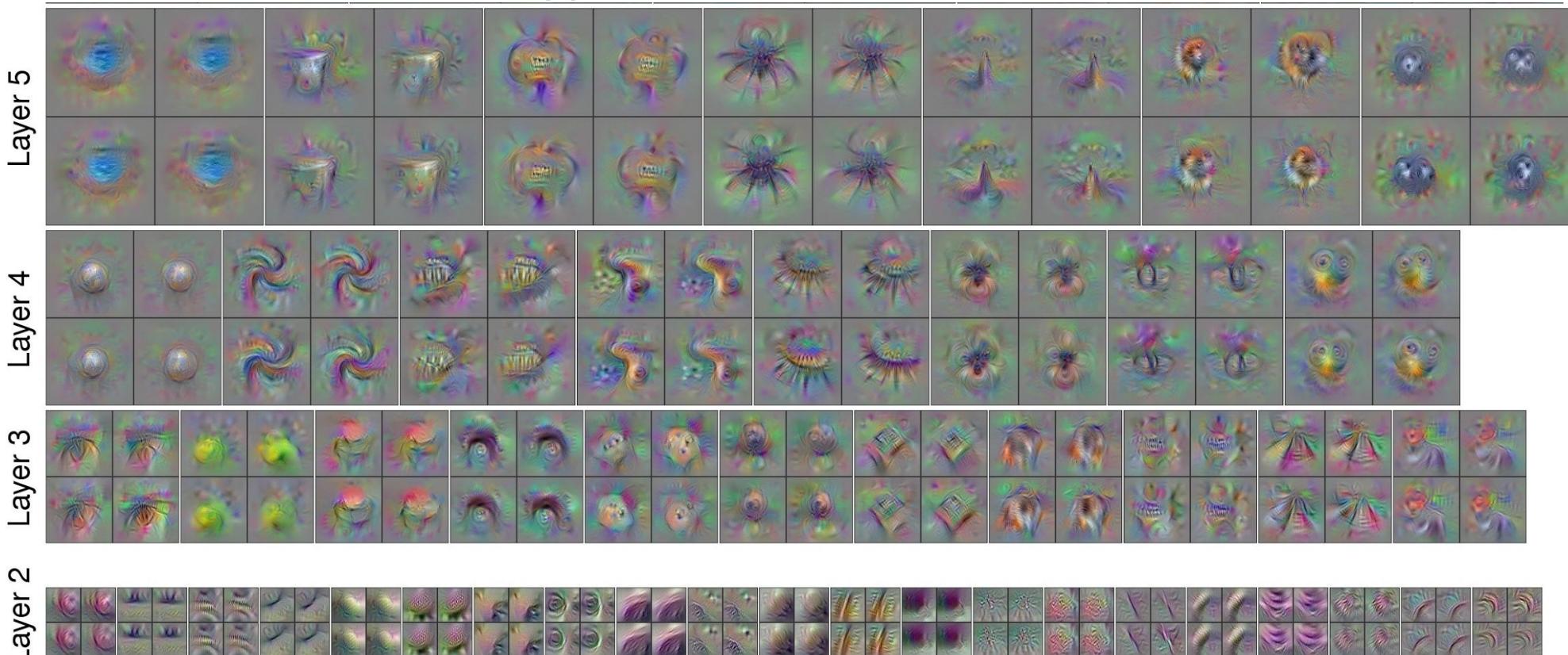
Billiard Table



Black Swan

# Visualizing CNN Features: Gradient Ascent

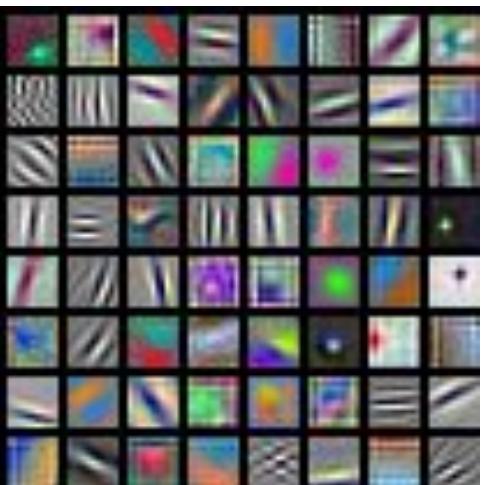
Use the same approach to visualize intermediate features



Yosinski et al, "Understanding Neural Networks Through Deep Visualization", ICML DL Workshop 2014.  
Figure copyright Jason Yosinski, Jeff Clune, Anh Nguyen, Thomas Fuchs, and Hod Lipson, 2014. Reproduced with permission.

# It's easy to visualize early layers

# First Layer: Visualize Filters



## AlexNet: 64 x 3 x 11 x 11



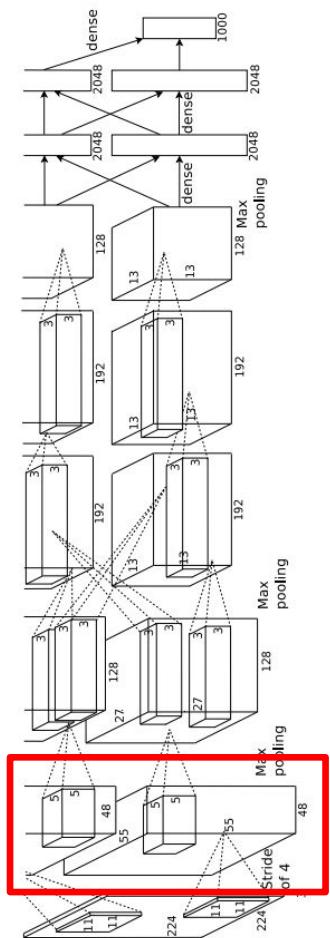
## ResNet-18: 64 x 3 x 7 x 7



# ResNet-101: 64 x 3 x 7 x 7



# DenseNet-121: 64 x 3 x 7 x 7



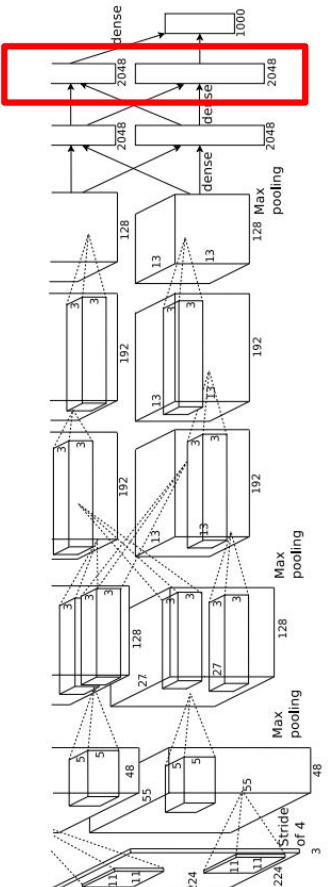
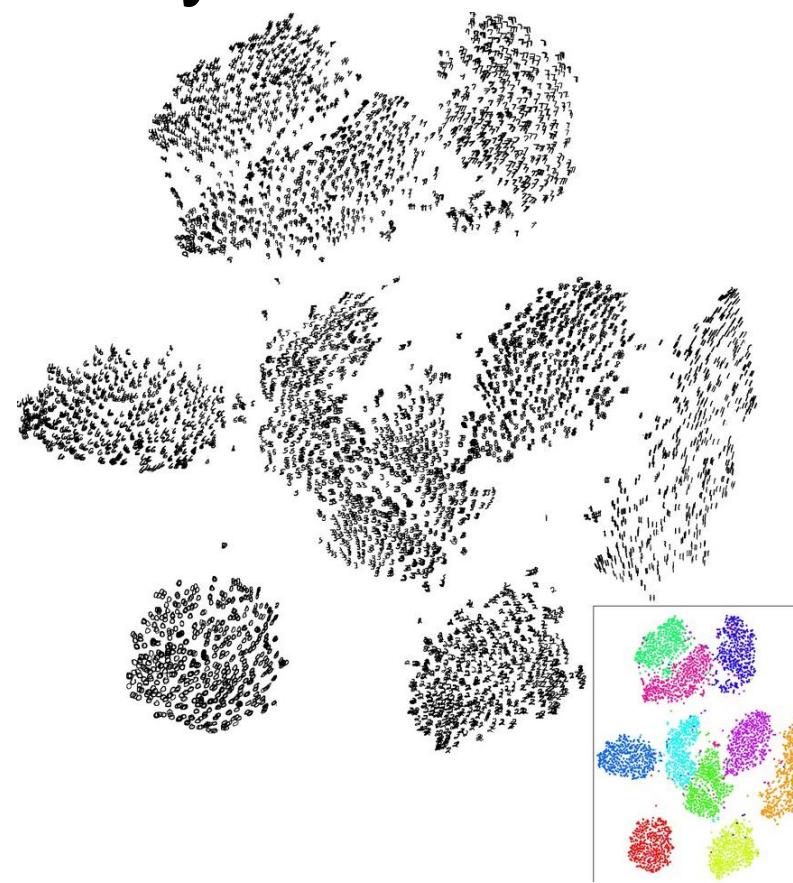
# Last layers are hard to visualize

## Last Layer: Dimensionality Reduction

Visualize the “space” of FC7 feature vectors by reducing dimensionality of vectors from 4096 to 2 dimensions

Simple algorithm: Principle Component Analysis (PCA)

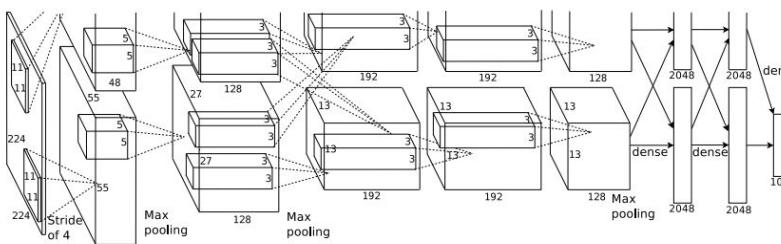
More complex: t-SNE



Van der Maaten and Hinton, “Visualizing Data using t-SNE”, JMLR 2008  
Figure copyright Laurens van der Maaten and Geoff Hinton, 2008. Reproduced with permission.

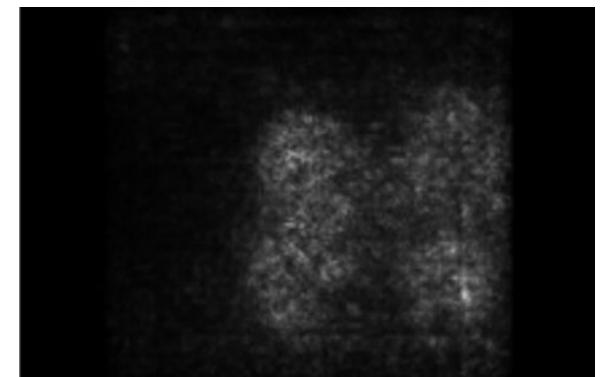
# Saliency Maps

How to tell which pixels matter for classification?



Dog

Compute gradient of (unnormalized) class score with respect to image pixels, take absolute value and max over RGB channels

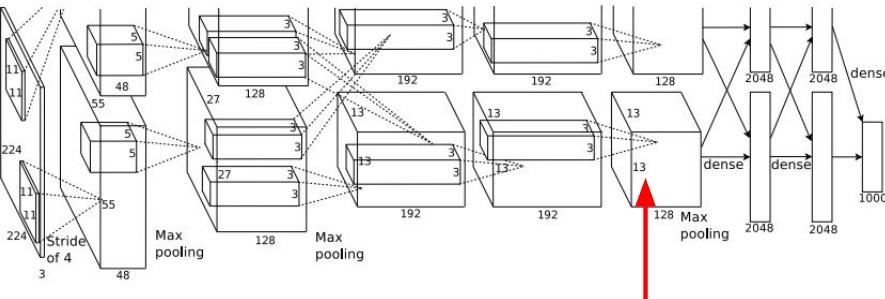


Simonyan, Vedaldi, and Zisserman, "Deep Inside Convolutional Networks: Visualising Image Classification Models and Saliency Maps", ICLR Workshop 2014.

Figures copyright Karen Simonyan, Andrea Vedaldi, and Andrew Zisserman, 2014; reproduced with permission.

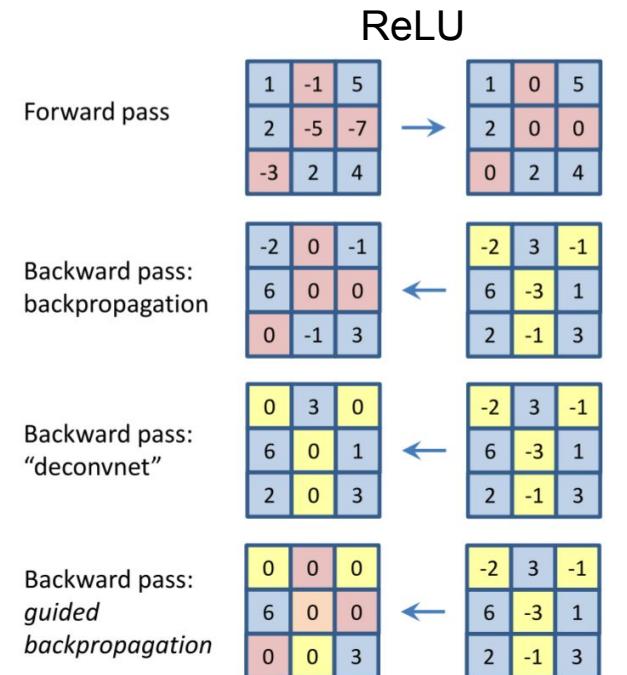
# Guided BP

## Intermediate features via (guided) backprop



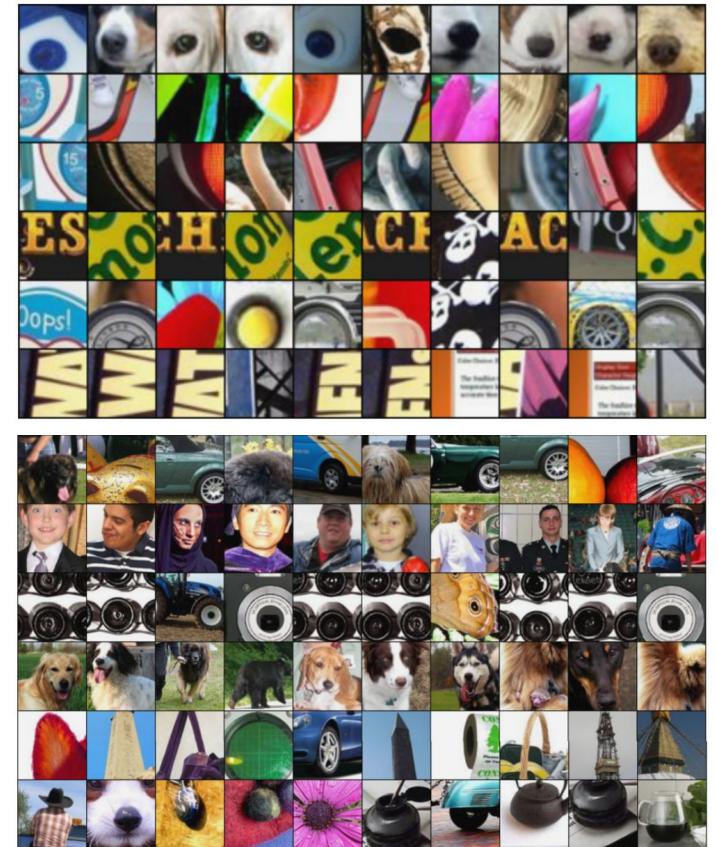
Pick a single intermediate neuron, e.g. one value in  $128 \times 13 \times 13$  conv5 feature map

Compute gradient of neuron value with respect to image pixels



Images come out nicer if you only backprop positive gradients through each ReLU (guided backprop)

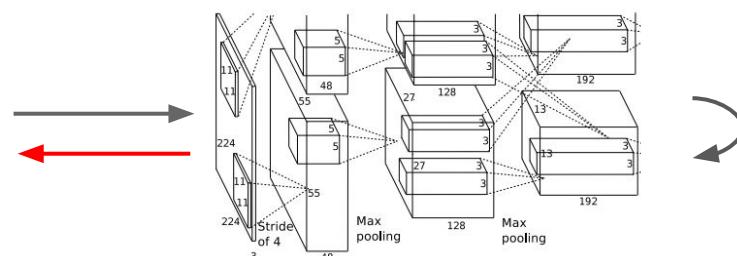
# Intermediate features via Guided BP



Zeiler and Fergus, "Visualizing and Understanding Convolutional Networks", ECCV 2014  
Springenberg et al, "Striving for Simplicity: The All Convolutional Net", ICLR Workshop 2015  
Figure copyright Jost Tobias Springenberg, Alexey Dosovitskiy, Thomas Brox, Martin Riedmiller, 2015; reproduced with permission.

# DeepDream: amplifying features

Rather than synthesizing an image to maximize a specific neuron, instead try to **amplify** the neuron activations at some layer in the network

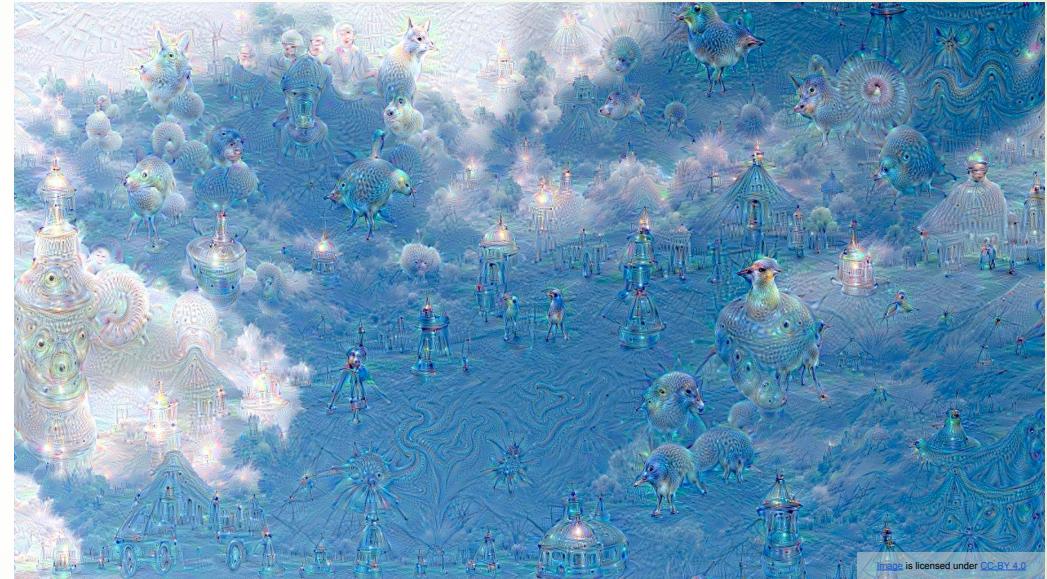


Choose an image and a layer in a CNN; repeat:

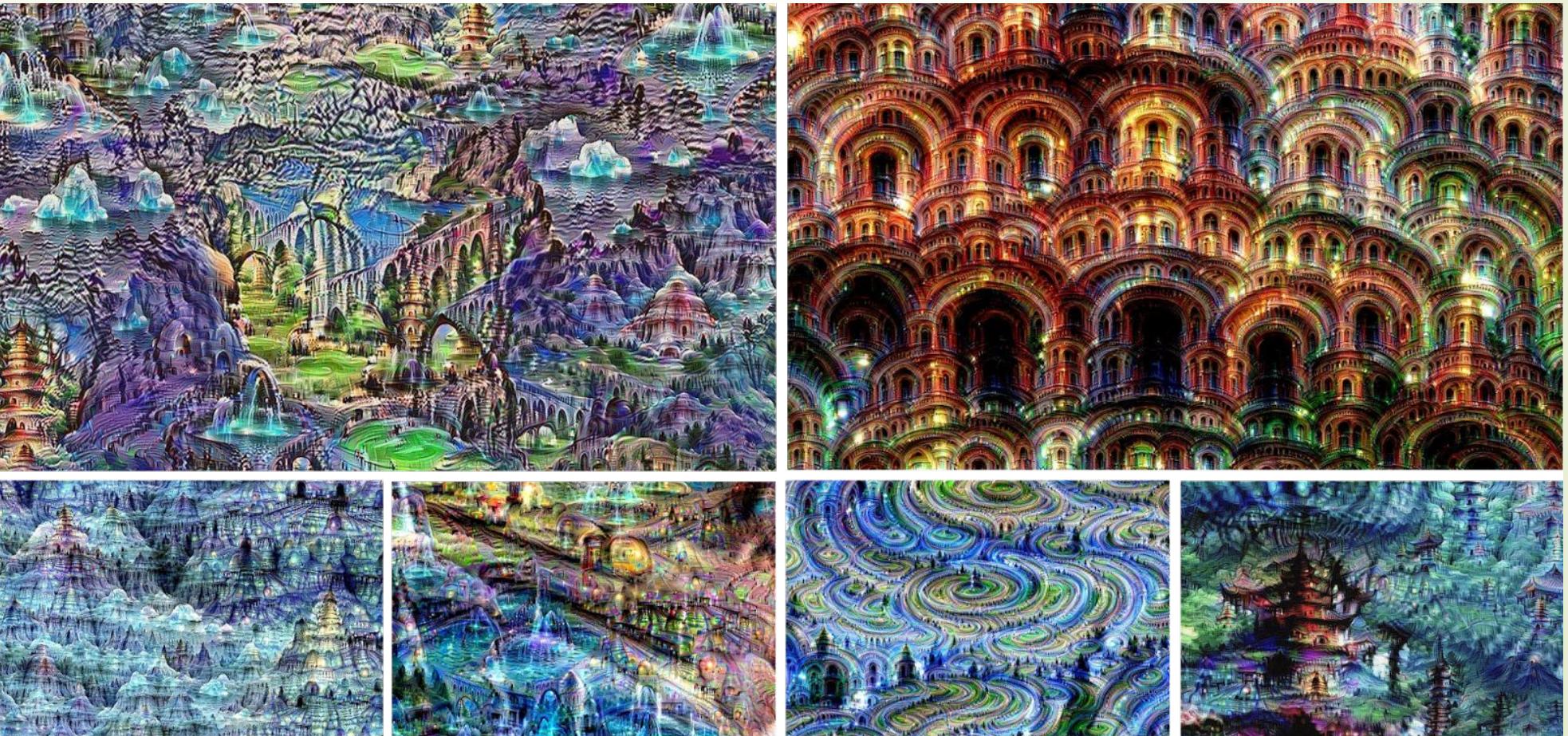
1. Forward: compute activations at chosen layer
2. Set gradient of chosen layer *equal to its activation*
3. Backward: Compute gradient on image
4. Update image

Equivalent to:  
 $I^* = \arg \max_I \sum_i f_i(I)^2$

# Example: DeepDream of Sky



# More Examples



[Image](#) is licensed under CC-BY 4.0

# Python Notebooks

- ▶ An interesting Pytorch Implementation of these visualizatoin methods
  - ▶ <https://github.com/utkuozbulak/pytorch-cnn-visualizations>
- ▶ Some examples demo



Neural Style

# Example: The Noname Lake in PKU

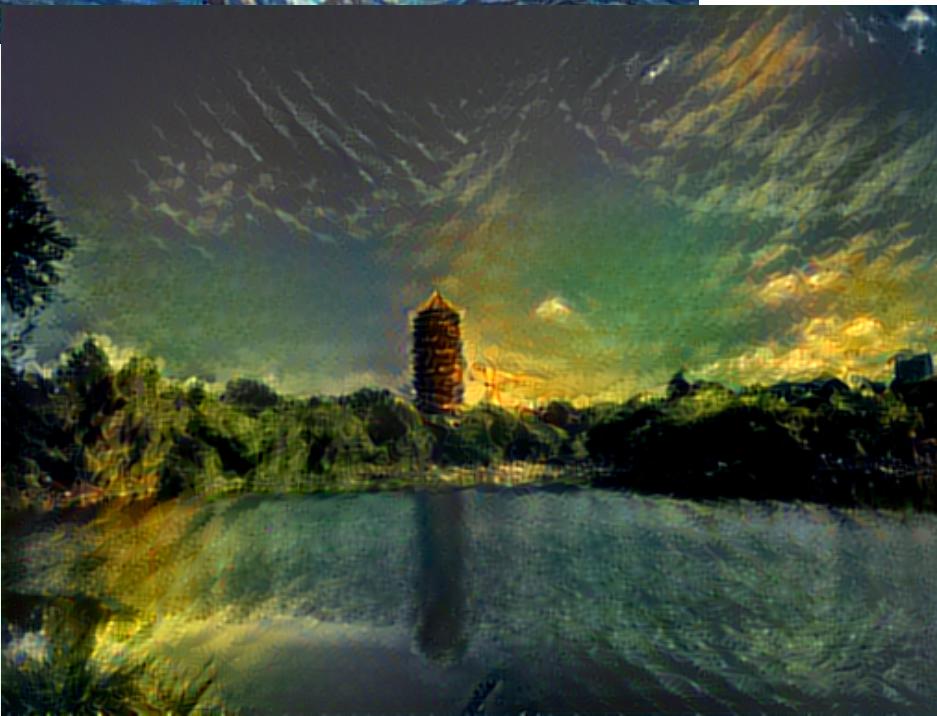
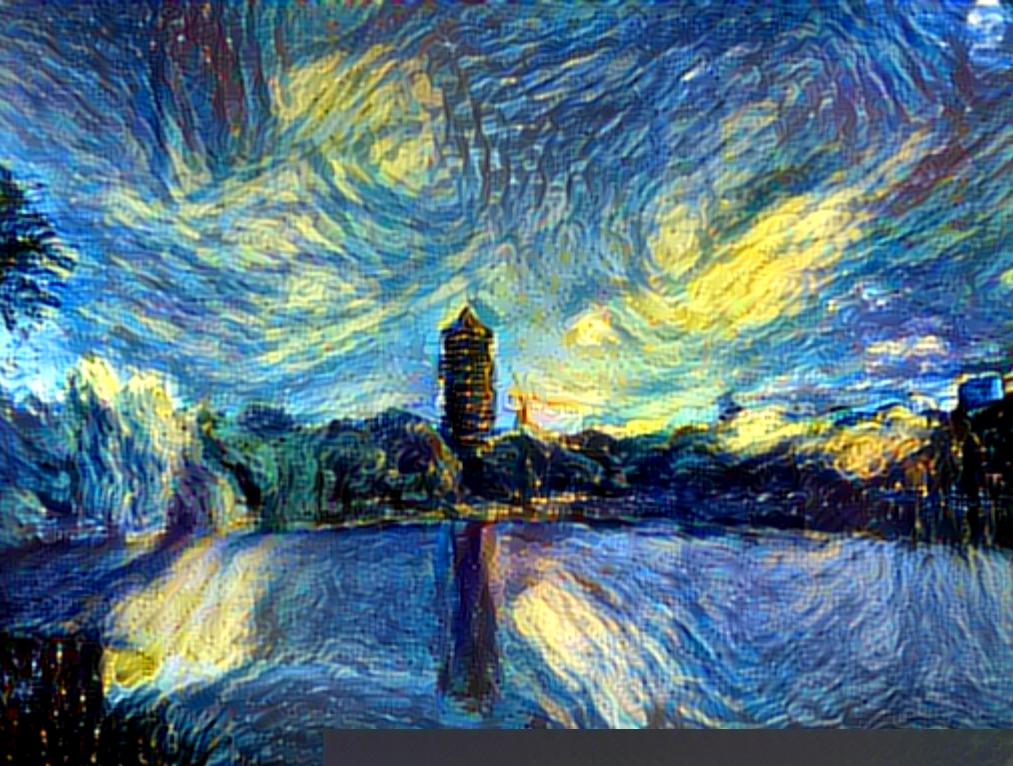




Left: Vincent Van Gogh, Starry Night  
Right: Claude Monet, Twilight Venice  
Bottom: William Turner, Ship Wreck



开始吧



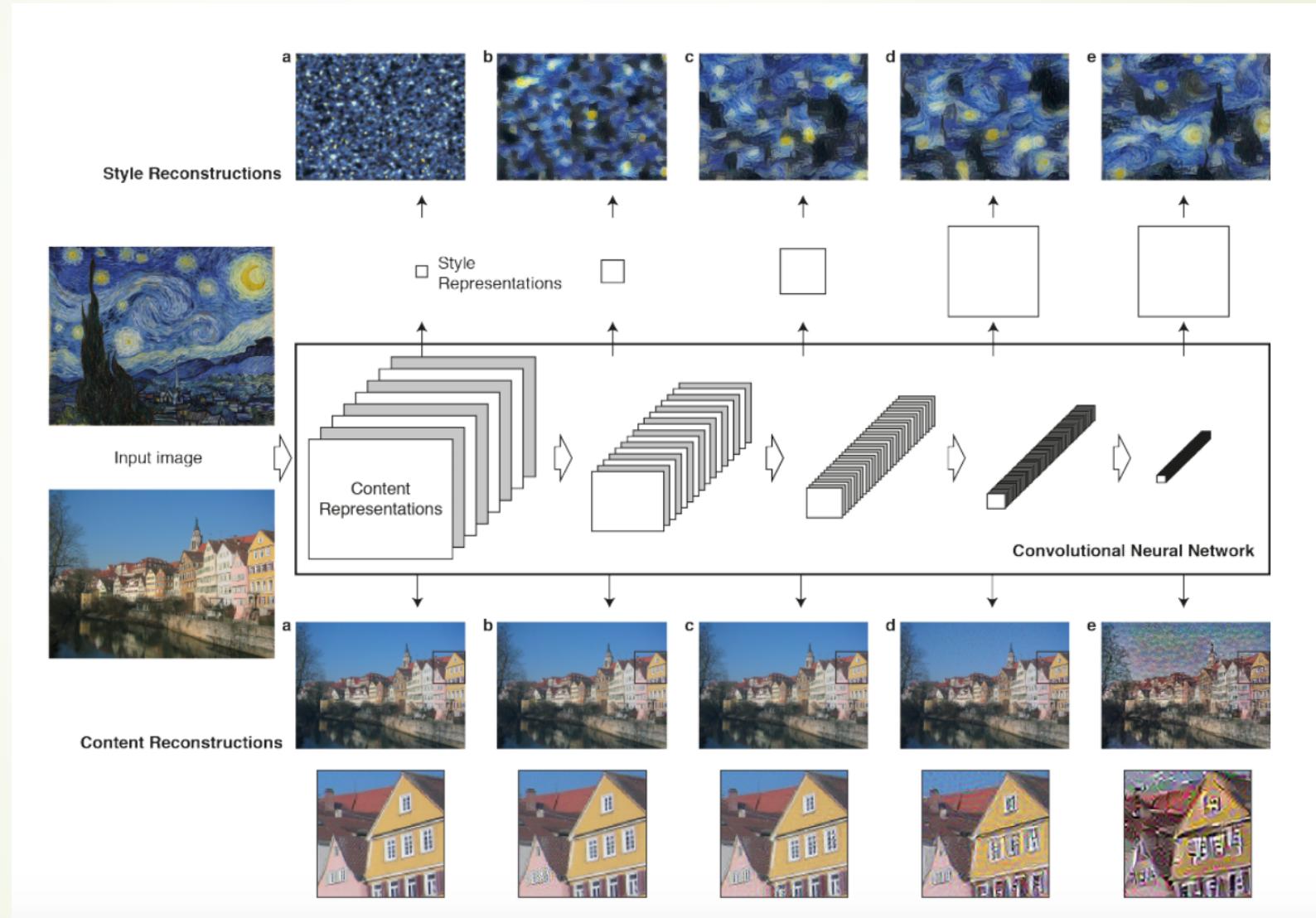
Application of Deep Learning:  
Content-Style synthetic  
pictures  
By “neural-style”



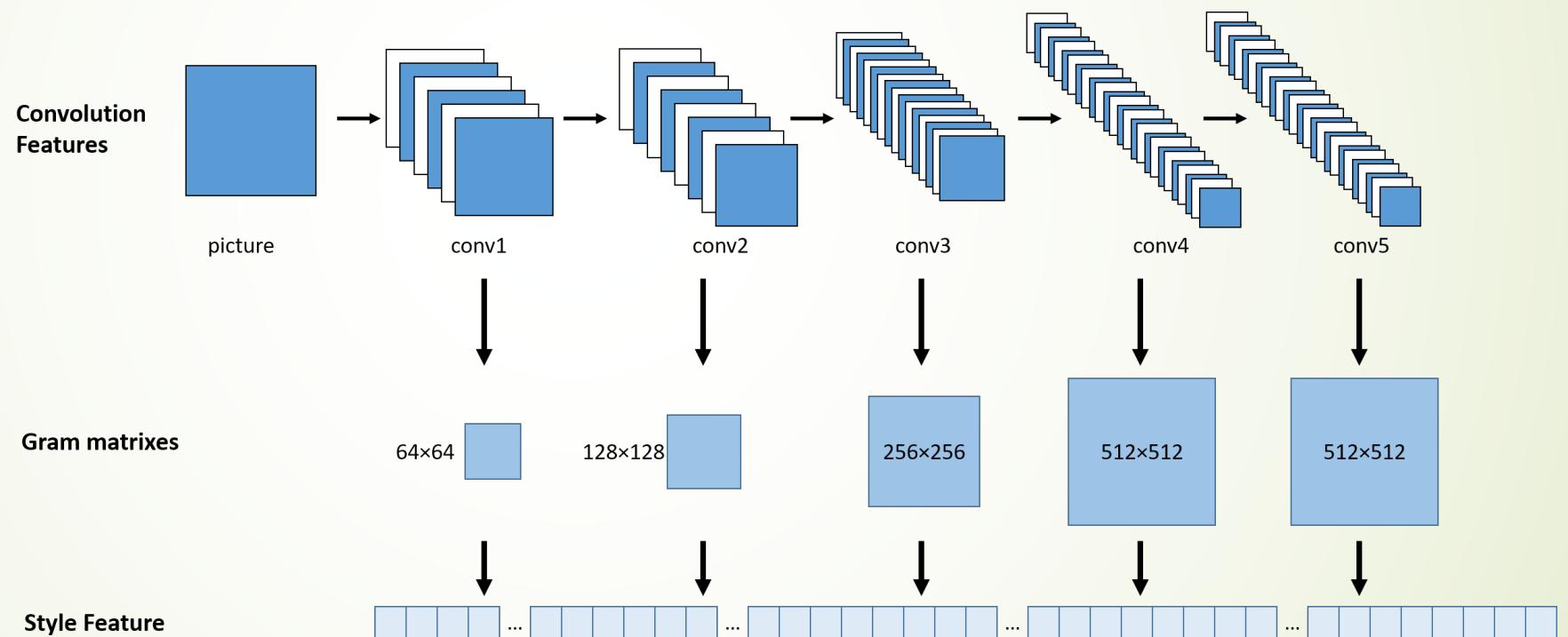
# Neural Style

- ▶ J C Johnson's Website: <https://github.com/jcjohnson/neural-style>
- ▶ A torch implementation of the paper
  - ▶ *A Neural Algorithm of Artistic Style*,
  - ▶ by Leon A. Gatys, Alexander S. Ecker, and Matthias Bethge.
  - ▶ <http://arxiv.org/abs/1508.06576>

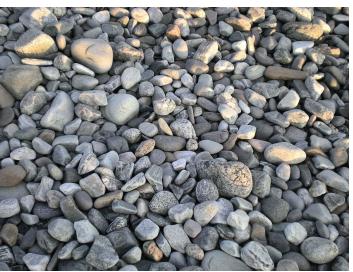
# Style-Content Feature Extraction



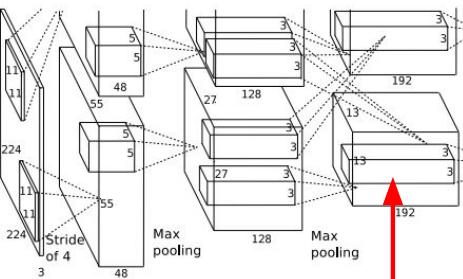
# Style Features as Second Order Statistics



# Neural Texture Synthesis



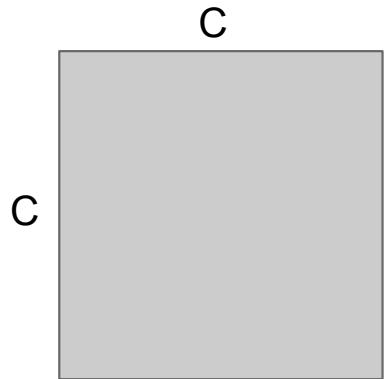
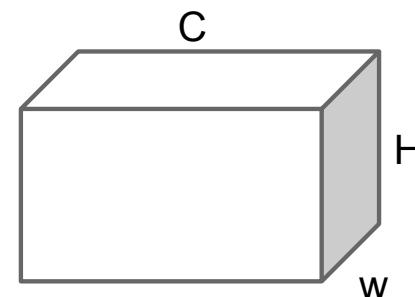
This image is in the public domain.



Each layer of CNN gives  $C \times H \times W$  tensor of features;  $H \times W$  grid of  $C$ -dimensional vectors

Outer product of two  $C$ -dimensional vectors gives  $C \times C$  matrix measuring co-occurrence

Average over all  $HW$  pairs of vectors, giving **Gram matrix** of shape  $C \times C$



Efficient to compute; reshape features from

$C \times H \times W$  to  $=C \times HW$

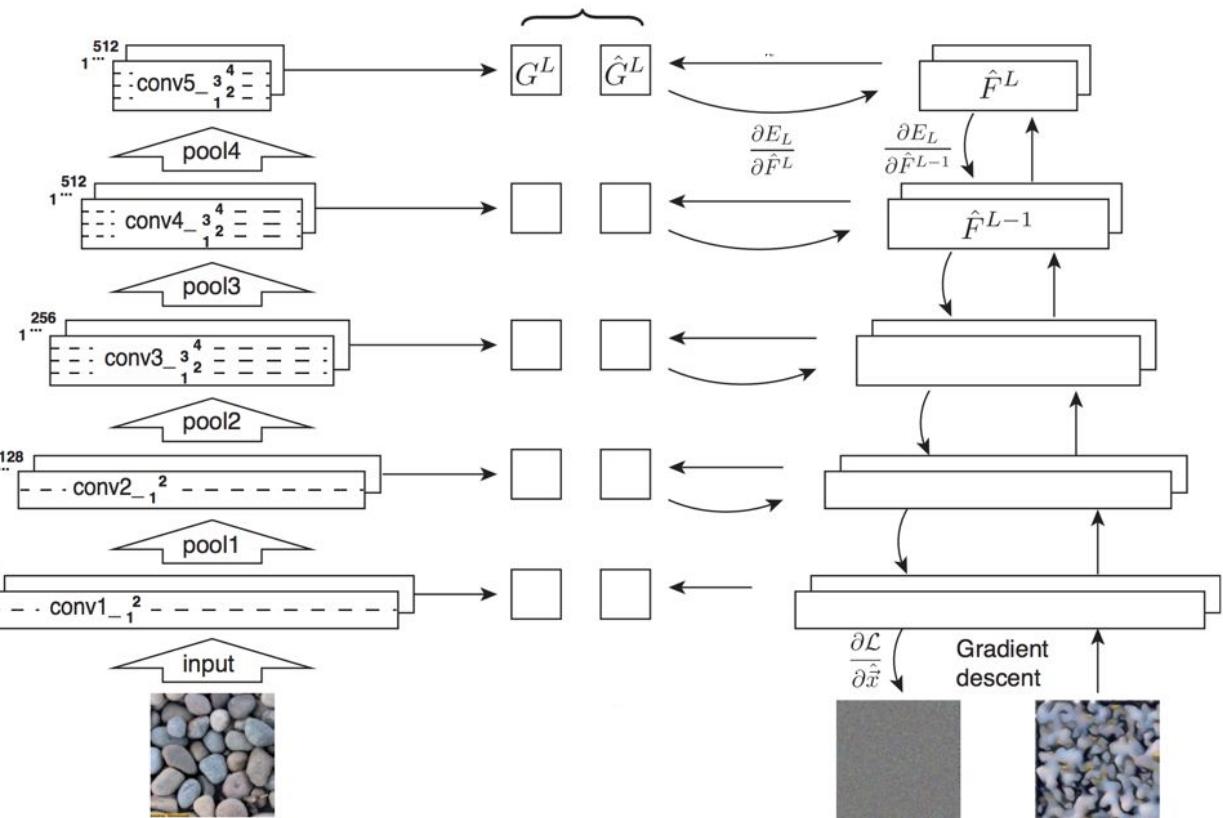
then compute  $G = FF^T$

# Neural Texture Synthesis

1. Pretrain a CNN on ImageNet (VGG-19)
2. Run input texture forward through CNN, record activations on every layer; layer  $i$  gives feature map of shape  $C_i \times H_i \times W_i$
3. At each layer compute the *Gram matrix* giving outer product of features:
$$G_{ij}^l = \sum_k F_{ik}^l F_{jk}^l \text{ (shape } C_i \times C_i\text{)}$$
4. Initialize generated image from random noise
5. Pass generated image through CNN, compute Gram matrix on each layer
6. Compute loss: weighted sum of L2 distance between Gram matrices
7. Backprop to get gradient on image
8. Make gradient step on image
9. GOTO 5

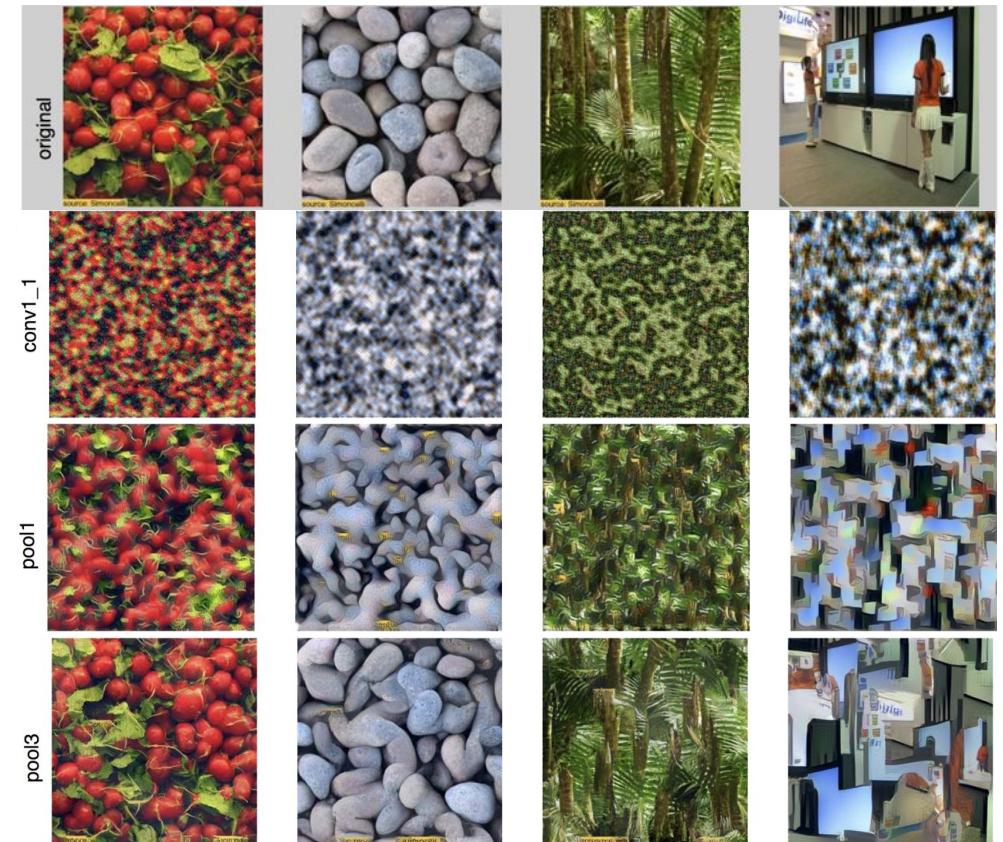
Gatys, Ecker, and Bethge, "Texture Synthesis Using Convolutional Neural Networks", NIPS 2015  
 Figure copyright Leon Gatys, Alexander S. Ecker, and Matthias Bethge, 2015. Reproduced with permission.

$$E_l = \frac{1}{4N_l^2 M_l^2} \sum_{i,j} (G_{ij}^l - \hat{G}_{ij}^l)^2 \quad \mathcal{L}(\vec{x}, \hat{\vec{x}}) = \sum_{l=0}^L w_l E_l$$



# Neural Texture Synthesis

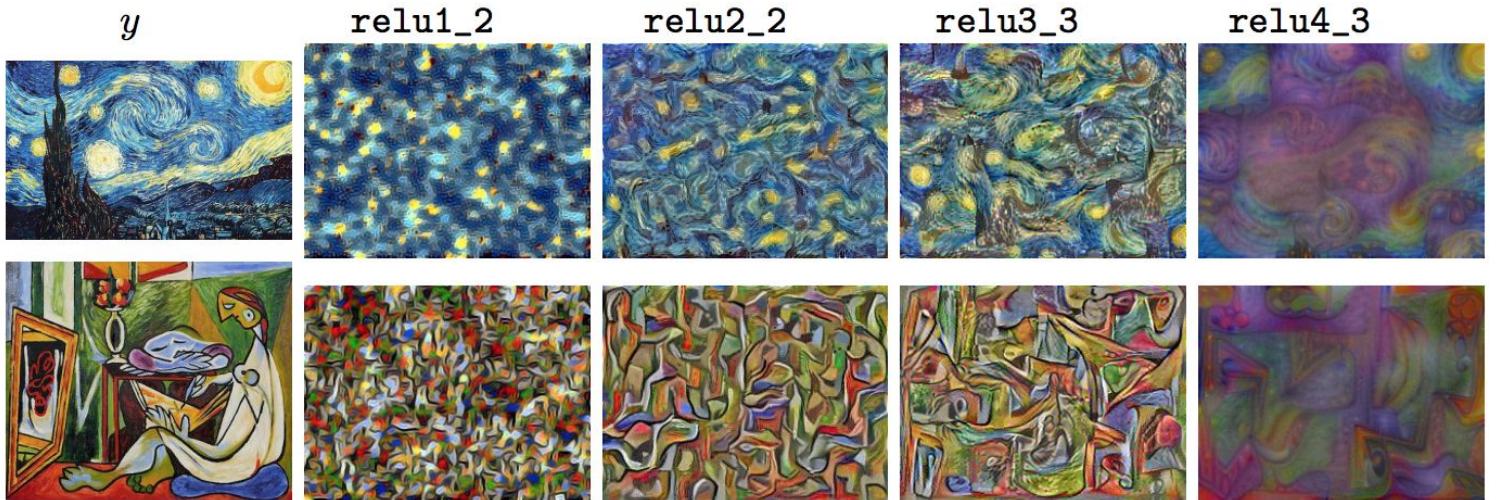
Reconstructing texture from higher layers recovers larger features from the input texture



Gatys, Ecker, and Bethge, "Texture Synthesis Using Convolutional Neural Networks", NIPS 2015  
Figure copyright Leon Gatys, Alexander S. Ecker, and Matthias Bethge, 2015. Reproduced with permission.

# Neural Texture Synthesis: Gram Reconstruction

Texture synthesis  
(Gram  
reconstruction)



# Feature Inversion

Given a CNN feature vector for an image, find a new image that:

- Matches the given feature vector
- “looks natural” (image prior regularization)

$$\mathbf{x}^* = \underset{\mathbf{x} \in \mathbb{R}^{H \times W \times C}}{\operatorname{argmin}} \ell(\Phi(\mathbf{x}), \Phi_0) + \lambda \mathcal{R}(\mathbf{x})$$

Given feature vector

Features of new image

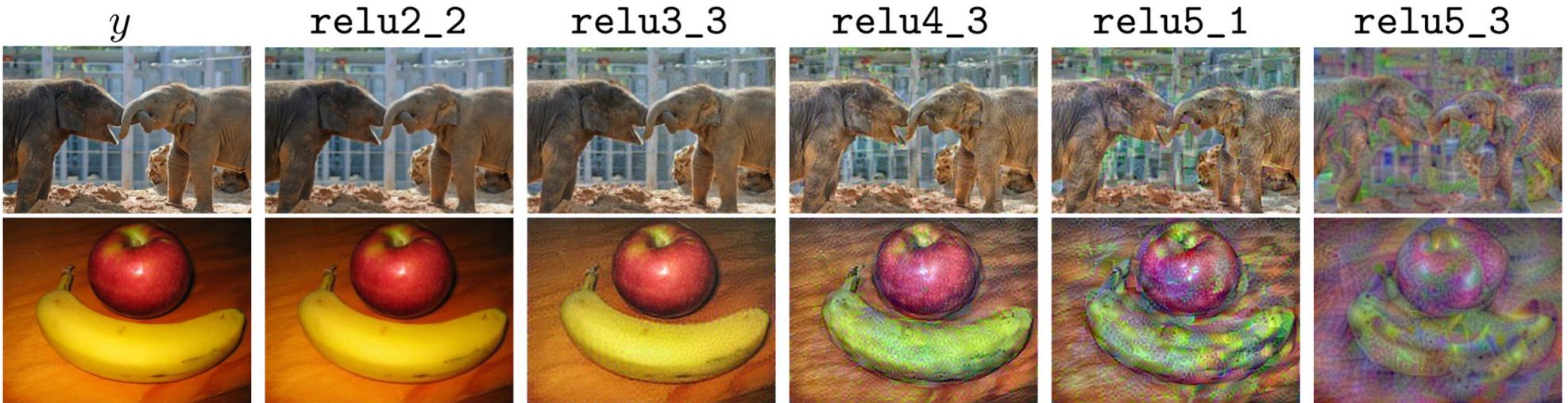
$$\ell(\Phi(\mathbf{x}), \Phi_0) = \|\Phi(\mathbf{x}) - \Phi_0\|^2$$

$$\mathcal{R}_{V^\beta}(\mathbf{x}) = \sum_{i,j} \left( (x_{i,j+1} - x_{ij})^2 + (x_{i+1,j} - x_{ij})^2 \right)^{\frac{\beta}{2}}$$

Total Variation regularizer  
(encourages spatial smoothness)

# Feature Inversion

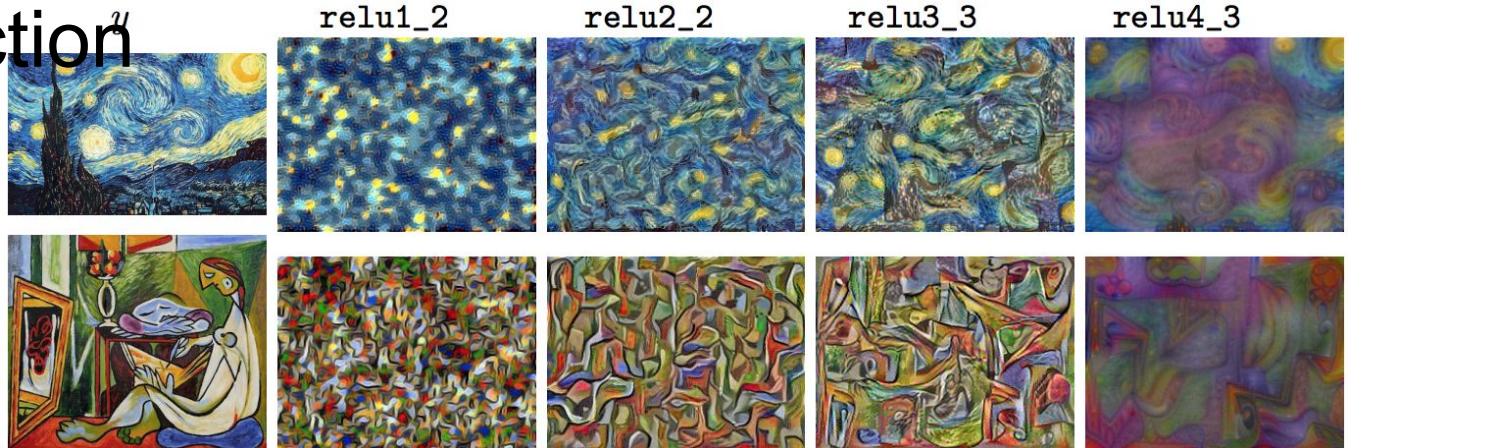
Reconstructing from different layers of VGG-16



Mahendran and Vedaldi, "Understanding Deep Image Representations by Inverting Them", CVPR 2015  
Figure from Johnson, Alahi, and Fei-Fei, "Perceptual Losses for Real-Time Style Transfer and Super-Resolution", ECCV 2016. Copyright Springer, 2016.  
Reproduced for educational purposes.

# Neural Style Transfer: Feature + Gram Reconstruction

Texture synthesis  
(Gram reconstruction)



Feature  
reconstruction

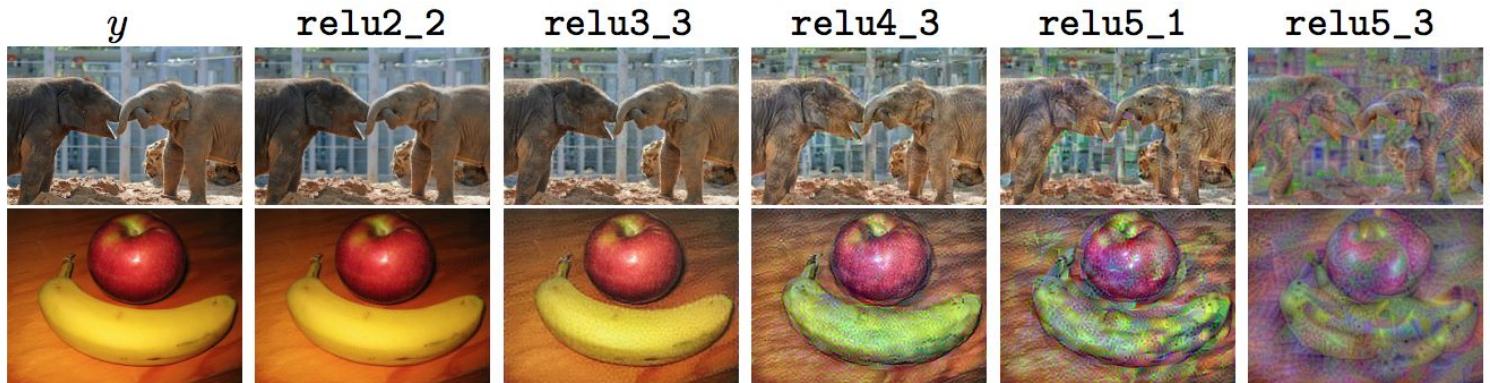


Figure from Johnson, Alahi, and Fei-Fei, "Perceptual Losses for Real-Time Style Transfer and Super-Resolution", ECCV 2016. Copyright Springer, 2016. Reproduced for educational purposes.



## Combined Loss for both Content (1<sup>st</sup> order statistics) and Style (2<sup>nd</sup> order statistics: Gram)

$$\mathcal{L}_{content}(\vec{p}, \vec{x}, l) = \frac{1}{2} \sum_{i,j} (F_{ij}^l - P_{ij}^l)^2 .$$

$$\mathcal{L}_{style}(\vec{a}, \vec{x}) = \sum_{l=0}^L w_l E_l$$

$$E_l = \frac{1}{4N_l^2 M_l^2} \sum_{i,j} (G_{ij}^l - A_{ij}^l)^2$$

$$G_{ij}^l = \sum_k F_{ik}^l F_{jk}^l.$$

# Neural Style Transfer

Content Image



[This image](#) is licensed under CC-BY 3.0

Style Image



[Starry Night](#) by Van Gogh is in the public domain

Style Transfer!

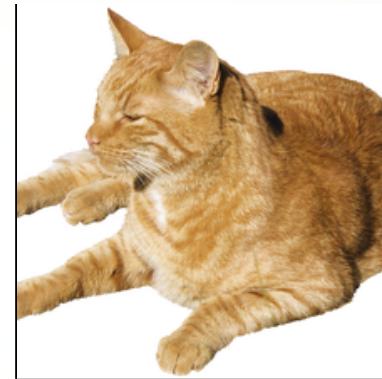


[This image](#) copyright Justin Johnson, 2015. Reproduced with permission.

# CNN learns **texture** features, not shapes!



(a) Texture image  
81.4% **Indian elephant**  
10.3% indri  
8.2% black swan



(b) Content image  
71.1% **tabby cat**  
17.3% grey fox  
3.3% Siamese cat



(c) Texture-shape cue conflict  
63.9% **Indian elephant**  
26.4% indri  
9.6% black swan

Geirhos et al. ICLR 2019

<https://videoken.com/embed/W2HvLBMhCJQ?tocitem=46>



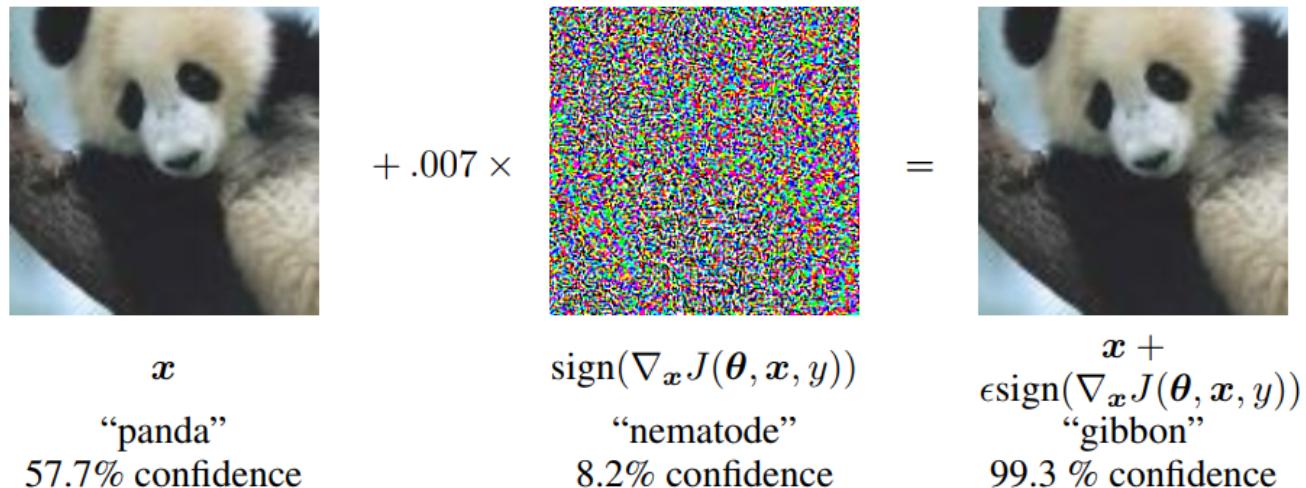
# Examples

- ▶ Jupyter Notebook Demo
- 



# Adversarial Examples and Robustness

# Deep Learning may be fragile: adversarial examples



[Goodfellow et al., 2014]

- Small but malicious perturbations can result in severe misclassification
- Malicious examples generalize across different architectures
- What is source of instability?
- Can we robustify network?

# Adversarial Examples: Fooling Images

- ▶ Start from an arbitrary image
- ▶ Pick an arbitrary class
- ▶ Modify the image to maximize the class
- ▶ Repeat until network is fooled

# Fooling Images/Adversarial Examples

African elephant



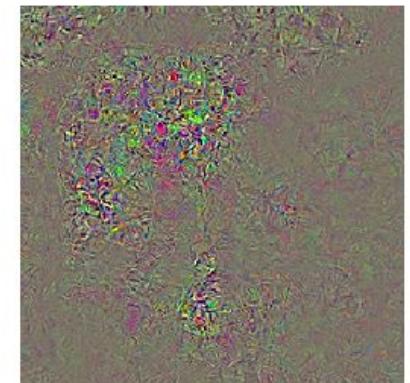
koala



Difference



10x Difference



schooner



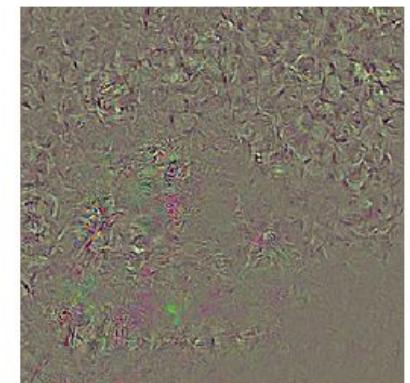
iPod



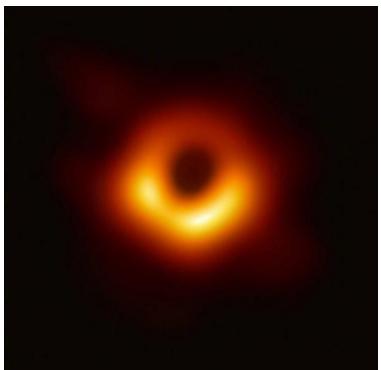
Difference



10x Difference



# Convolutional Networks lack Robustness

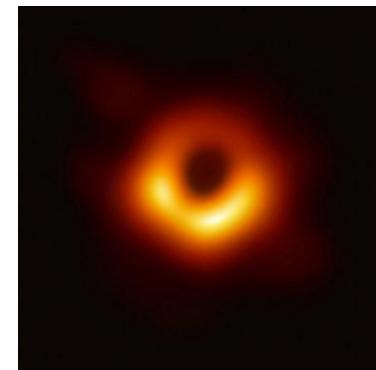


“black hole”  
87.7% confidence

+ .007 ×



=

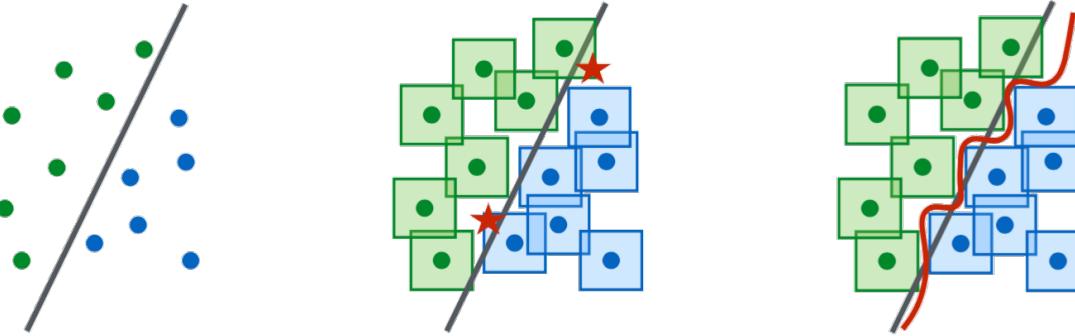


“donut”  
99.3% confidence



Courtesy of Dr. Hongyang ZHANG.

# Adversarial Robust Training



- Traditional training:

$$\min_{\theta} J_n(\theta, \mathbf{z} = (x_i, y_i)_{i=1}^n)$$

- e.g. square or cross-entropy loss as negative log-likelihood of logit models

- Robust optimization (Madry et al. ICLR'2018):

$$\min_{\theta} \max_{\|\epsilon_i\| \leq \delta} J_n(\theta, \mathbf{z} = (x_i + \epsilon_i, y_i)_{i=1}^n)$$

- robust to any distributions, yet computationally hard

Thank you!

