Advanced Prediction Models

Deep Learning, Graphical Models and Reinforcement Learning

Today's Outline

- Visualizing CNNs
- Transfer Learning
- Neural Net Training Tricks
  - Data Augmentation
  - Weight Initialization/Batch Normalization/Dropout

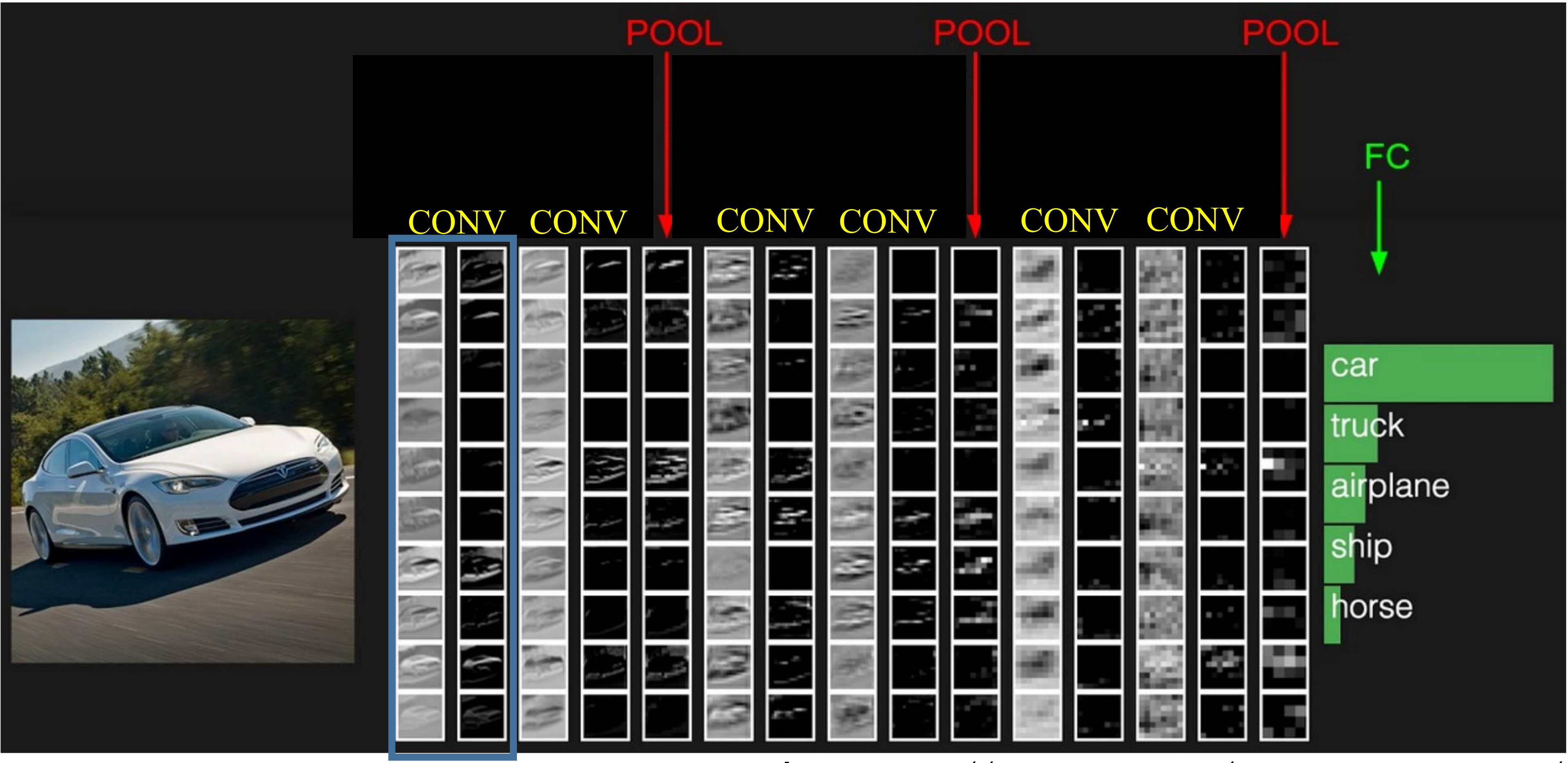
Quick Review: Convolutional Neural Networks

Recap of CNN Architecture

- Typically a CONV is followed by a POOL
- Closer to the output, use FC layers
- In CONV, smaller filters are preferred (say $3 * 3 * z$)
- Input image should ideally be divisible by 2 many times

Input → CONV → POOL → CONV → POOL → CONV → POOL → FC → FC

Example: A CNN Architecture



[1]Figure: http://cs231n.github.io/convolutional-networks/

- A different sequence of layers
- Number of filters (layer depth) is 10
- Activation tensors (flattened along depth) are shown

Example: CONV Layer Parameter Count

- Input tensor of size $90 * 90 * 10$
- Say we have 5 filters, each is $3 * 3 * 10$
- Stride is 1 and zero padding is 1
- Then output tensor will be $90 * 90 * 5$
- We can calculate manually for other strides and padding values

- Number of parameters is $5 * (3 * 3 * 10 \ + \ 1) = 455$
- Contrast with Fully connected net:
  - Number of inputs is 81000
  - Number of hidden layer neurons is 40500
  - Hence, the number of parameters is $> 3{,}280{,}500{,}000$

CNN and Backpropagation

- Backpropagation through a CONV layer
  - Constitutes a set of matrix-matrix products and whatever is the behavior for the nonlinearity
- Backpropagation through a POOL layer
  - Essentially like ReLU where one can keep track of the index of the maximum
- (You will not have to do this by hand in real-life)

Questions?

Visualizing CNNs

Combating Non-Interpretability

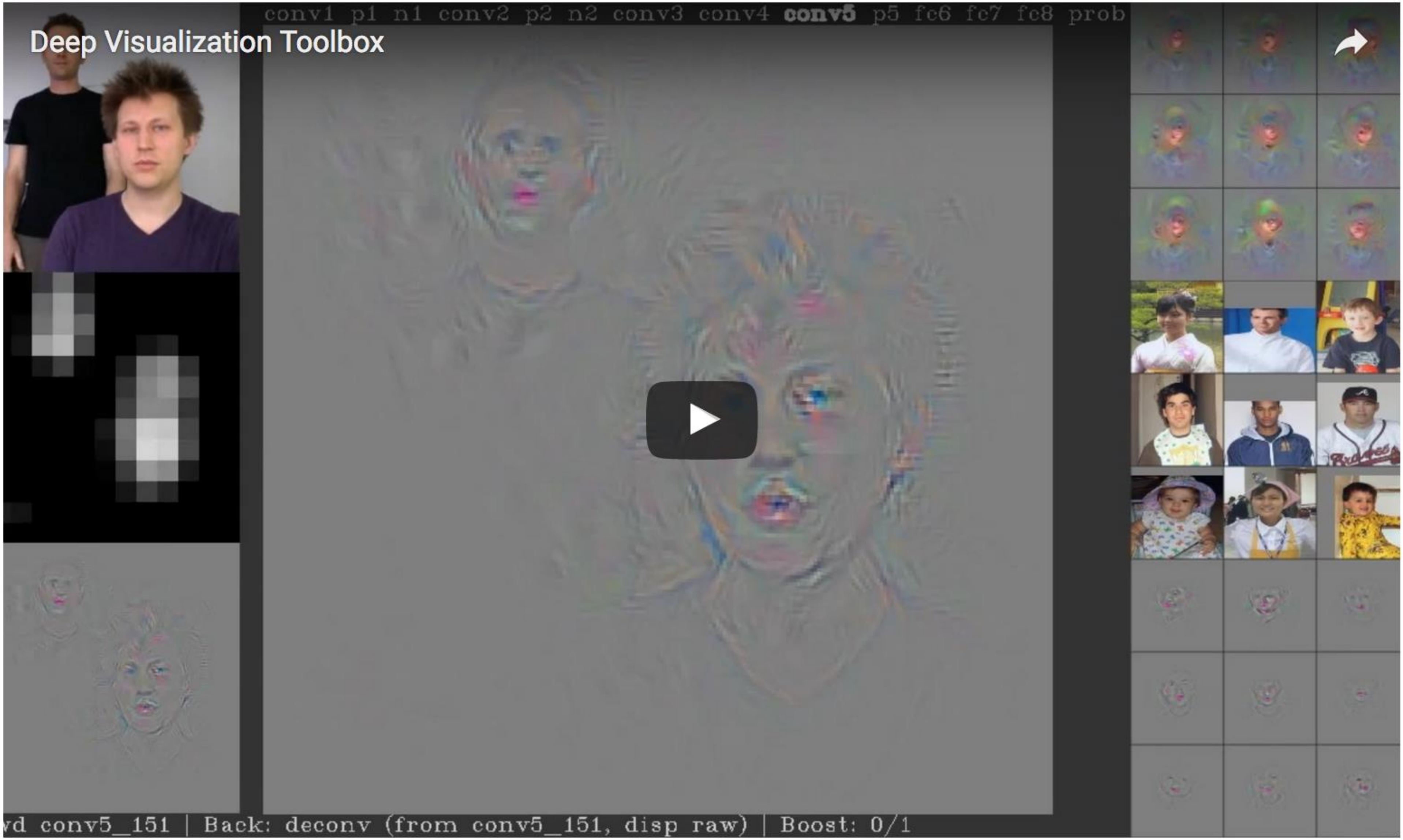
- Common criticism: learned features are not interpretable

- We will look at 4 attempts
  - Look at activations
  - Look at weights
  - Look at images in an embedded space
  - Look at impact of occlusion
  - Look at images that activate neurons highly

An Example CNN Visualization Tool

- Online tool by Adam Harley
  - http://scs.ryerson.ca/~aharley/vis/conv/flat.html

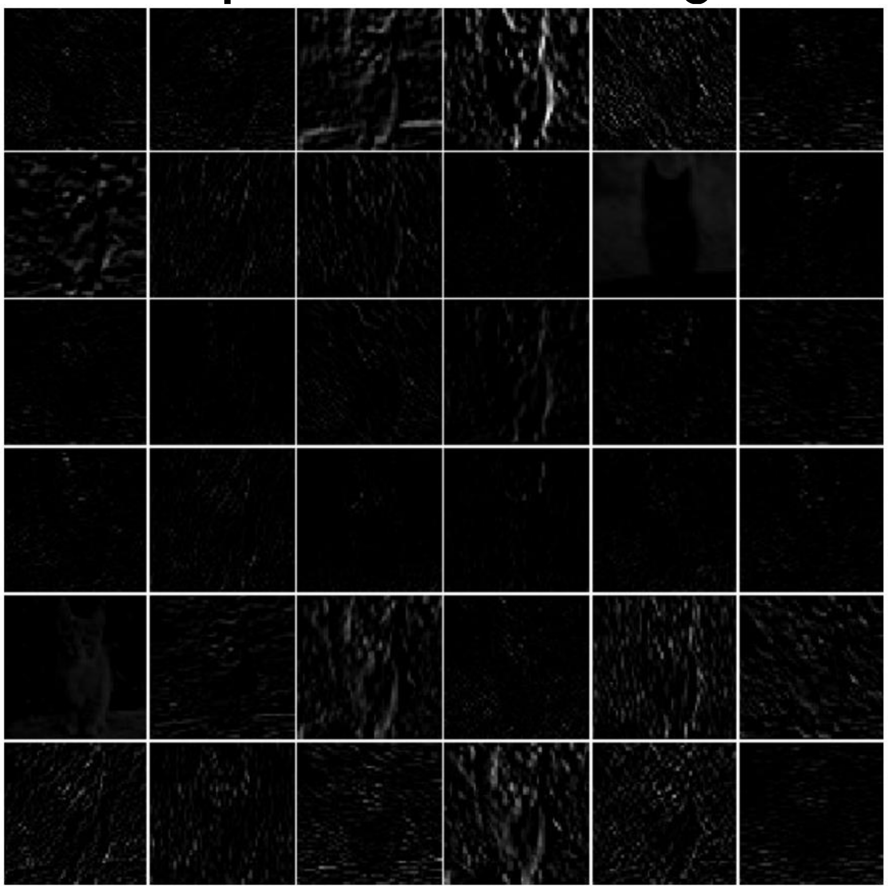
Another Example Tool



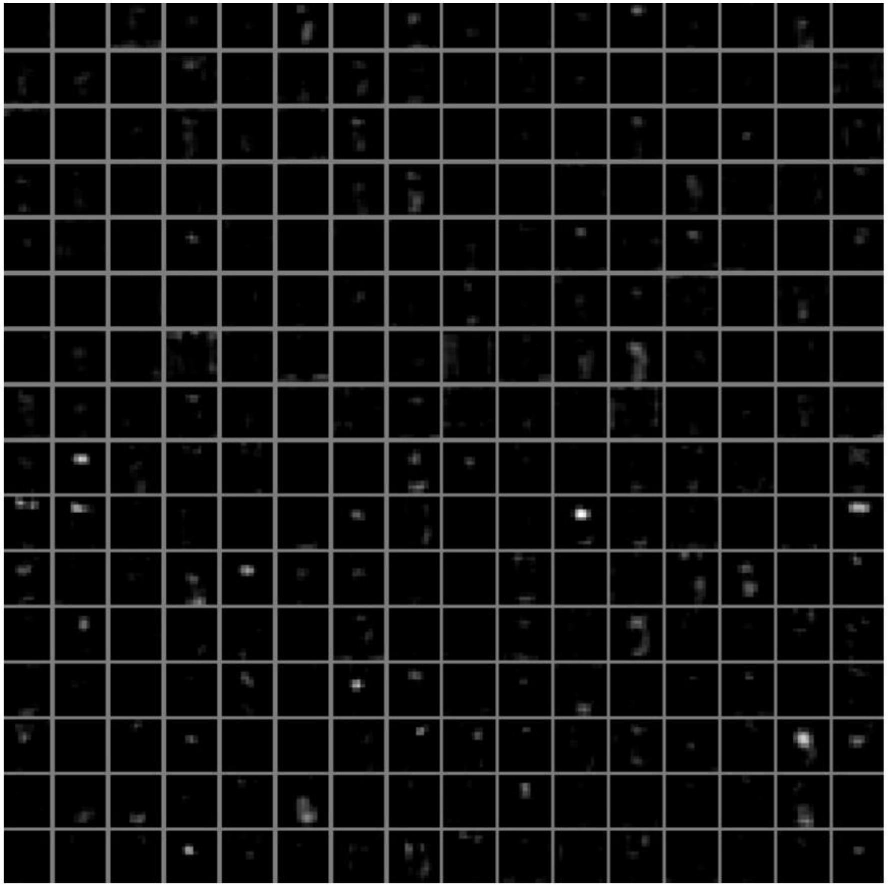
[1]Figure: http://yosinski.com/deepvis

Visualize: Activations

- Useful to debug 'dead' filters (e.g., when using ReLU)
- Input is a cat image



1st CONV

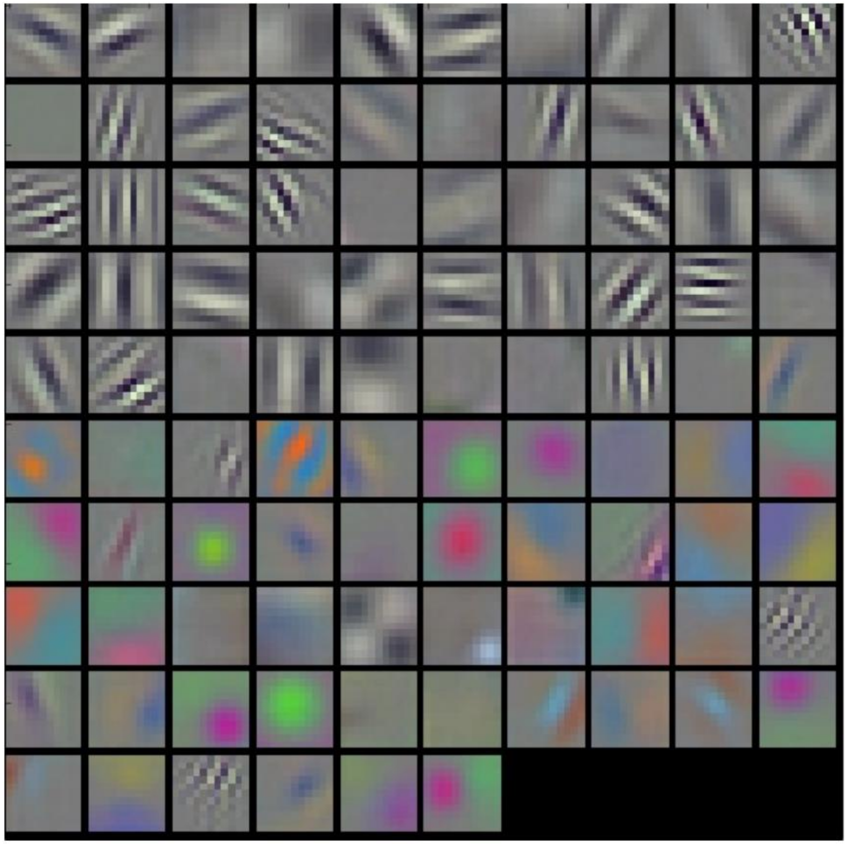


5th CONV

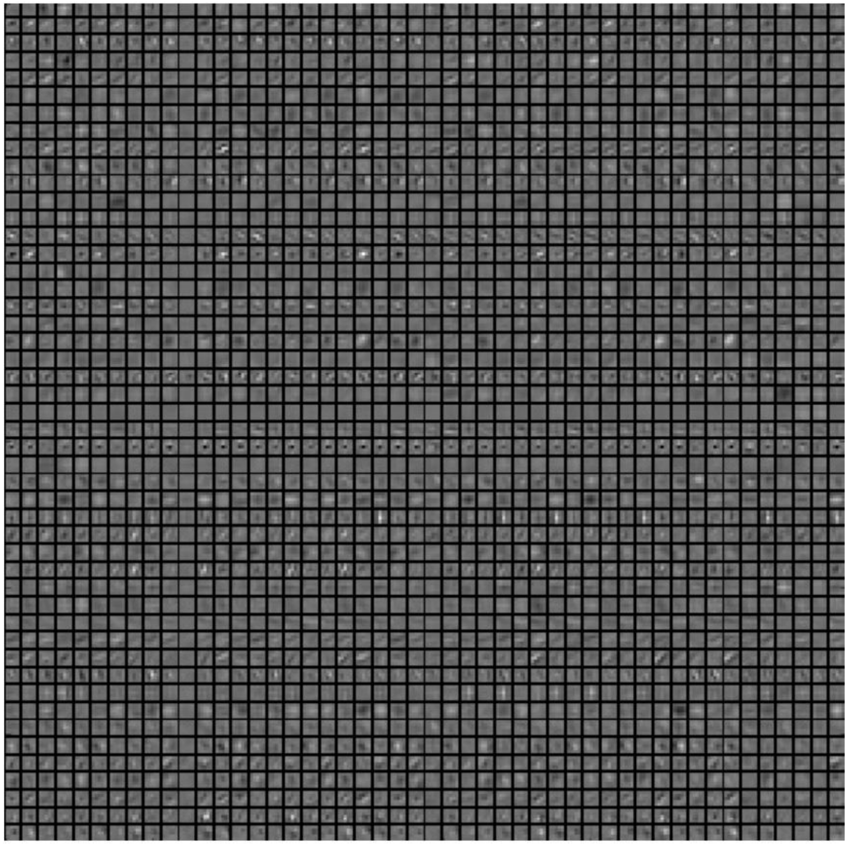
[1]Figure: http://cs231n.github.io/understanding-cnn/

Visualize: Weights

- Useful to debug if training needs to be run more (if patterns are noisy)



1st CONV



2nd CONV

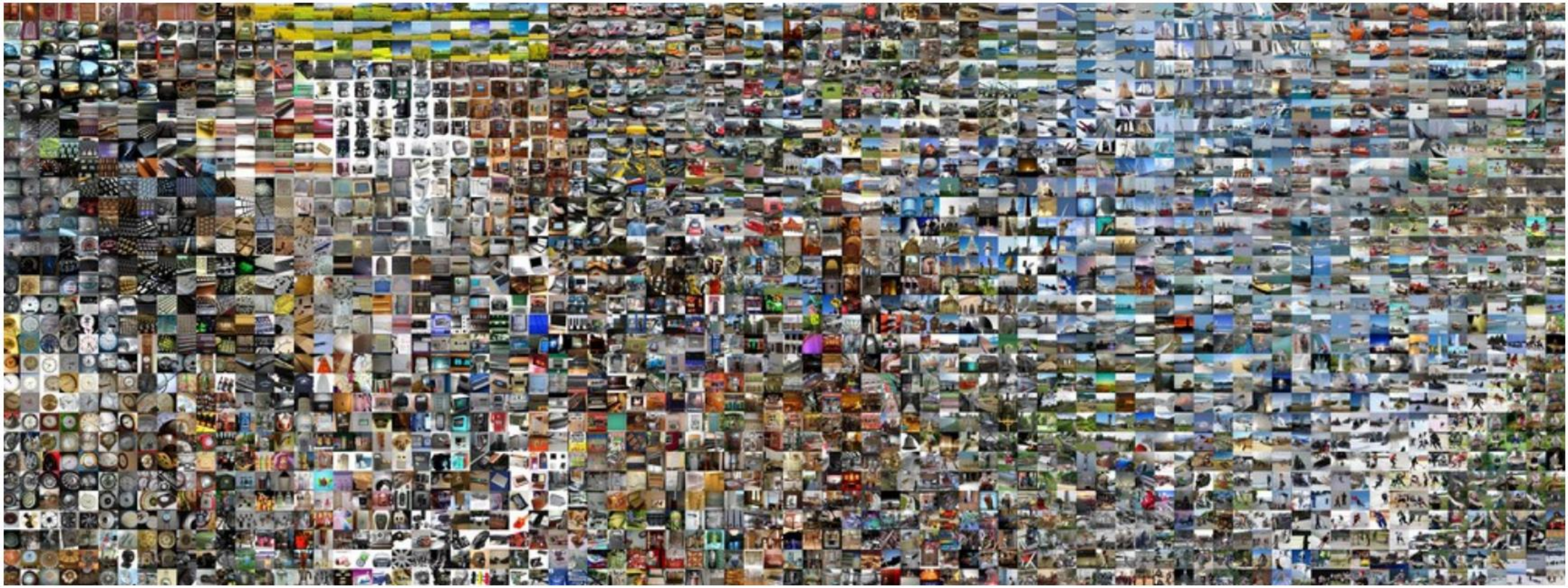
[1]Figure: http://cs231n.github.io/understanding-cnn/

Visualize: Low-Dimensional Embeddings

- CNN
  - Input: Image
  - Output: Scores
- The input to the layer that computes scores:
  - $s = W\max(0, h) + b = Wa + b$
- Activation a can be considered as a representation of the input image
- Embed a's into a 2D space
  - Such that distance properties are preserved

Visualize: Low-Dimensional Embeddings

- In Alexnet, the output of layer before FC layer is 4096 dim
- The t-SNE embedding is shown below:



- Similarities are class-based and semantic rather than color and pixel based
  - Implies: images close to each other are similar for the CNN

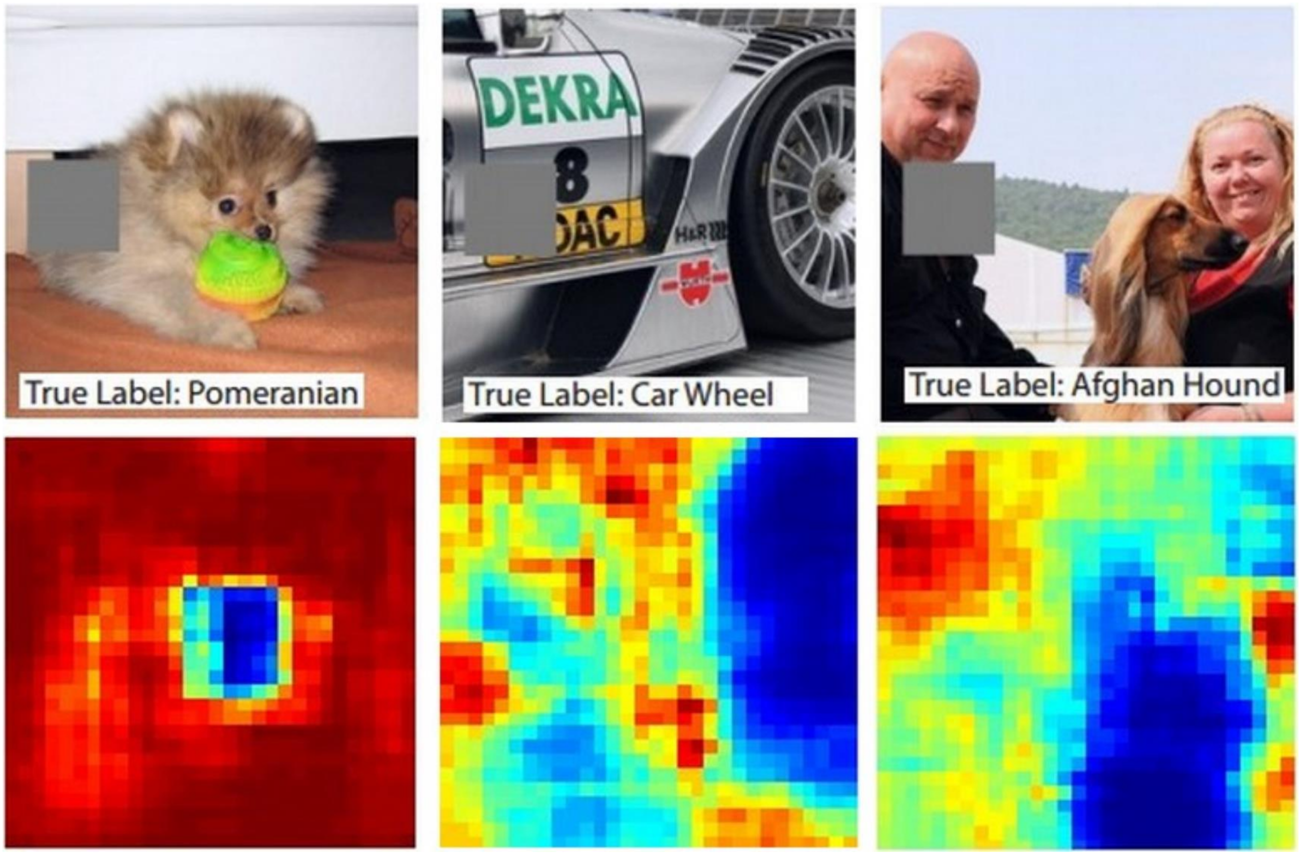
[1]Figure: http://cs231n.github.io/understanding-cnn/

Visualize: By Occlusion

- To figure out which part of the image is leading to a certain classification
- Plot the probability of class of interest as a function of occlusion

Visualize: By Occlusion

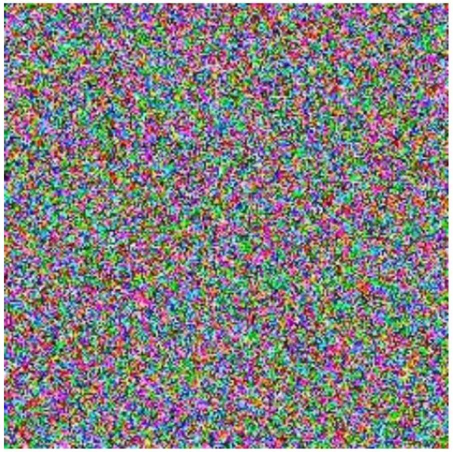
- Occlusion in grey is slid over the images and plot probability of correct class

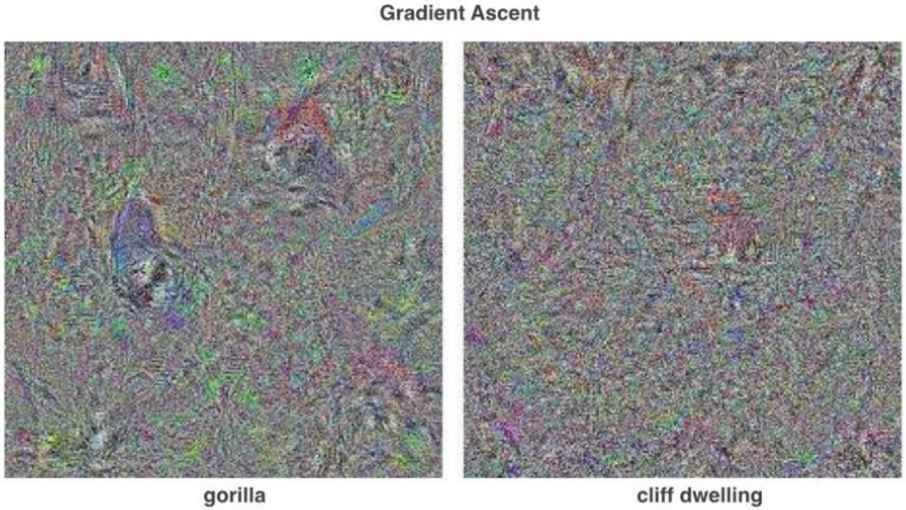


[1]Figure: http://cs231n.github.io/understanding-cnn/

Visualize: Synthesize Images

- Find images that activate a neuron the most



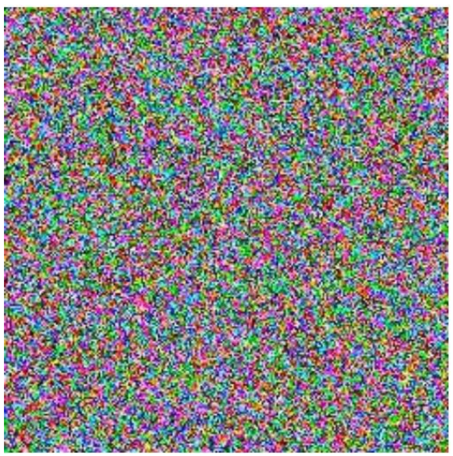


- Seed with ‘natural’ image priors

[1]Figure: http://yosinski.com/deepvis

Visualize: Synthesize Images

- Find images that activate a neuron the most



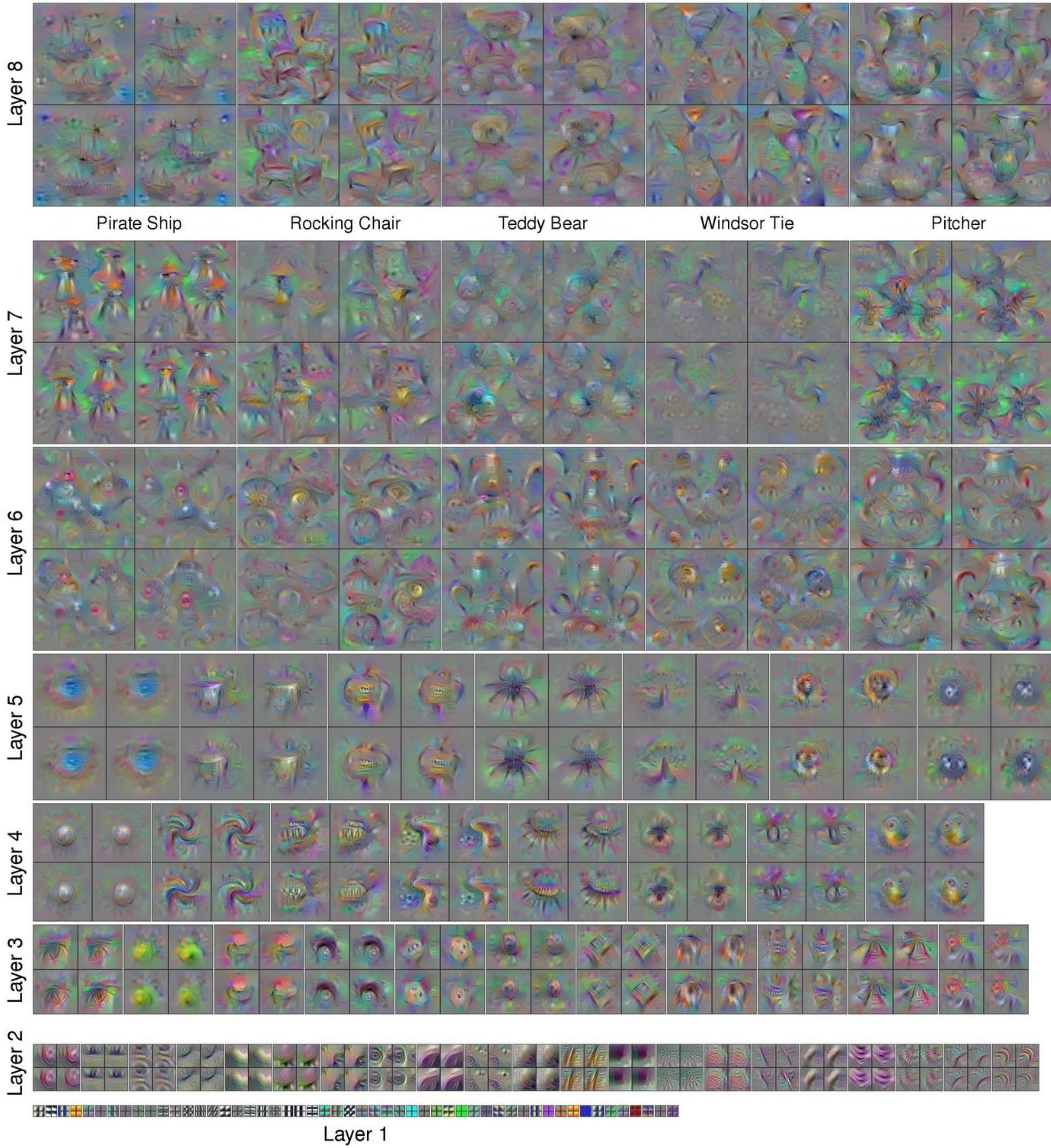
goose

ostrich

- Seed with ‘natural’ image priors

[1]Figure: http://yosinski.com/deepvis

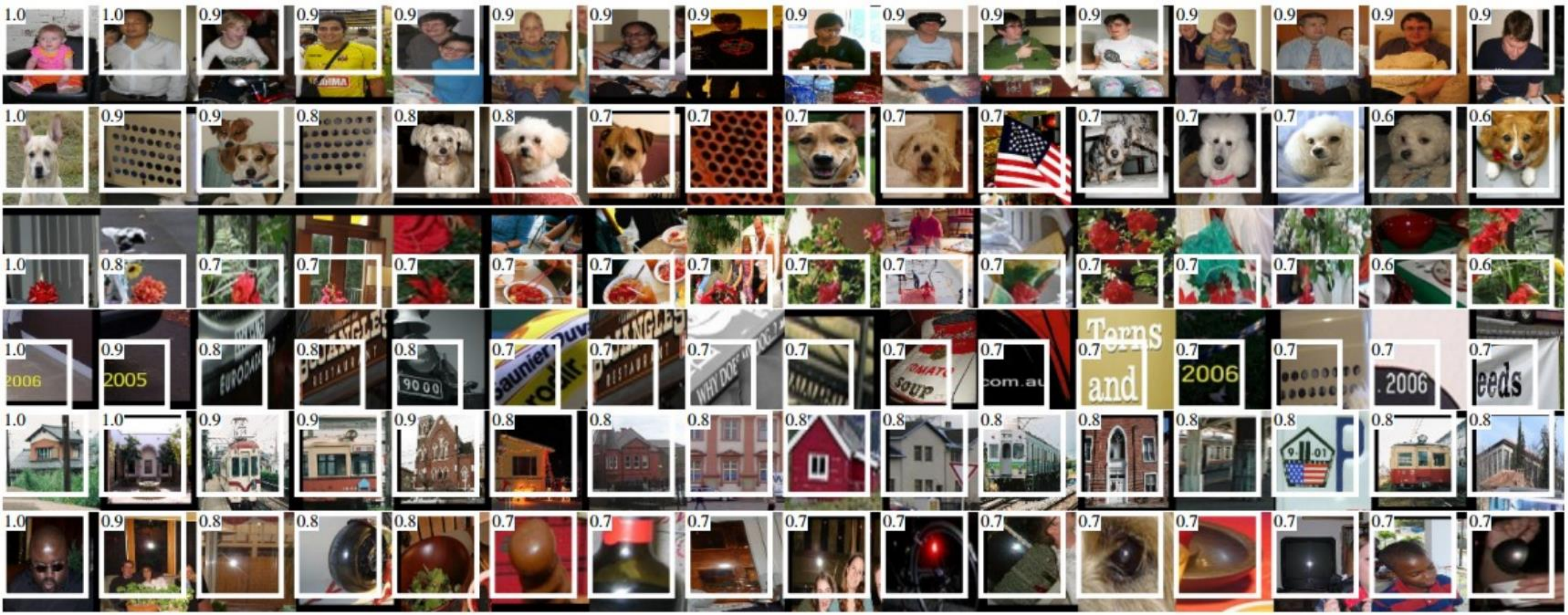
Visualize: Synthesize images



[1]Figure: http://yosinski.com/deepv

Visualize: Images that Activate a Neuron

- Track which images maximally activate a neuron
  - Understand what the neuron is tracking



5th POOL Activation values and receptive fields of some neurons in Alexnet (May not be a good idea…)

[1]Figure: http://cs231n.github.io/understanding-cnn/

Questions?

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Transfer Learning

Transfer Learning

- Very few people train a deep feedforward net or a CNN from scratch

- Myth: "We need a lot of data to use Deep Neural Networks"

- We will see two approaches if we have small data
  - Feature extraction
  - Fine-tuning
- Both these are loosely termed as Transfer learning

Transfer by Feature Extraction (I)

- Get a pretrained CNN
  - Example: VGG or AlexNet that was trained on Imagenet
- Remove the last FC (that outputs 1000 dim score)
- Pass new training data to get embeddings

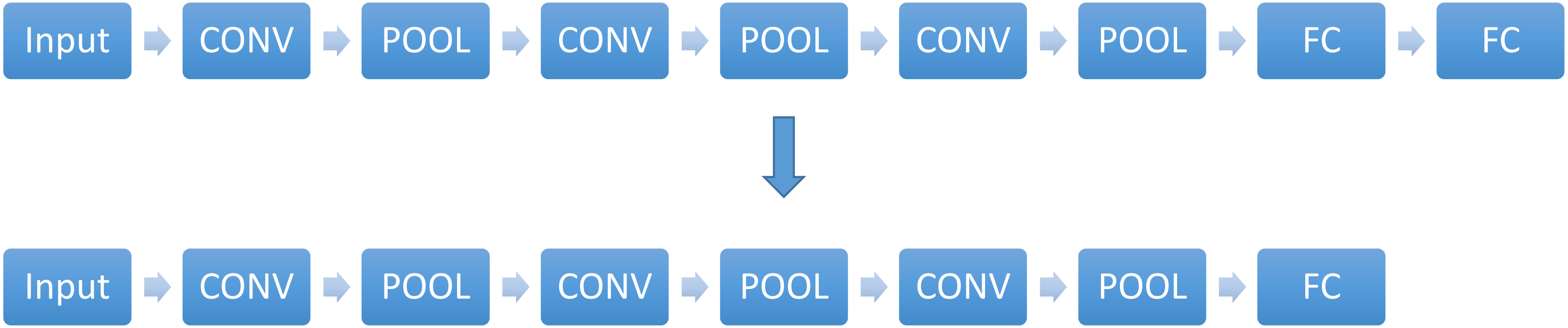
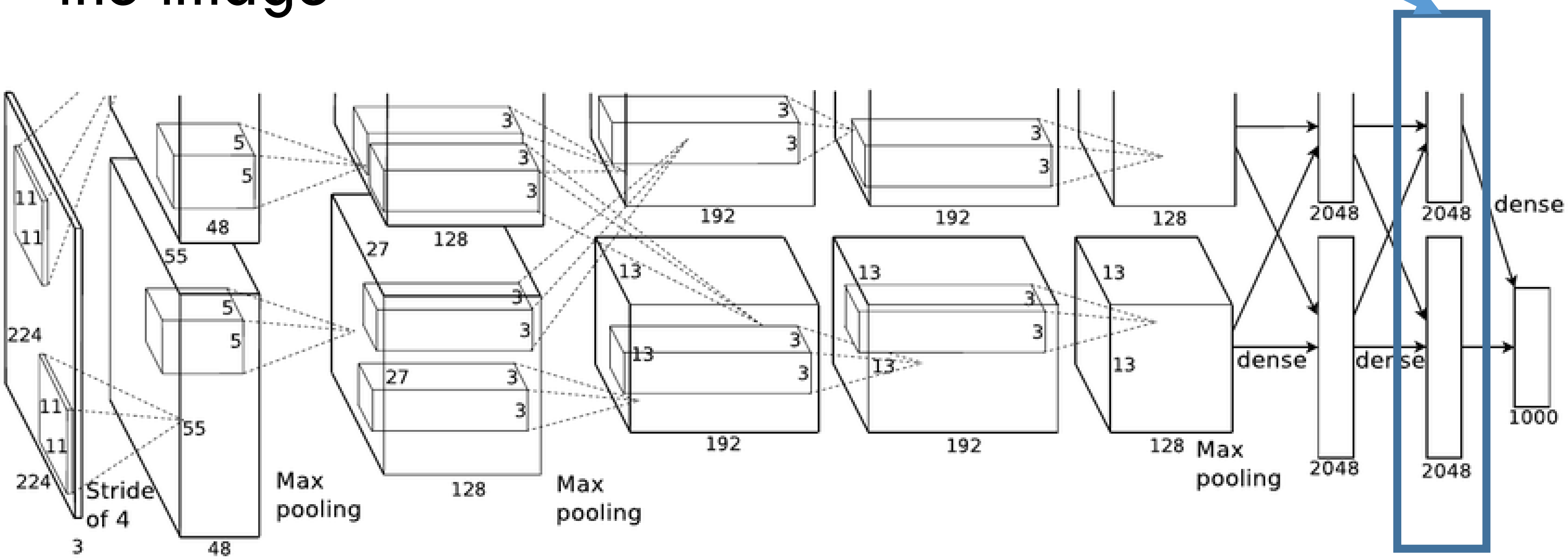


Image Embeddings

- We can think of the penultimate hidden layer activations (a 4096 dim vector) as an embedding of the image

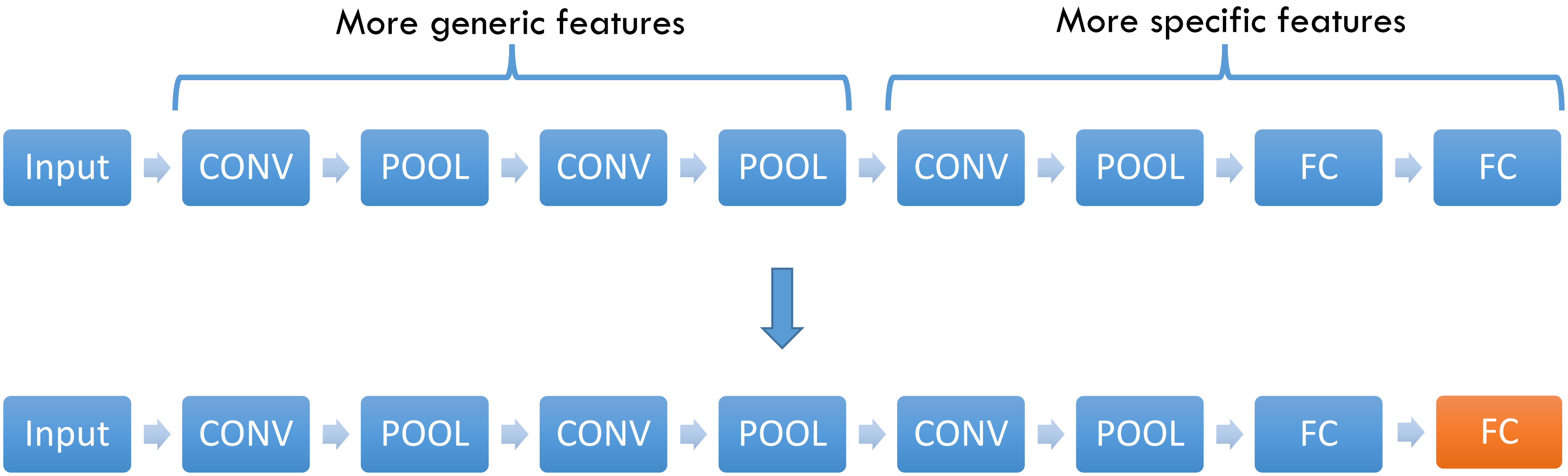


- This is the activation vector or the representation or the CNN code of the image

[1]Figure: https://papers.nips.cc/paper/4824-imagenet-classification-with-deep-convolutional-neural-networks.pdf

Transfer by Feature Extraction (II)

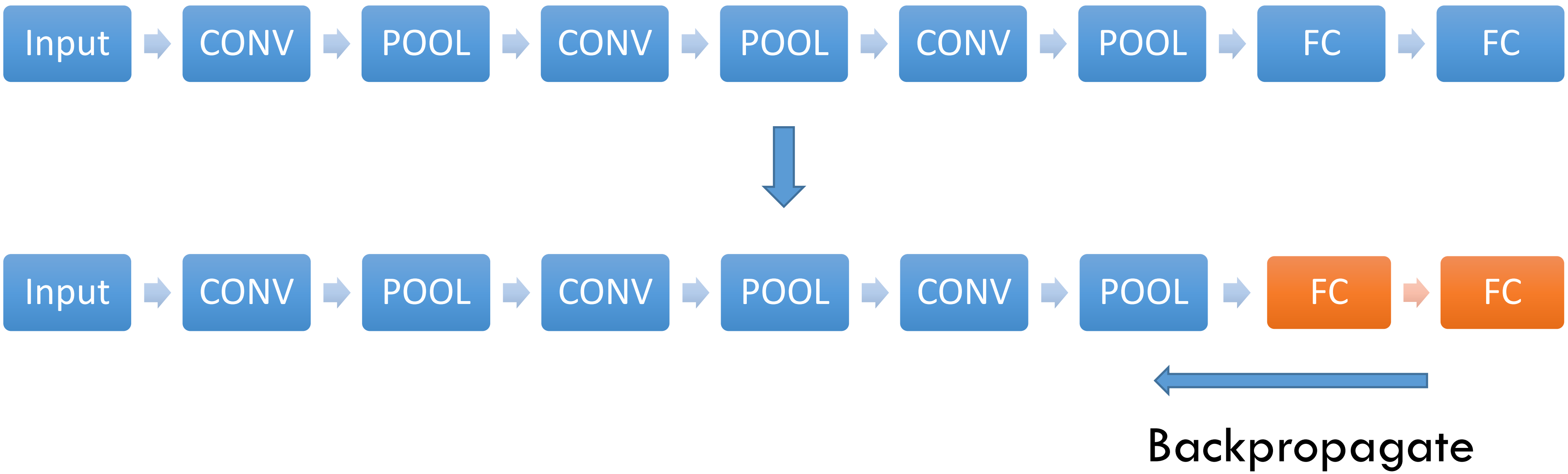
- Input these to a linear or non-linear classifier!



- For example, for imagenet output 1000 dim scores
- For our data, output say 2 scores (cat vs dog)

Transfer by Fine-tuning

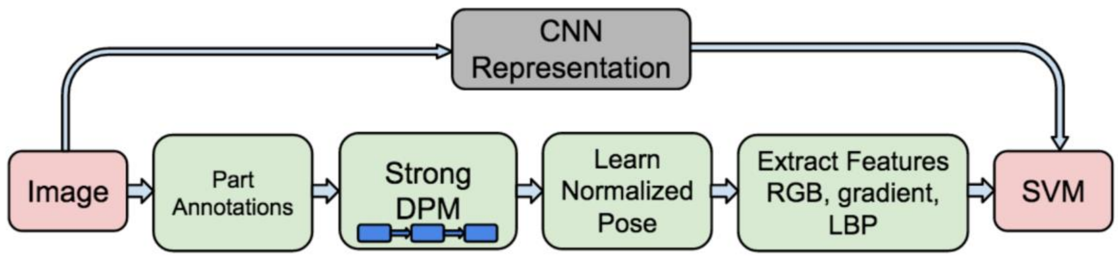
- Retrain or finetune additional layers of the pre-trained if we have more data

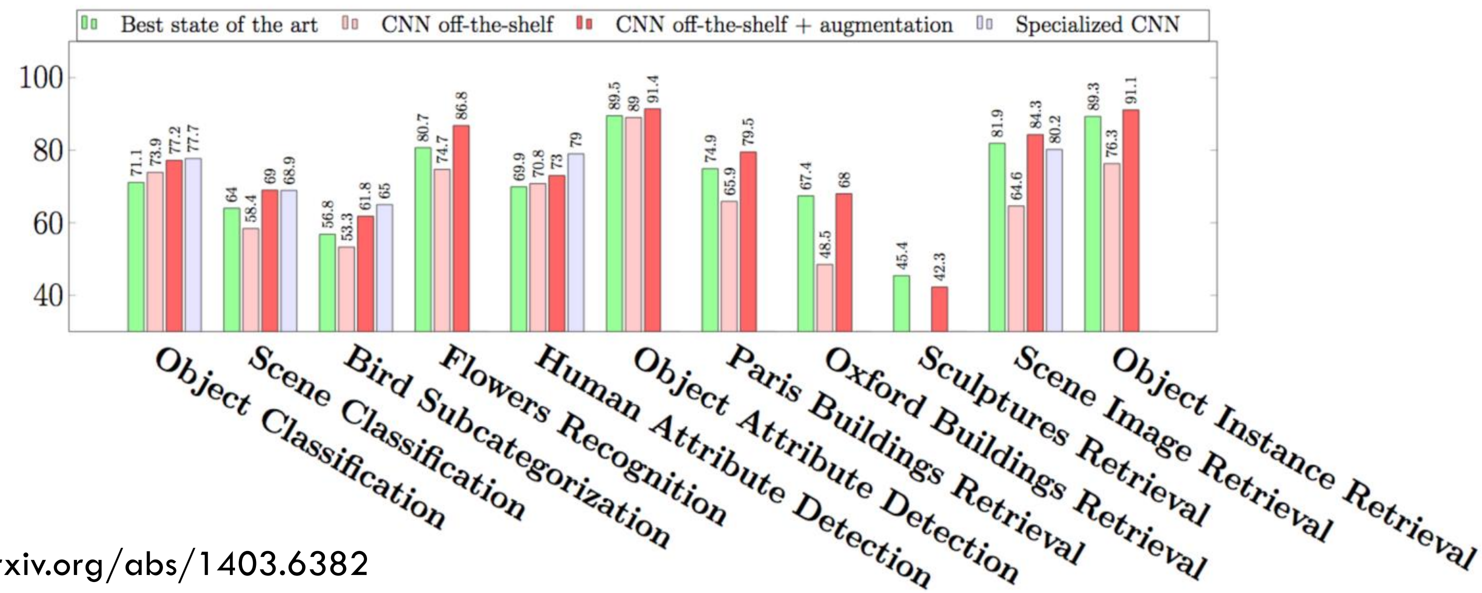


- We can even go all the way back to the first layer if there is a lot of training data available

Benefits of Transfer

- We can get a significant boost in performance compared to hand engineered classification/machine-learning pipelines

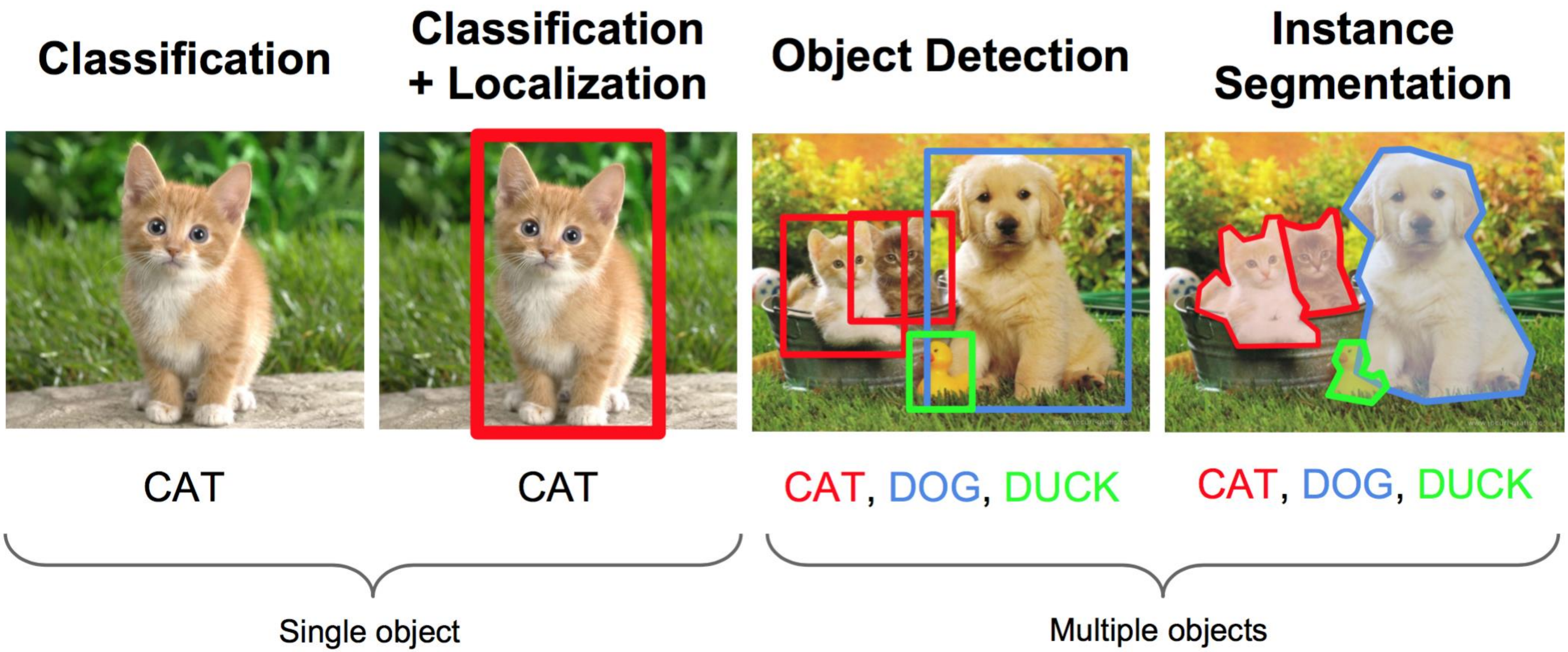




[1]Figure: https:// arxiv.org/abs/1403.6382

Aside: Other Vision Tasks

- Some example vision tasks are given below



[1]Figure: http://cs231n.stanford.edu/

Transfer Learning Choices

- When to transfer

	Similar dataset	Different dataset
Small data	Feature extract	NA
Large data	Fine-tune a bit	Fine-tune a lot

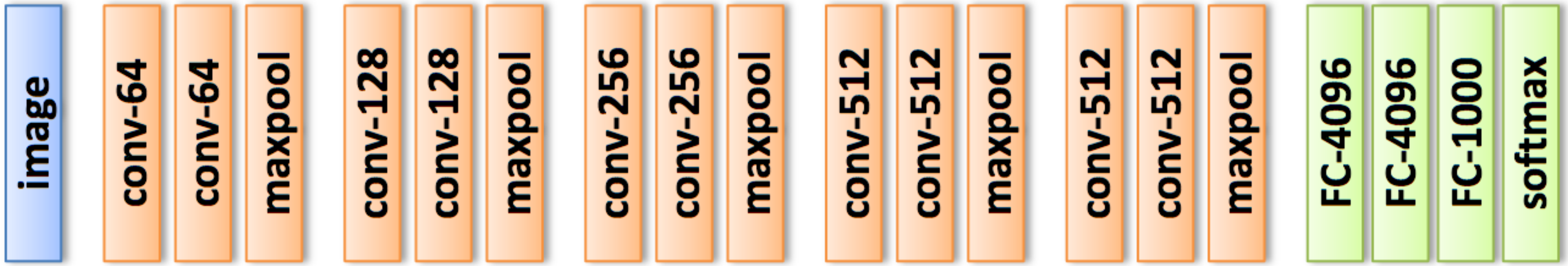
- How to transfer
  - Get pre-trained models for popular software systems
    - Tensorflow Models
    - Keras Model Zoo
    - Caffe Model Zoo

This is key for projects!

VGG Net in Keras

- 2nd in the 2014 ILSVRC classification task
- 3x3 conv filters with stride 1
- ReLU non-linearity
- 5 POOL layers
- 3 FC layers

https://gist.github.com/baraldilorenzo/07d7802847aaad0a35d3



[1]Figure: http://www.robots.ox.ac.uk/%7Evgg/research/very_deep/

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Neural Net Training Tricks

Neural Nets in Practice

- There are a few empirically validated techniques that improve the performance (classification accuracy) of feedforward nets and CNNs

- We will look at some of these
  - Data: data augmentation
  - Model: initalization, batch normalization, dropout

- For our discussion, we will fix the optimization technique to be a gradient based method. We will revisit related algorithmic enhancements later.

Data

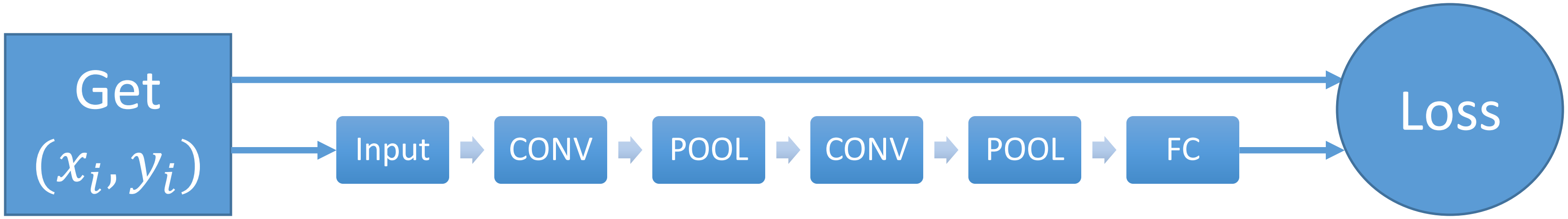
- Data:
  - How is it handled?
  - What is it quality?

- Handling:
  - Deep nets may need to read lots of data (images), so keep them in contiguous spaces of hard-disk

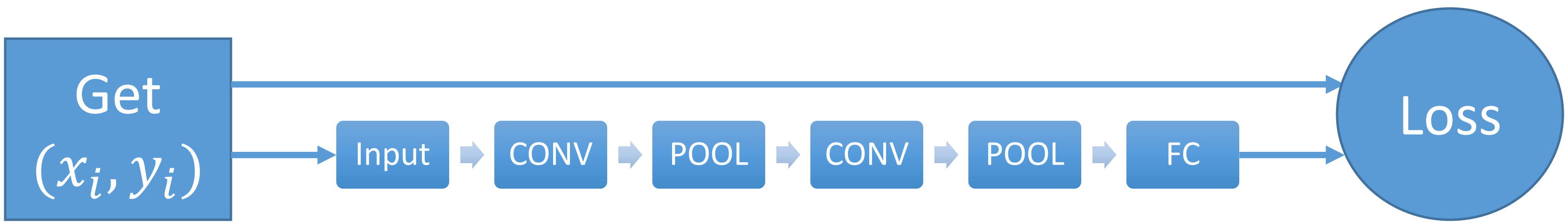
- Quality:
  - Collect as much clean data as possible. At the same time, unclean may also be good enough

Next: Extract the most out of existing data for CNNs

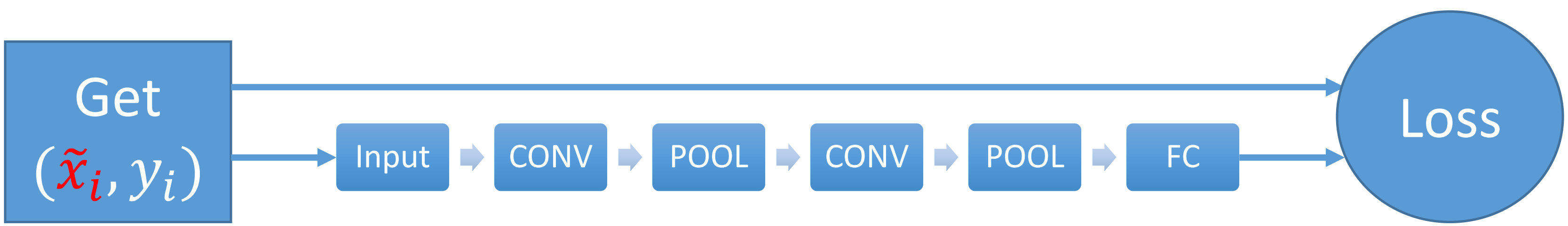
Augmenting Data (I)



Augmenting Data (I)



And



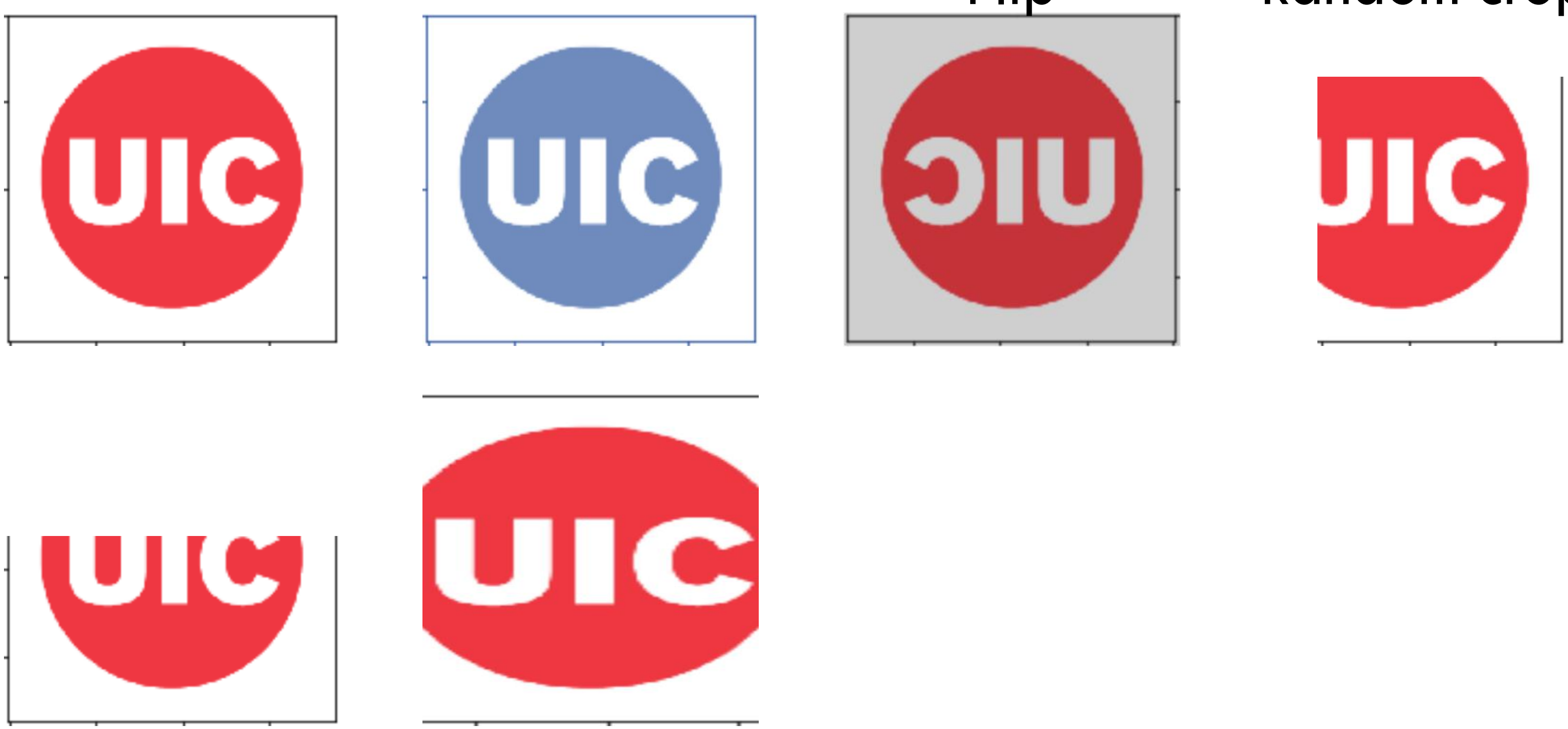
Where $\tilde{x}_i = g(x)$ is a transformation

Augmenting Data (II)

- We are changing the input without changing the label
- We then add this new example to our training set
- Widely used technique!

Flip

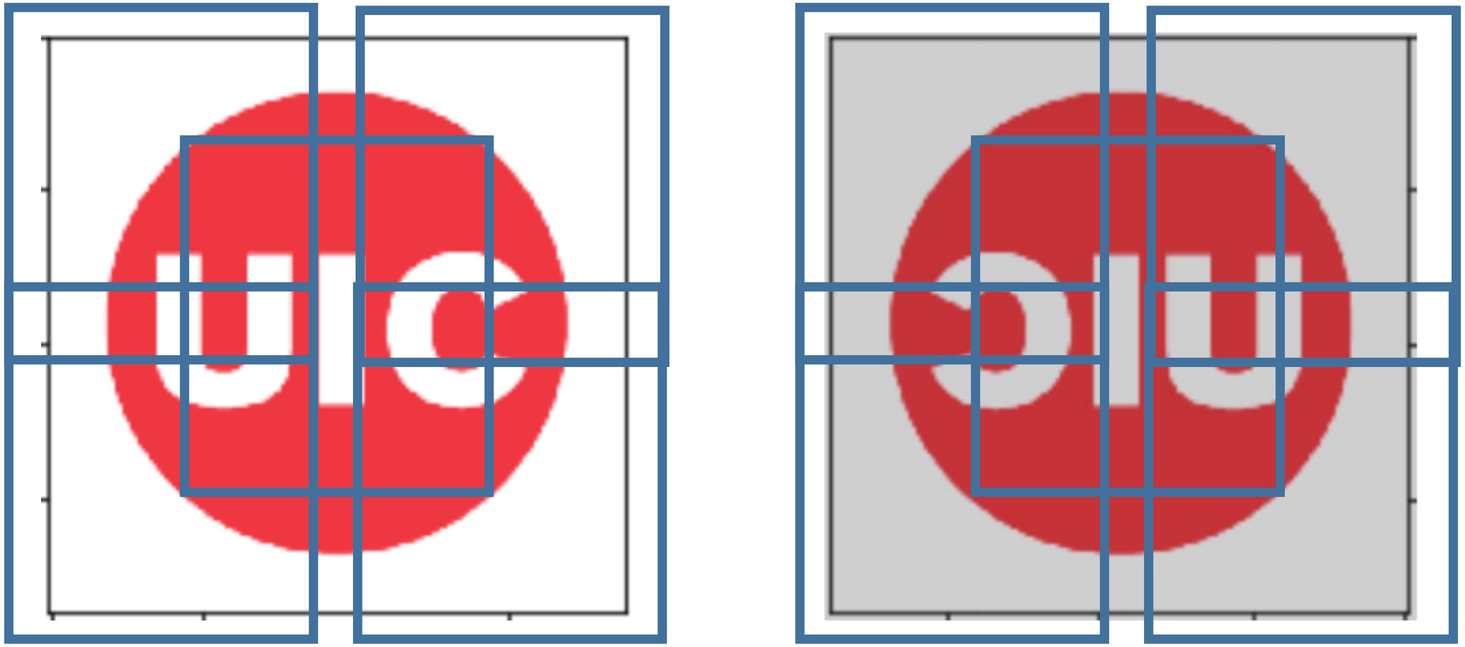
Random crop



Random scale

Augmenting Data (III)

- At test time, average the predictions of a fixed set of transformations
- Example (for Resnet, the ILSVRC 2015 winner):
  - Image at 5 scales: 224,256,384,460 and 640
  - At each scale, get 10 224*224 crops



Augmenting Data (IV)

- Other ways to augment data include
  - Changing contrast and color
  - Mix translations, rotations, stretching, shearing, distortions

- This is very useful for small datasets

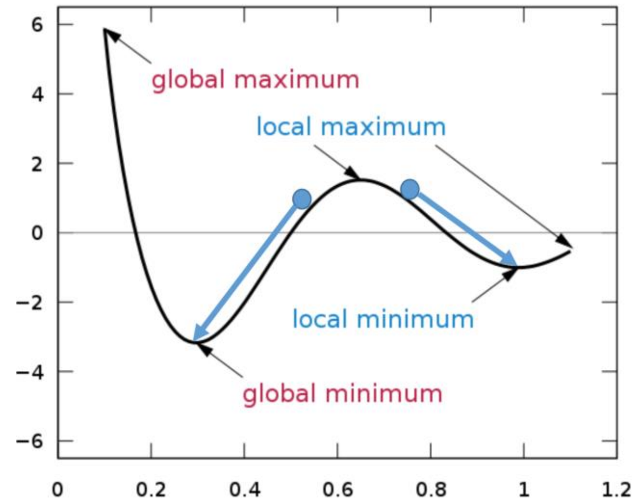
- From one point of view, this is essentially
  - Adding some noise during training
  - Marginalizing noise out at test

Model

- We have already seen few choices
  - Activation function or nonlinearities
  - Number of layers and number of neurons per layer
  - CNN filter choices …
- There are other choices while training deep neural nets (including CNNs) that also make a difference
  - Weight initialization
  - Batch normalization
  - Dropout

Model: Weight Initialization

- Weight initialization plays a key role in training deep networks
  - Example: $W = 0$ may be bad



- Not just the issue of local optima
- But also the magnitudes of gradients in backprop
  - Activation statistics (mean and variance) influence gradients
- Heuristics available in the literature to initialize W

Model: Batch Normalization

- Activations magnitudes and their statistics depend on the dataset, the network and the nonlinearity used

- Their statistics influence gradient propagation, hence also learning

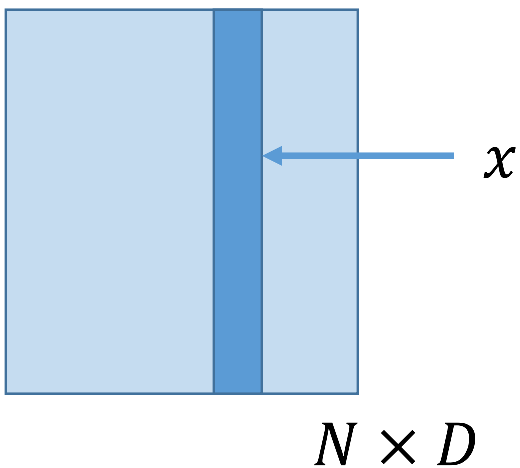
- Is there a way to control them?
  - Yes, through batch normalization!

Model: Batch Normalization

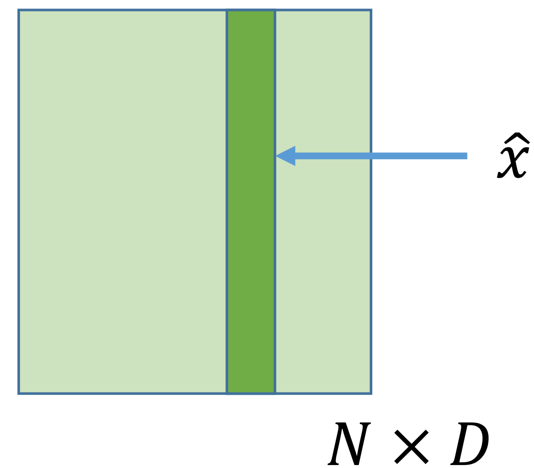
- Idea: Make each activation unit-Gaussian by subtracting the mean and then dividing by standard deviation

Batch-size $= N$

Number of output neurons $= D$



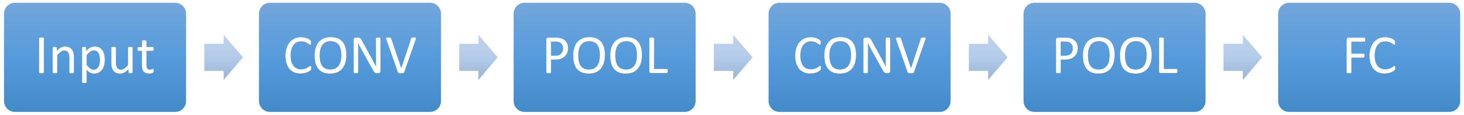
$$\hat{x} = \frac{\gamma(x - E[x])}{\sqrt{Var[x]}} + \beta$$



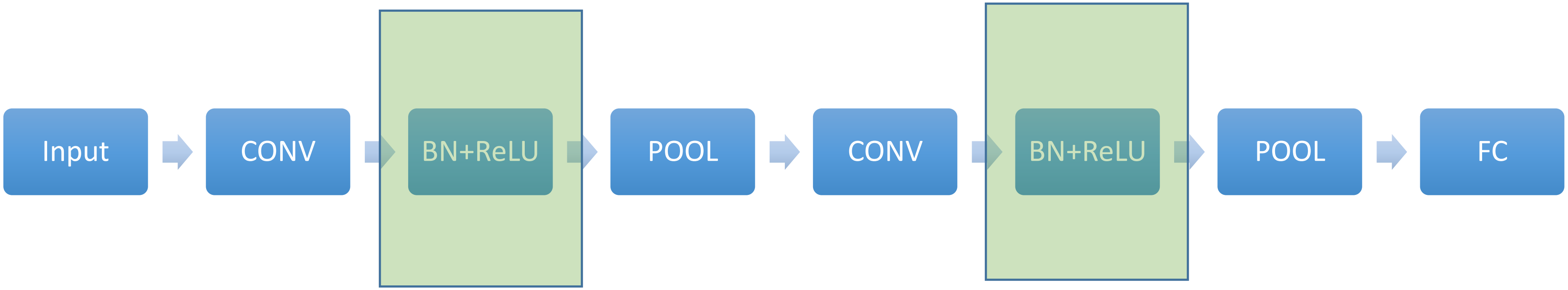
- Is a differentiable function: hence no issue with backpropagation
- At test time, there is no batch. Use the training data means and variances

Model: Batch Normalization

- Previously,



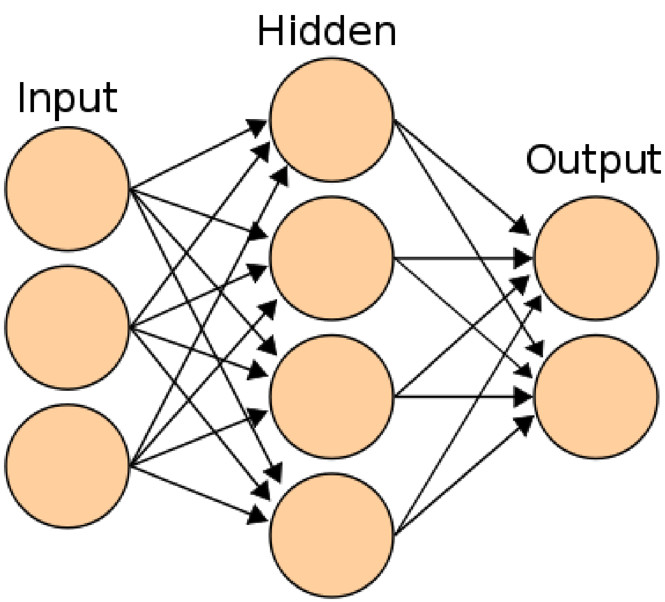
- Now
  - Insert a Batch Normalization layer between CONV and nonlinearity (ReLU)



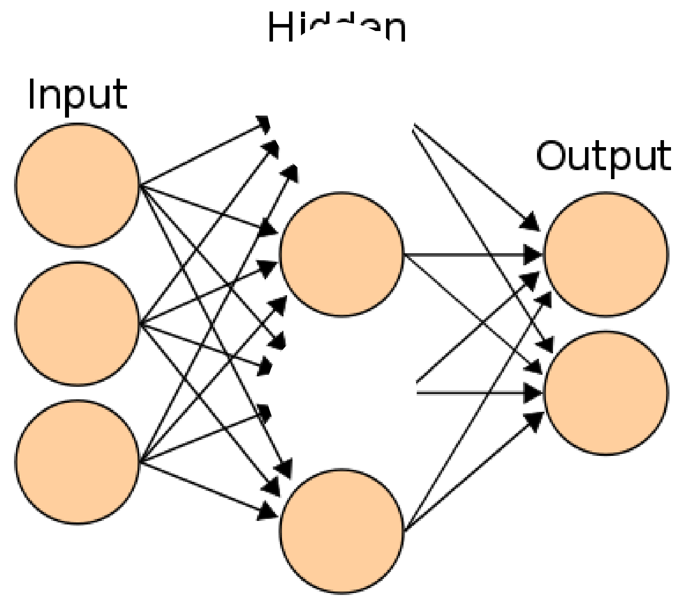
- Empirically observed: improved gradient flows, less sensitive to initialization.

Model: Dropout (Regularization)

- Idea: During training, every time we forward pass, we set the output of a few neurons to zero with some probability



Without dropout



One pass with dropout

[1]Figure: http://cs231n.stanford.edu/

Model: Dropout (Regularization)

- Intuitively, it is
  - Making us use smaller capacity of the network. Hence, can think of it as a regularization
  - Forcing all the neurons to be useful. Hence there is over-representation or redundency

- Also think of it as
  - Subsampling a part of the network for each example
  - Thus, we get an ensemble of neural networks that share parameters

Model: Dropout (Regularization)

- Higher probability means stronger regularization

- At test time,
  - Instead of doing many forward passes
  - Perform no dropout
  - Scale all activations by the probability of dropout

- Example:
  - Say dropout with probability p
  - Originally: $f(x, W_1, b_1, W_2, b_2) = W_2 \max(0, W_1 x + b_1) + b_2$
  - With dropout: $W_2 * p * \max(0, W_1 x + b_1) + b_2$

Summary (I)

- CNN are very effective in image related applications.
  - State of the art!
- Exploit specific properties of images
  - Hierarchy of features
  - Locality
  - Spatial invariance
- Lots of design choices that have been empirically validated and are intuitive. Still, there is room for improvement.

Summary (II)

- We saw
  - Visualizations to understand how CNNs work
  - Transfer learning applied to CNNs (important for applications)
    - An excellent way to get a deep learning solution working
    - There is no need for large datasets to get started

Summary (III)

- Neural Nets Training Tricks
  - Revisited data: data augmentation
  - Revisited models: initialization, batch norm, dropout

  - To train state of the art deep learning systems, you have to rethink:
    - (a) data, (b) models, and (c) optimization[1]
    - What is the most bang per buck for your business?

- If the deep learning system is core to the business, look at engineering best practices (we saw some today)

[1]We did not cover this in this lecture

Appendix

Sample Questions

- How does a 2 layer feedforward net differ from a linear classifier?
- Describe why nonlinearities are introduced in a neural network? Why is the ReLU non-linearity called a gradient gate?
- Describe the parameter sharing property of a convolutional layer
- How is backpropagation used while optimizing the parameters of a neural network?

Advice

- In spite of all these design choices, for 90% of the applications, pick an architecture that works well on an established dataset (e.g., Imagenet)

- Focus on the application and business considerations, not architectural decisions!

Ref: http://cs231n.github.io/convolutional-networks/

Practical Considerations

- Model choice: nonlinearity, number of layers, number of neurons
- Data preprocessing: batch normalization, subtracting mean of inputs
- Parameter initialization: random or zeroes?
- Learning rate: How to change?
- Batch normalization: re-normalizing activations
- Monitoring learning: plot graphs of training and validation
- Cross validation: hyper-parameter tuning is non-trivial

Partial Robustness to Input Size

- The input image size determines the tensors in intermediate stages
- Example
  - Alexnet requires 224*224*3 sized images

- What if we have a larger sized image?
  - We can 'convert' FC layers to equivalent CONV layers for efficiency
  - Then slide the original CNN over the larger image!
    - This leads to a 'single' forward pass

Partial Robustness to Input Size

- Instead of a single vector of scores, now we get a bunch of scores