Convolutional Neural Networks

INTELLIGENT SYSTEMS FOR PATTERN RECOGNITION (ISPR)

DAVIDE BACCIU – DIPARTIMENTO DI INFORMATICA - UNIVERSITA' DI PISA

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Module Outline

- Foundational models
  - Convolutional Neural Networks
  - Deep Autoencoders and RBM
  - Gated Recurrent Networks (LSTM, GRU, …)
  - Coding lectures: Keras/TF and Pytorch
- Advanced models
  - Advanced recurrent models (multiscale memories, …)
  - Advanced sequential models (seq-to-seq, …)
  - Attention and memory (Transformers, Neural Turing machines, …)

More advanced topics in the generative DL module and in the final module

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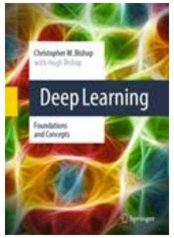
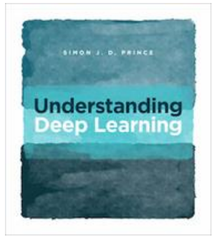
Reference Books (all freely available online)

Your choice between one of the two below:

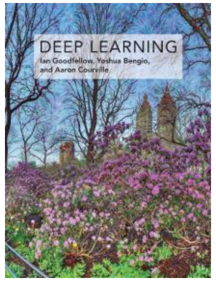


Chris Bishop, Hugh Bishop, Deep Learning Foundations and Concepts , Springer (2024)



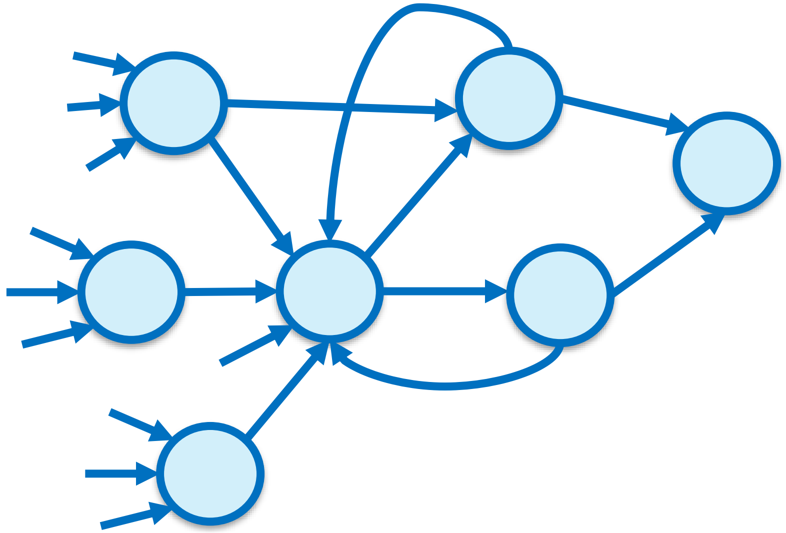
Simon J.D. Prince, Understanding Deep Learning, MIT Press (2023)

Previously was:



Ian Goodfellow and Yoshua Bengio and Aaron Courville, Deep Learning, MIT Press

Module's Prerequisites



- Formal model of neuron
- Neural network
  - Feed-forward
  - Recurrent
- Cost function optimization
  - Backpropagation/SGD
  - Regularization
- Neural network hyper-parameters and model selection

Lecture Outline

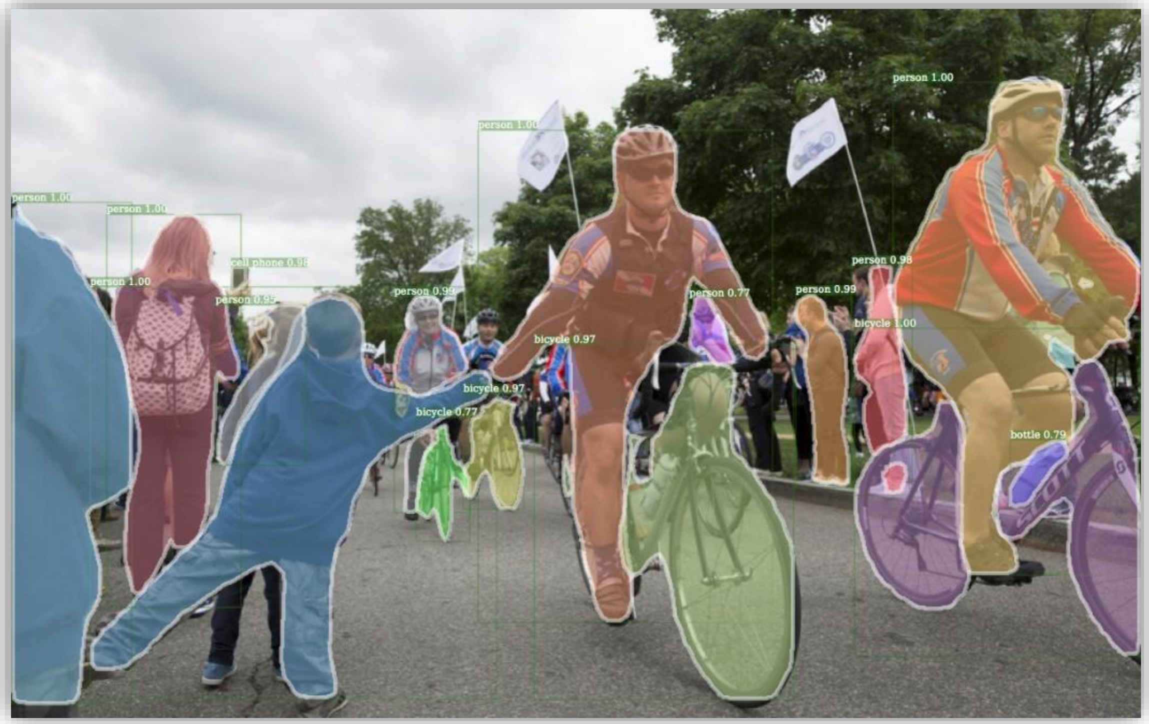
- Introduction and historical perspective
- Dissecting the components of a CNN
  - Convolution, stride, pooling
- CNN architectures for machine vision
  - Putting components back together
  - From LeNet to ResNet
- Advanced topics
  - Interpreting convolutions
  - Advanced models and applications

Split in two lectures

CNN Lecture – Part I

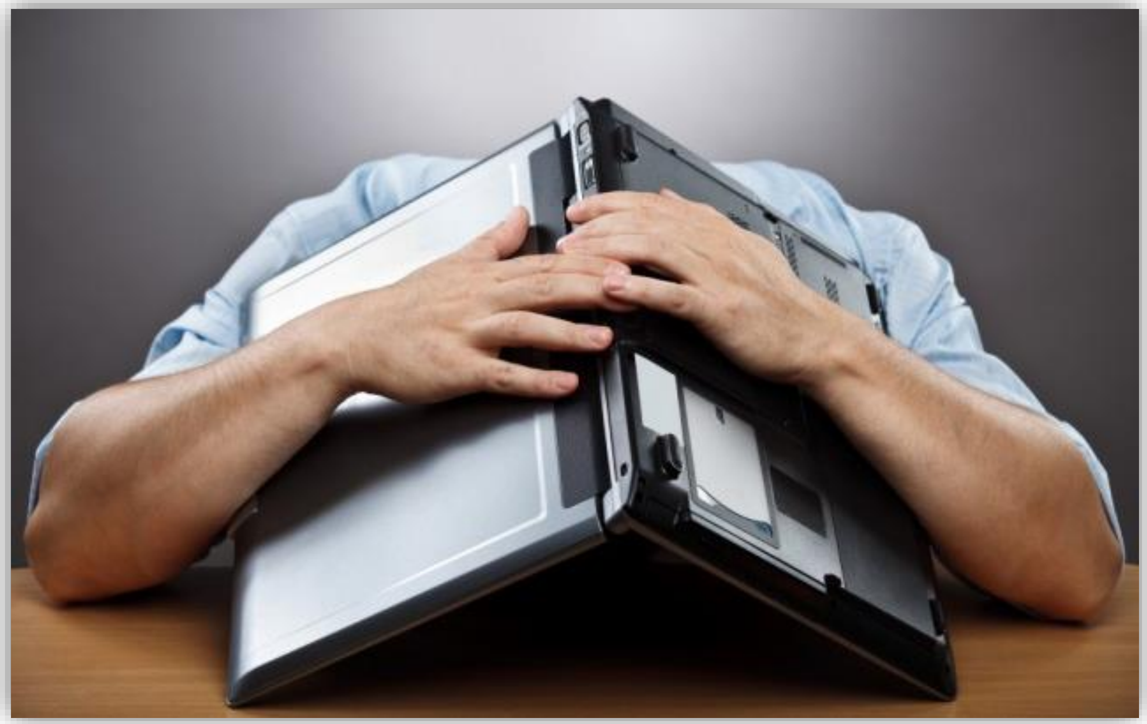
Introduction

Convolutional Neural Networks



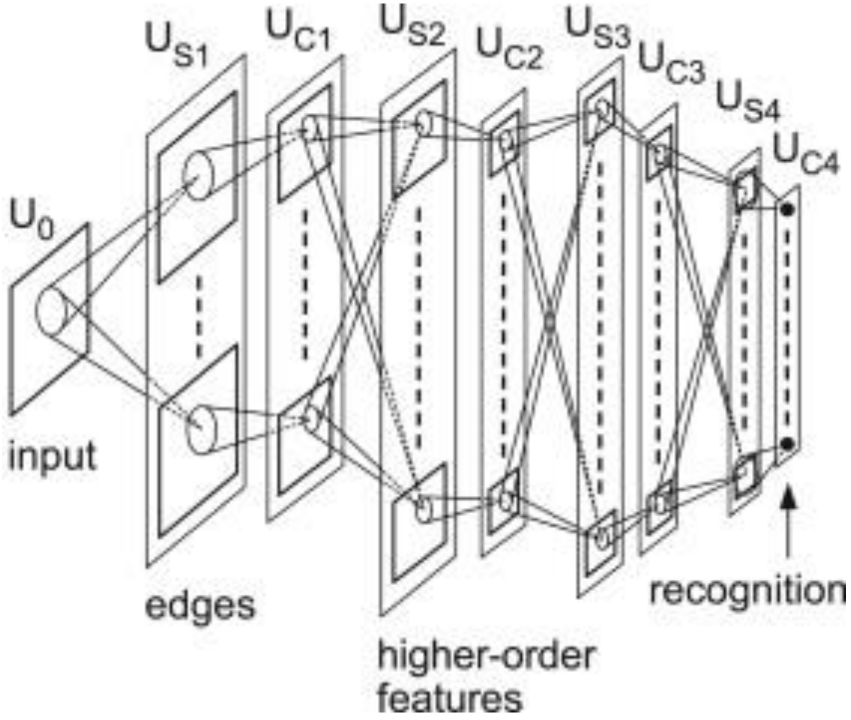
Introduction

Convolutional Neural Networks



Destroying Machine Vision research since 2012

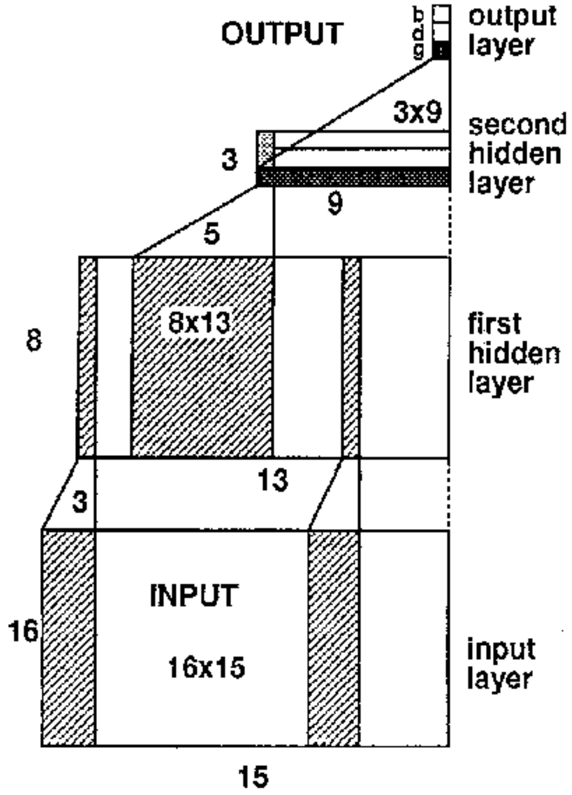
Neocognitron



- Hubel-Wiesel ('59) model of brain visual processing
  - Simple cells responding to localized features
  - Complex cells pooling responses of simple cells for invariance
- Fukushima ('80) built the first hierarchical image processing architecture exploiting this model

Trained by unsupervised learning

CNN for Sequences

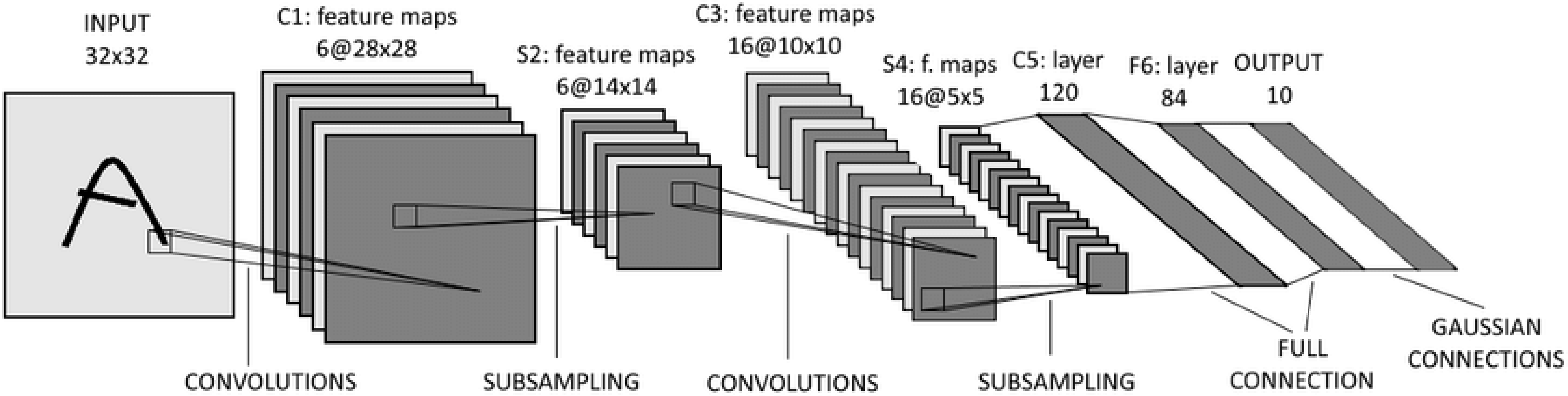


Time delay neural network (Waibel & Hinton, 1987)

- Apply a bank of 16 convolution kernels to sequences (windows of 15 elements)
- Trained by backpropagation with parameter sharing
- Guess who introduced it?

  …yeah, HIM!

CNN for Images



First convolutional neural network for images dates back to 1989 (LeCun)

Dense Vector Multiplication

Processing images: the dense way

32x32x3 image

Reshape it into a vector

An input-sized weight vector for each hidden neuron

$\boldsymbol{x}$

3072

$\boldsymbol{W}$

100x3072

$\boldsymbol{W}\boldsymbol{x}^{T}$

Each element contains the activation of 1 neuron

100

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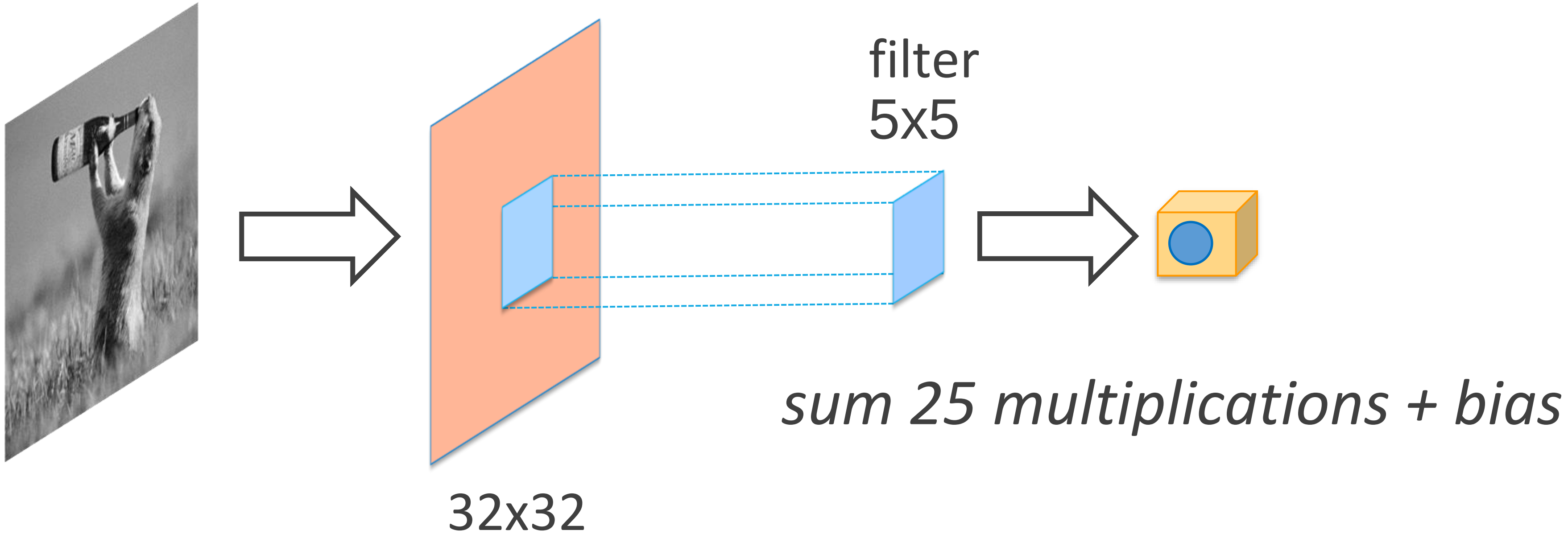
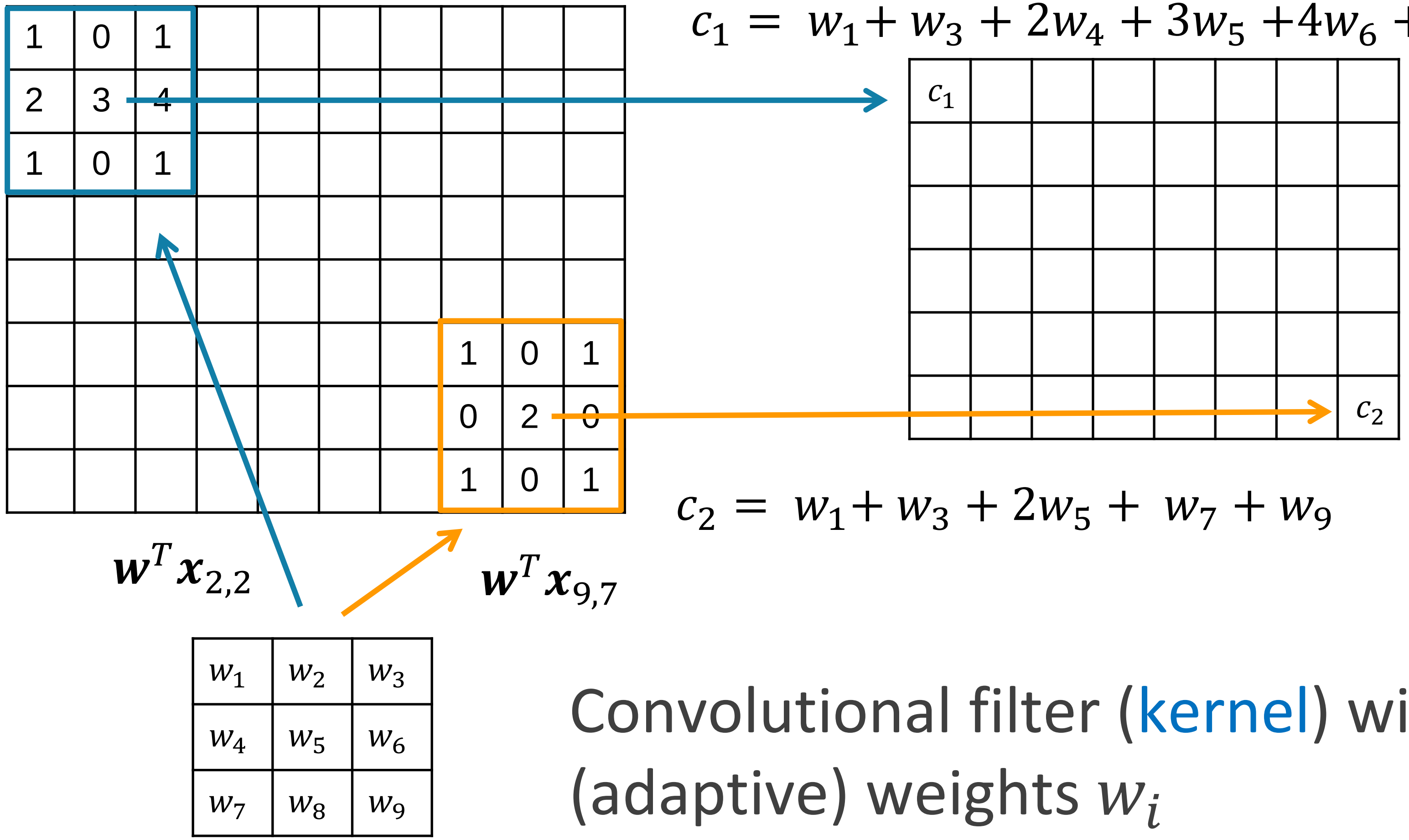
Convolution (Refresher)



Matrix input preserving
spatial structure

Adaptive Convolution

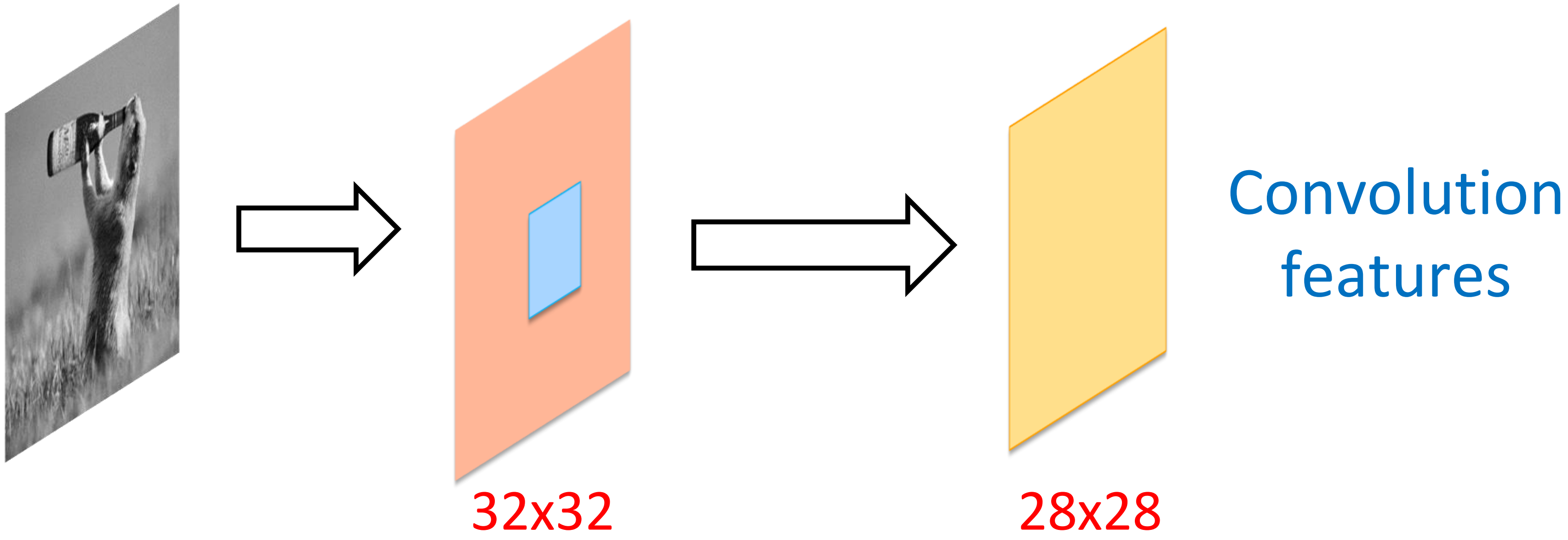


$$c_1 = w_1 + w_3 + 2w_4 + 3w_5 + 4w_6 + w_7 + w_9$$

$$c_2 = w_1 + w_3 + 2w_5 + w_7 + w_9$$

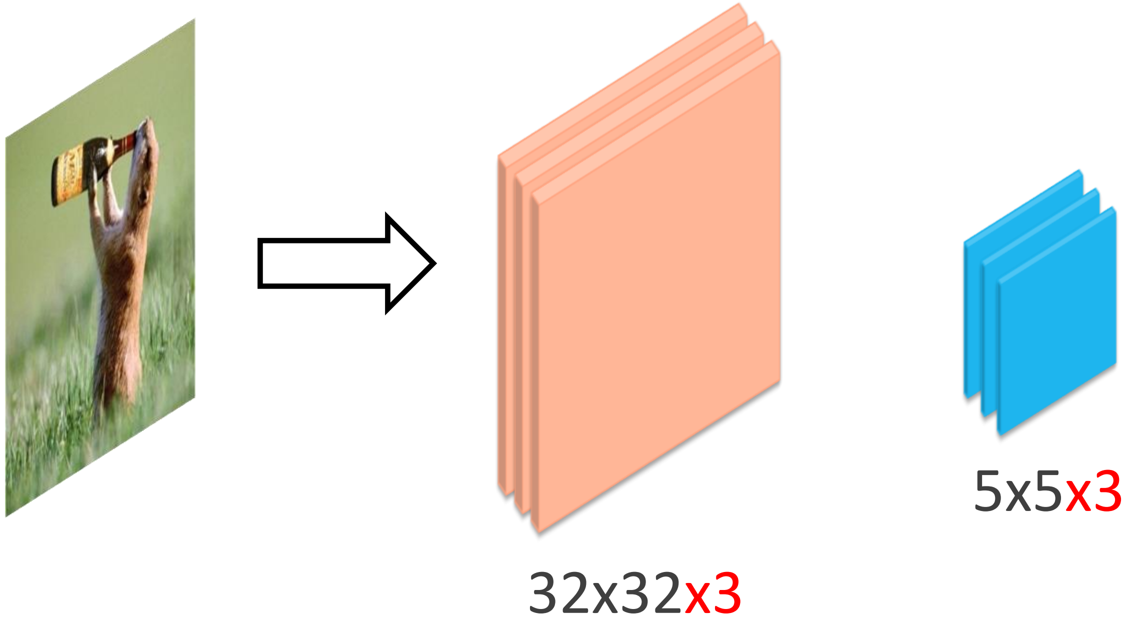
Convolutional filter (kernel) with (adaptive) weights w_i

Convolutional Features



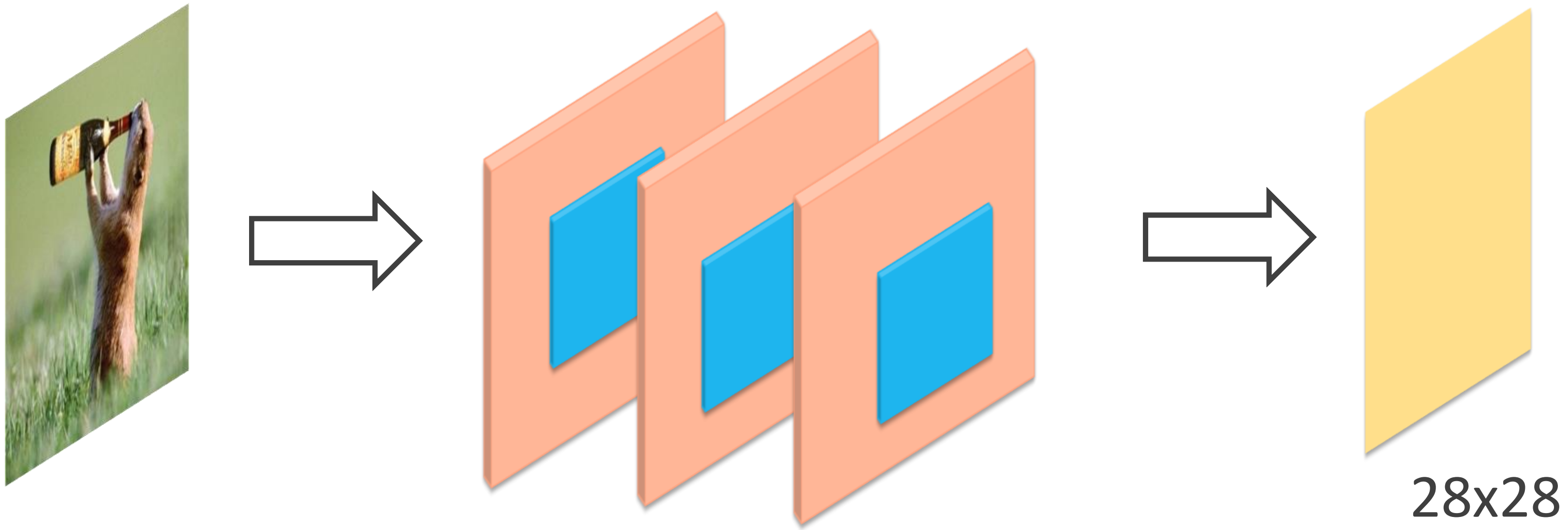
Slide the filter on the image computing elementwise products and summing up

Multi-Channel Convolution



Convolution filter has a number of slices equal to the number of image channels

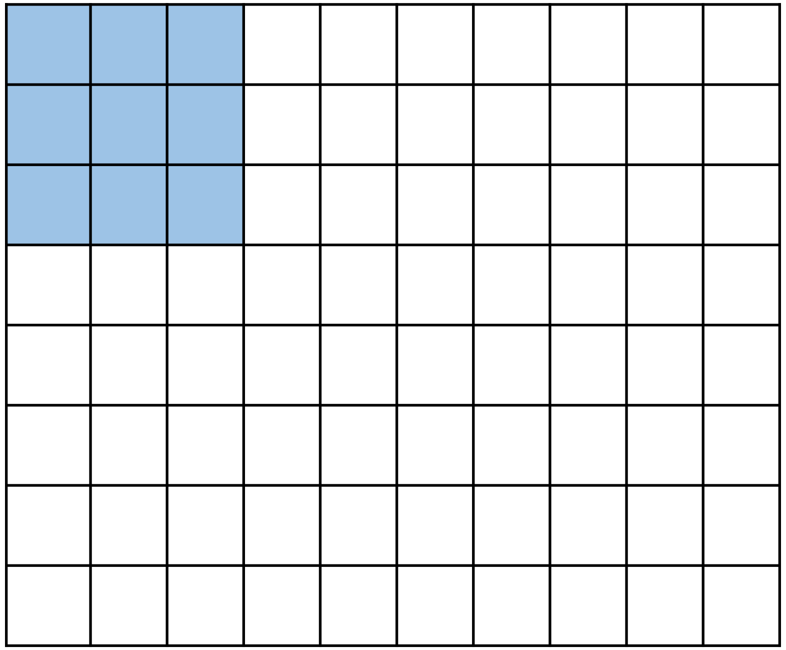
Multi-Channel Convolution



All channels are typically convolved together

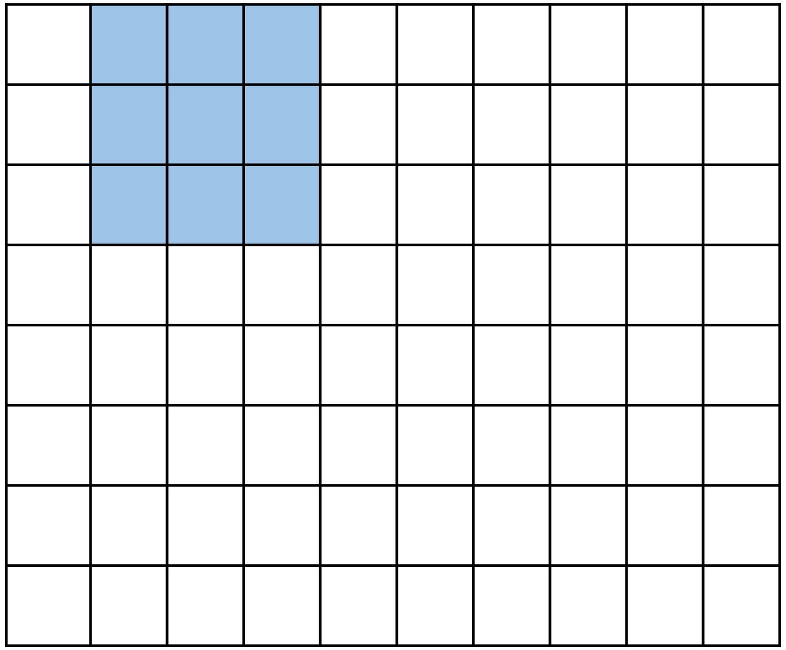
- They are summed-up in the convolution
- The convolution map stays bi-dimensional

Stride



- Basic convolution slides the filter on the image one pixel at a time
    - Stride = 1

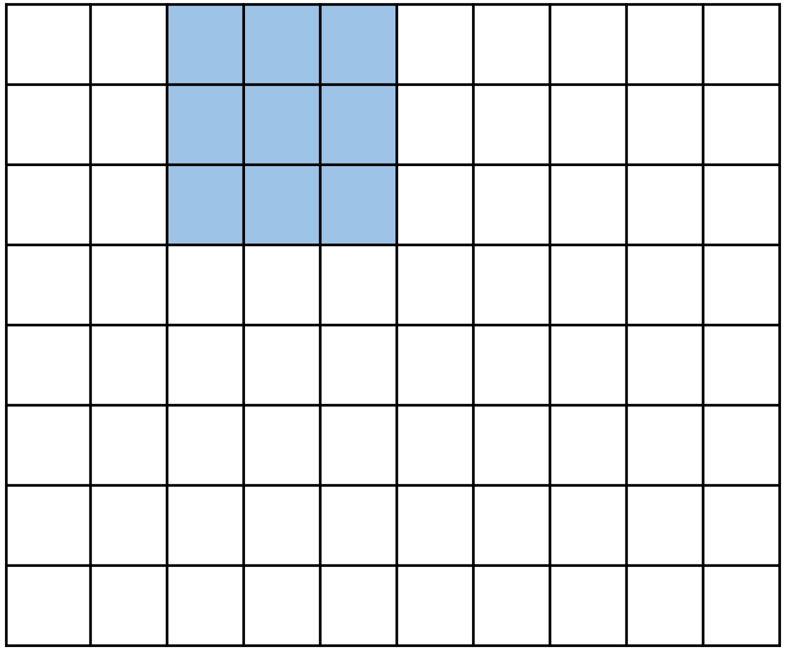
Stride



stride = 1

- Basic convolution slides the filter on the image one pixel at a time
  - Stride = 1

Stride



stride = 1

- Basic convolution slides the filter on the image one pixel at a time
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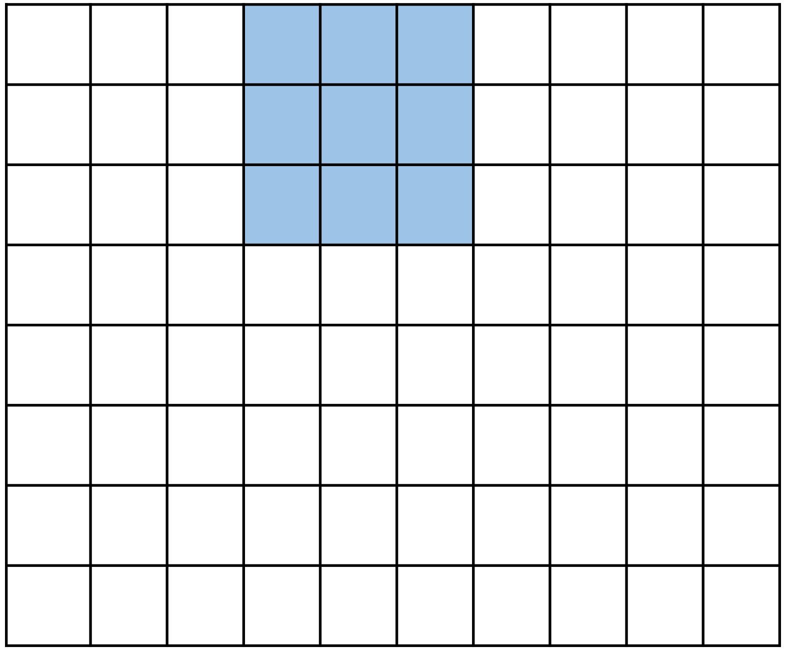
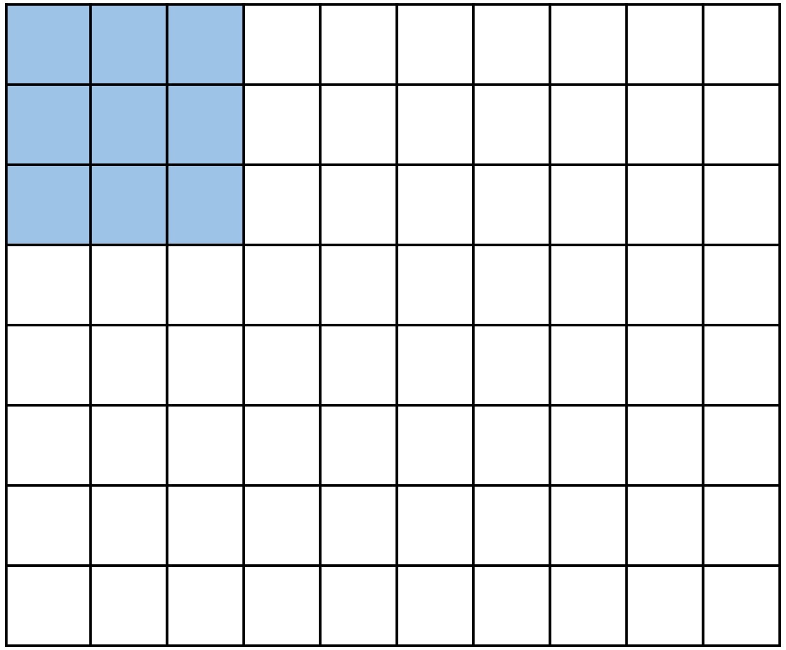
Stride



stride = 1

- Basic convolution slides the filter on the image one pixel at a time
  - Stride = 1

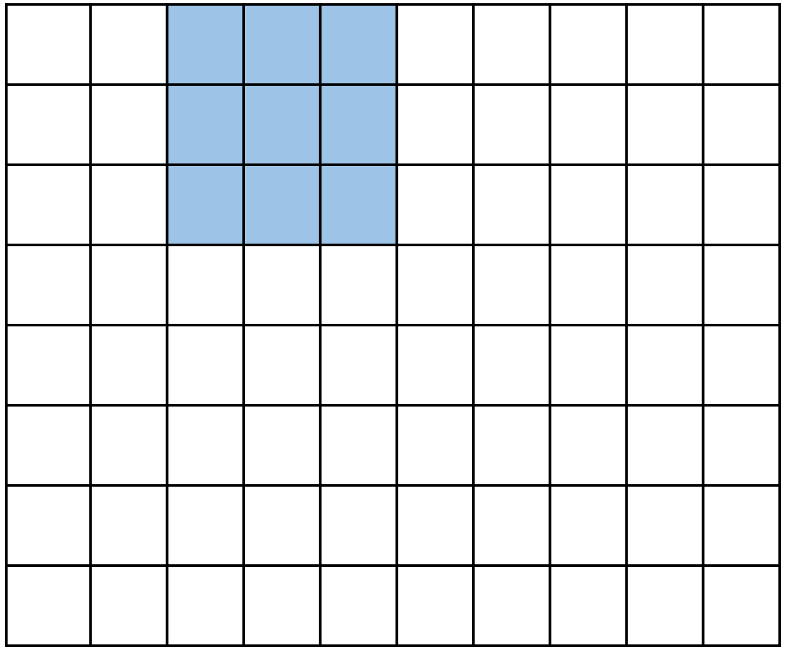
Stride



stride = 2

- Basic convolution slides the filter on the image one pixel at a time
  - Stride = 1
- Can define a different stride
  - Hyperparameter

Stride



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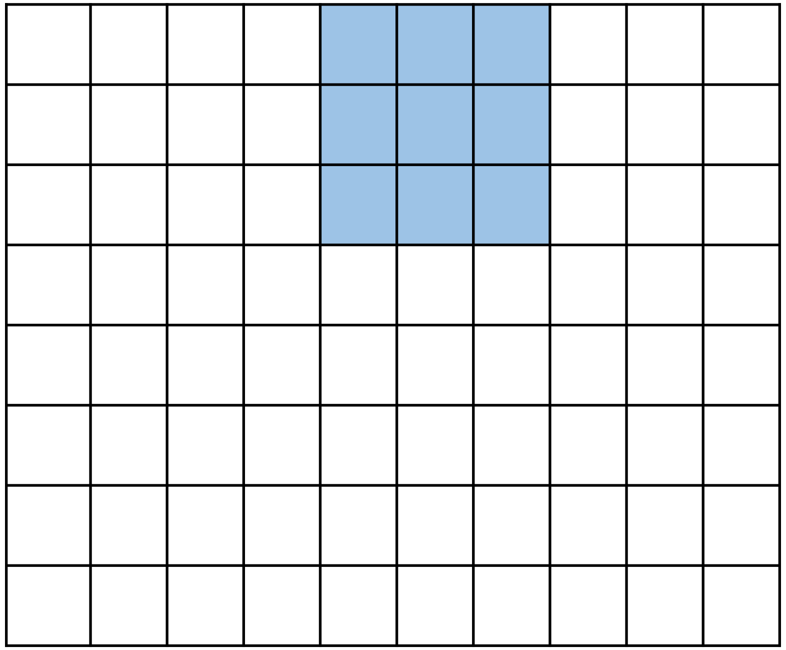
Stride



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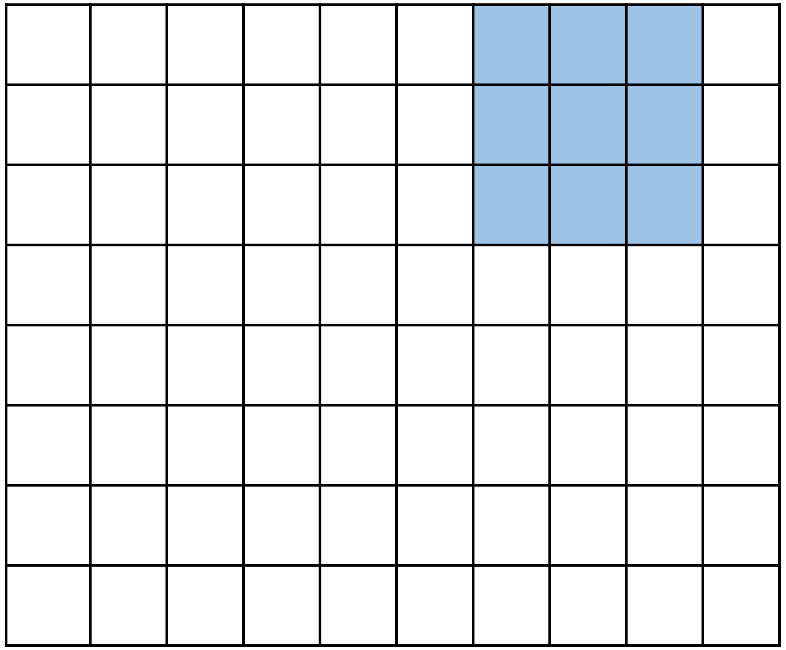
- Basic convolution slides the filter on the image one pixel at a time
  - Stride = 1
- Can define a different stride
  - Hyperparameter

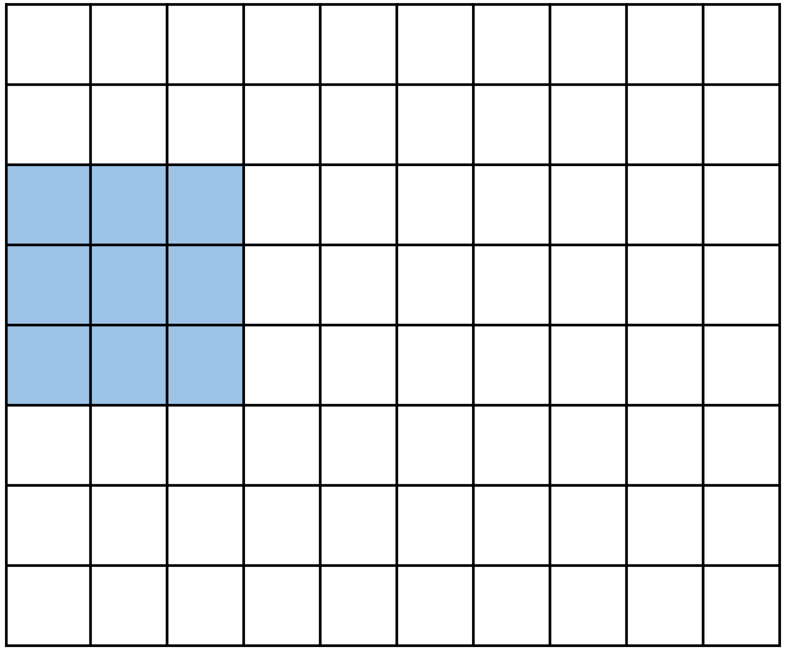
Stride



stride = 2

- Basic convolution slides the filter on the image one pixel at a time
  - Stride = 1
- Can define a different stride
  - Hyperparameter

Stride

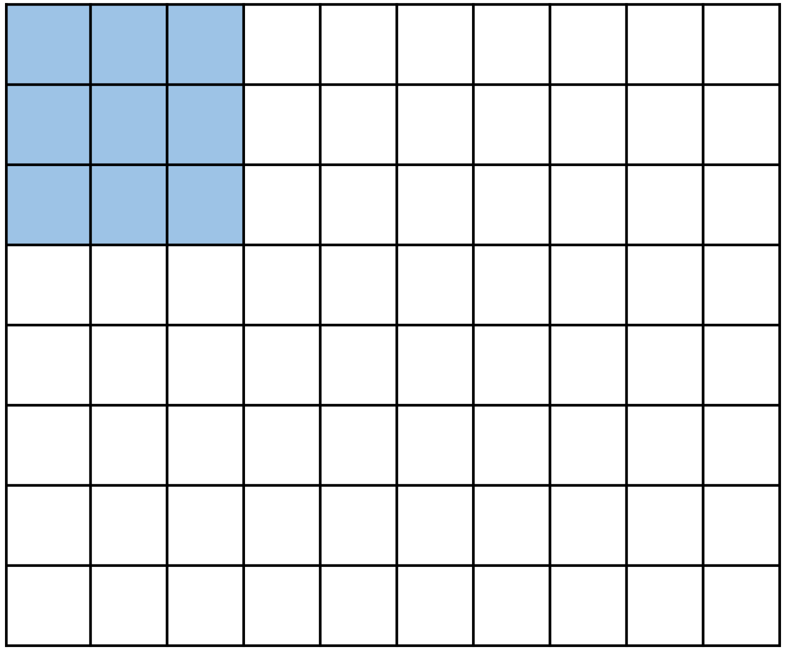


stride = 2

Works in both directions!

- Basic convolution slides the filter on the image one pixel at a time
  - Stride = 1
- Can define a different stride
  - Hyperparameter

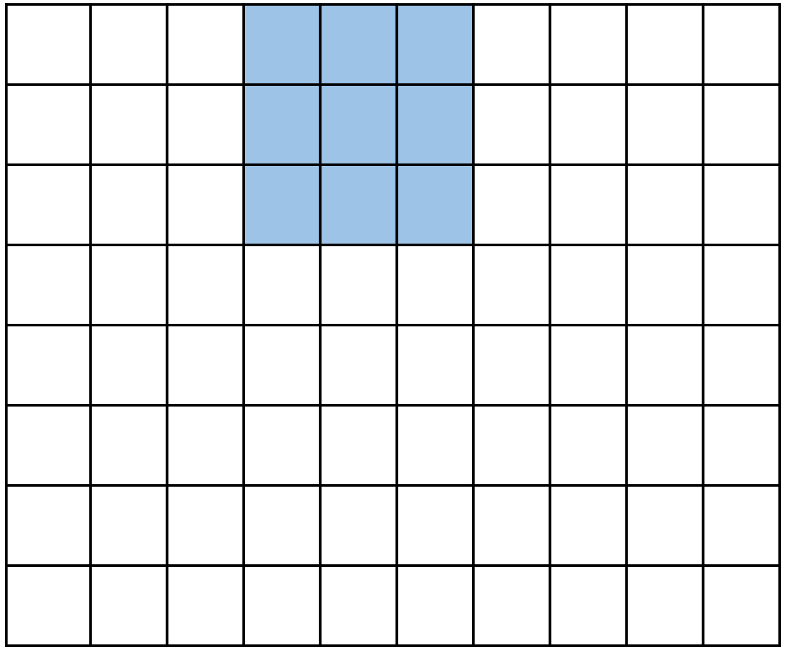
Stride



stride = 3

- Basic convolution slides the filter on the image one pixel at a time
  - Stride = 1
- Can define a different stride
  - Hyperparameter
- Stride reduces the number of multiplications
  - Subsamples the image

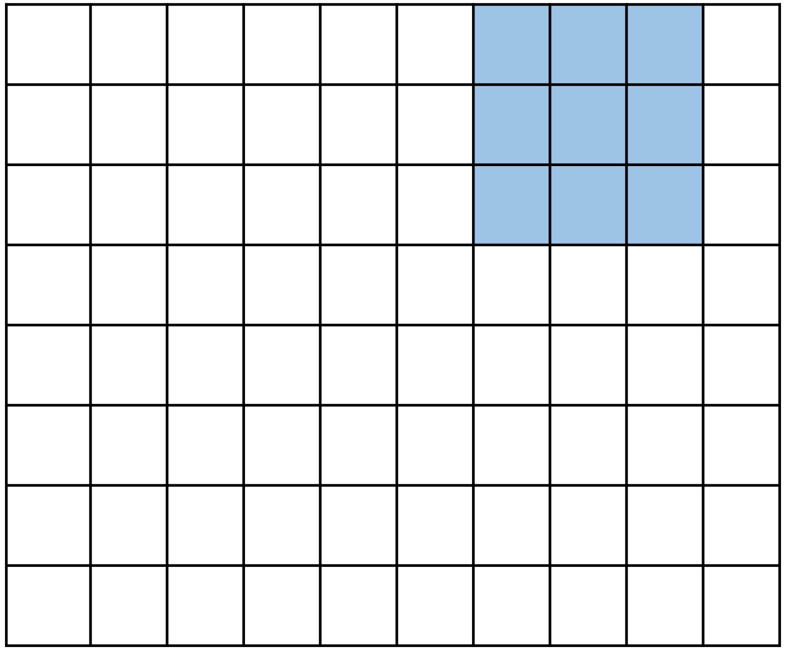
Stride



stride = 3

- Basic convolution slides the filter on the image one pixel at a time
  - Stride = 1
- Can define a different stride
  - Hyperparameter
- Stride reduces the number of multiplications
  - Subsamples the image

Stride

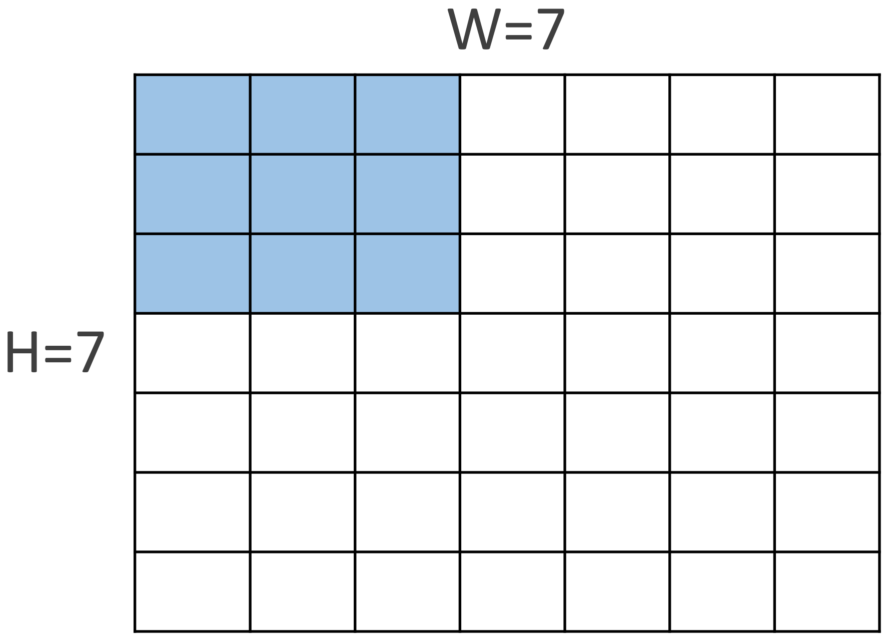


stride = 3

- Basic convolution slides the filter on the image one pixel at a time
  - Stride = 1
- Can define a different stride
  - Hyperparameter
- Stride reduces the number of multiplications
  - Subsamples the image

Activation Map Size

What is the size of the image after application of a filter with a given size and stride?



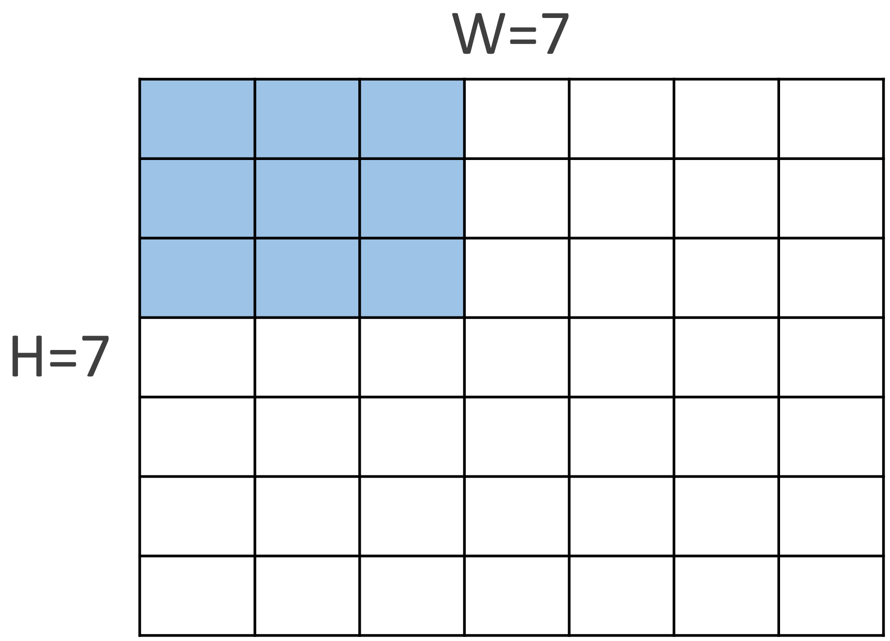
Take a 3x3 filter with stride 1

K=3, S=1

Output image is: 5x5

Activation Map Size

What is the size of the image after application of a filter with a given size and stride?



Take a 3x3 filter with stride 2

K=3, S=2

⇩

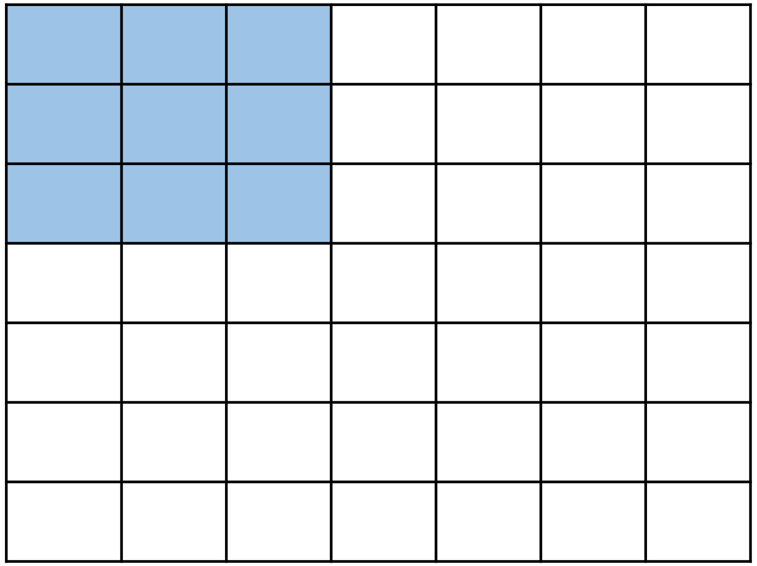
Output image is: 3x3

Activation Map Size

What is the size of the image after application of a filter with a given size and stride?

W=7

H=7



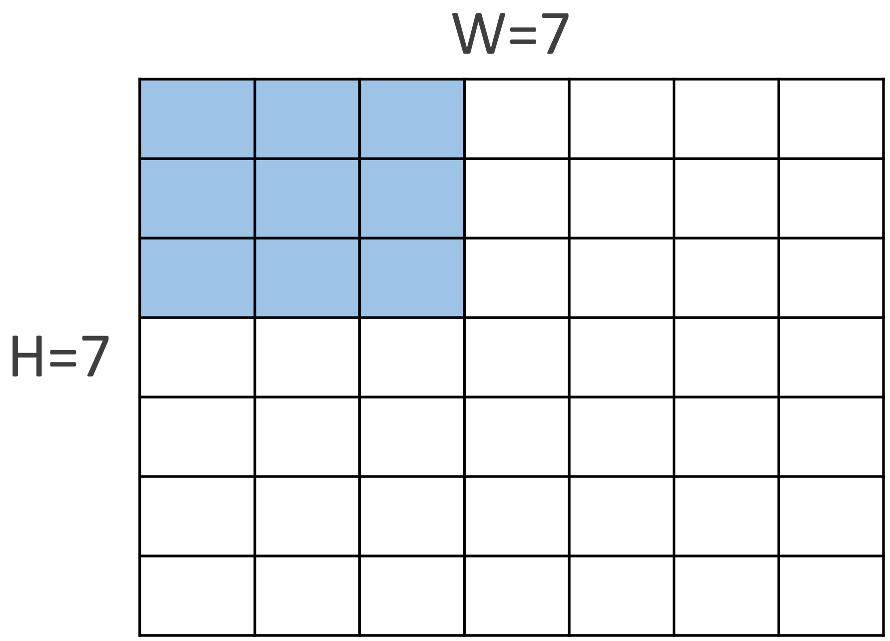
General rule

$$W' = \frac{W - K}{S} + 1$$

$$H' = \frac{H - K}{S} + 1$$

Activation Map Size

What is the size of the image after application of a filter with a given size and stride?



Take a 3x3 filter with stride 3

K=3, S=3

Output image is: not really and image!

Zero Padding

Add columns and rows of zeros to the border of the image

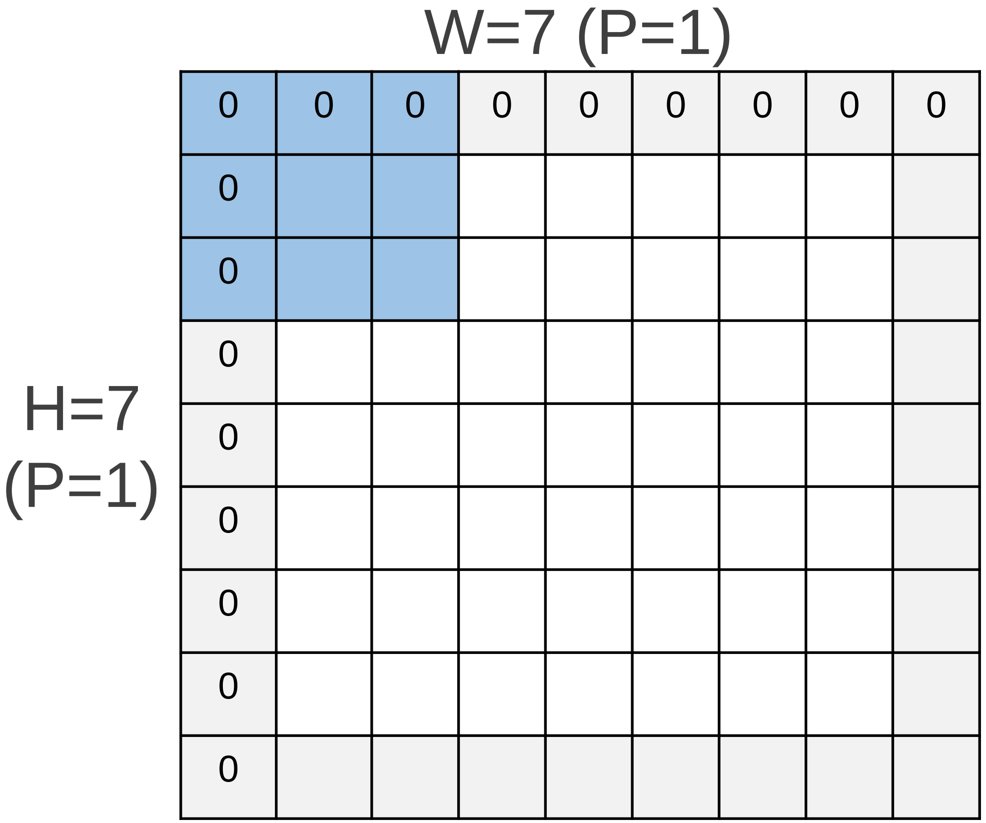
W=7

H=7

0	0	0	0	0	0	0	0	0
0								
0								
0								
0								
0								
0								
0								
0								

Zero Padding

Add columns and rows of zeros to the border of the image



K=3, S=1

⇩

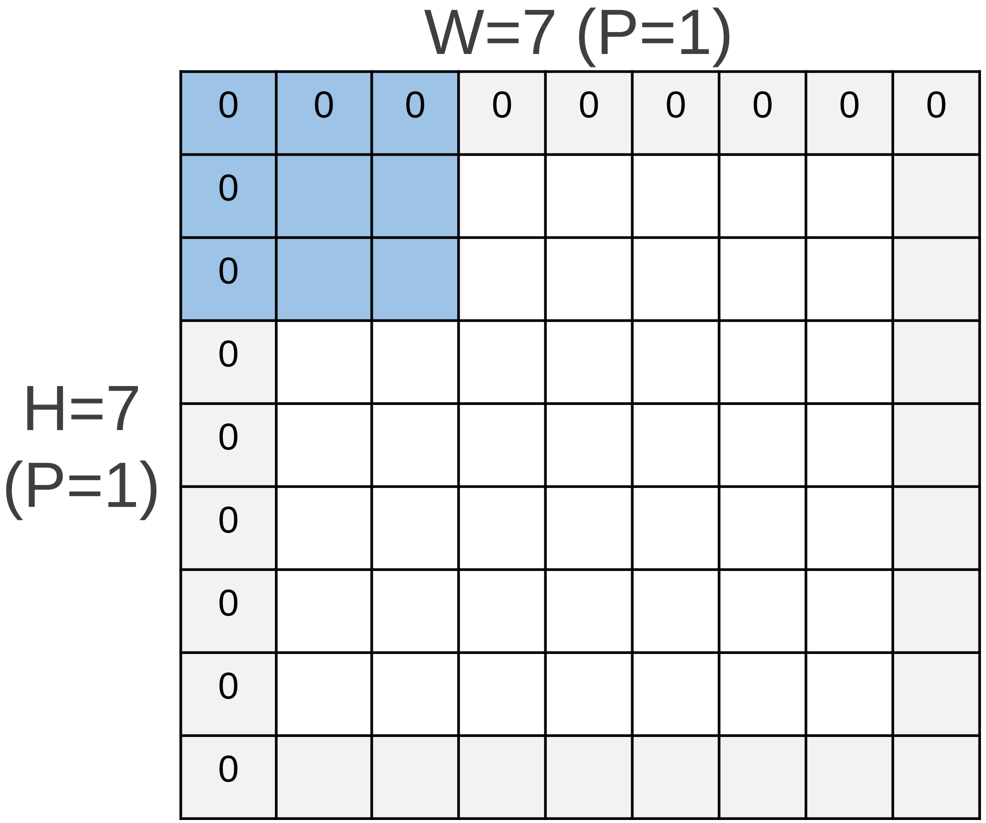
Output image is?

$$W' = \frac{W - K + 2P}{S} + 1$$

7x7

Zero Padding

Add columns and rows of zeros to the border of the image

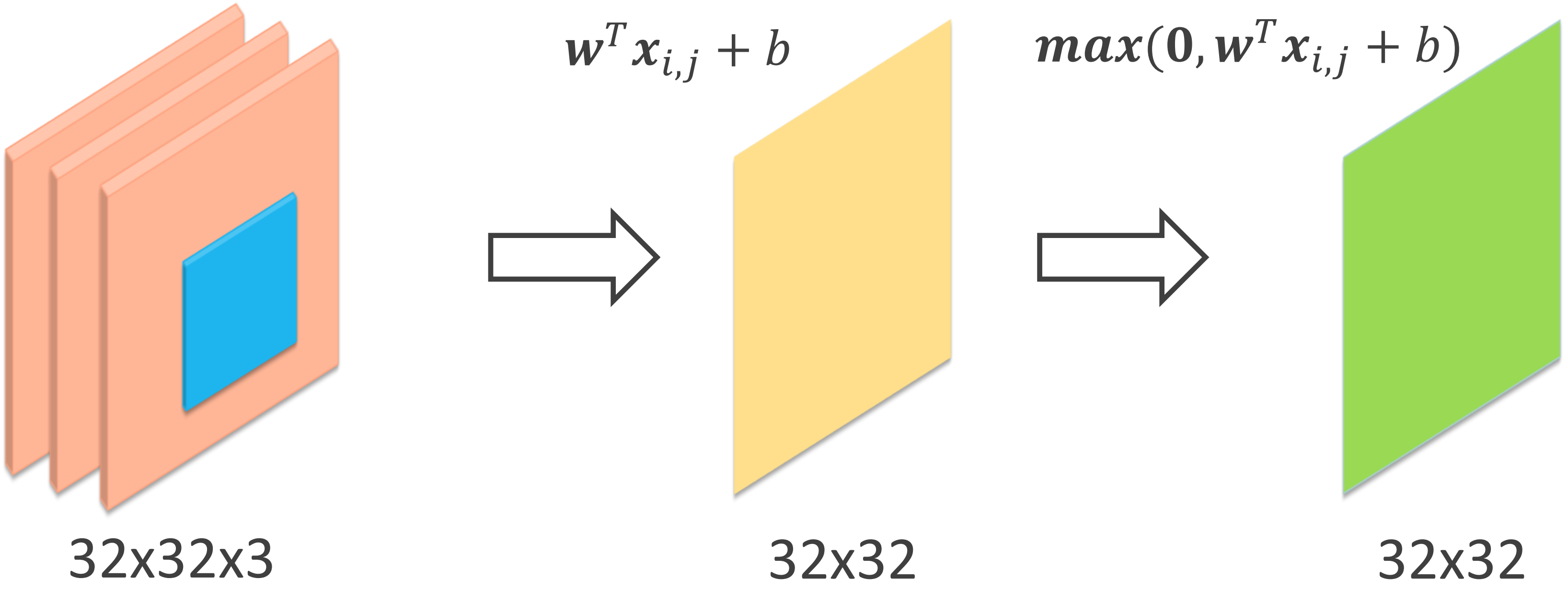


Zero padding serves to retain the original size of image

$$P = \frac{K-1}{2}$$

Pad as necessary to perform convolutions with a given stride S

Feature Map Transformation



- Convolution is a linear operator
- Apply an element-wise nonlinearity to obtain a transformed feature map

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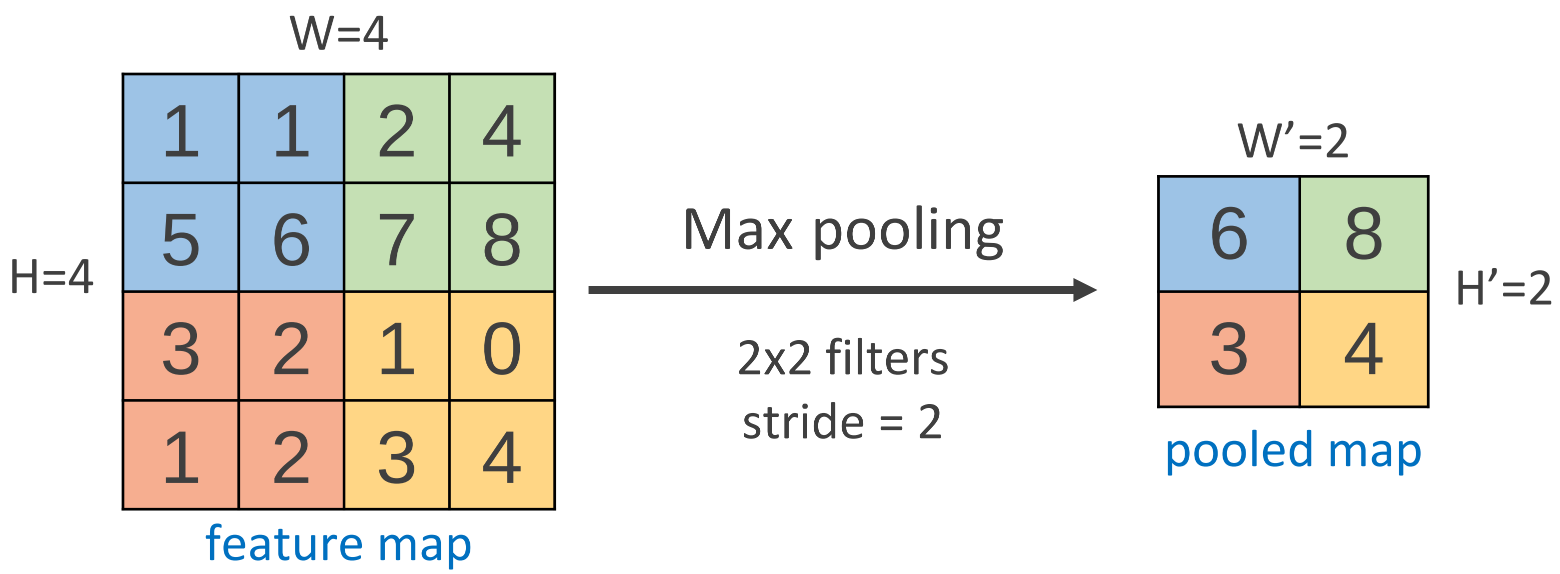
Pooling

- Operates on the feature map to make the representation
  - Smaller (subsampling)
  - Robust to (some) transformations



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Pooling Facts

- Max pooling is the one used more frequently, but other forms are possible
  - Average pooling
  - L2-norm pooling
  - Random pooling
- It is uncommon to use zero padding with pooling

$$W' = \frac{W - K}{S} + 1$$

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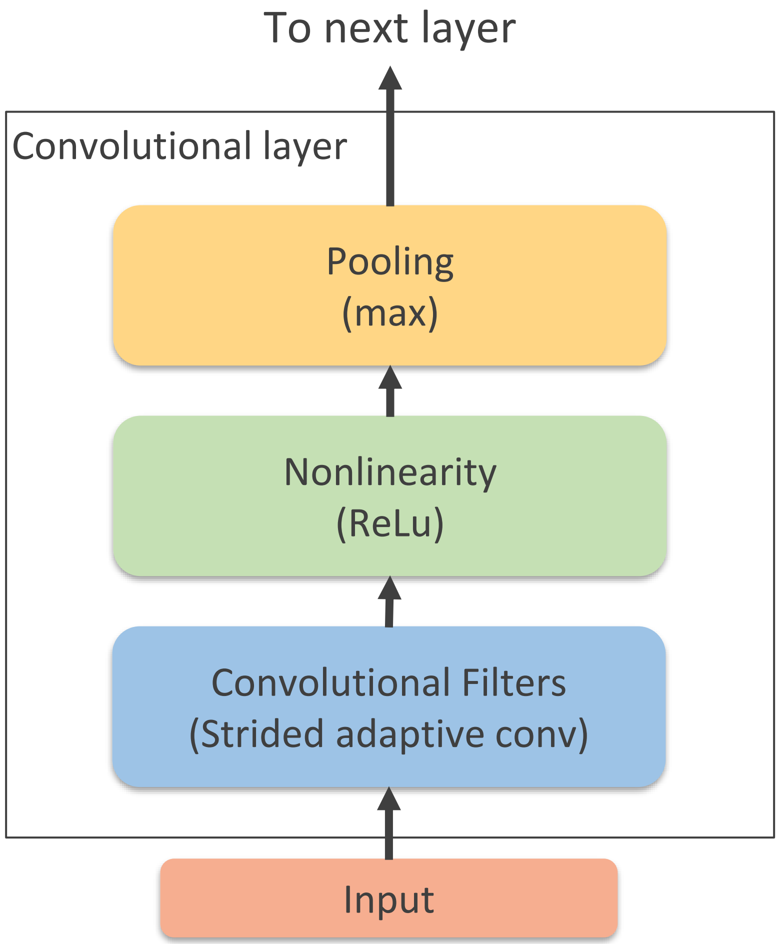
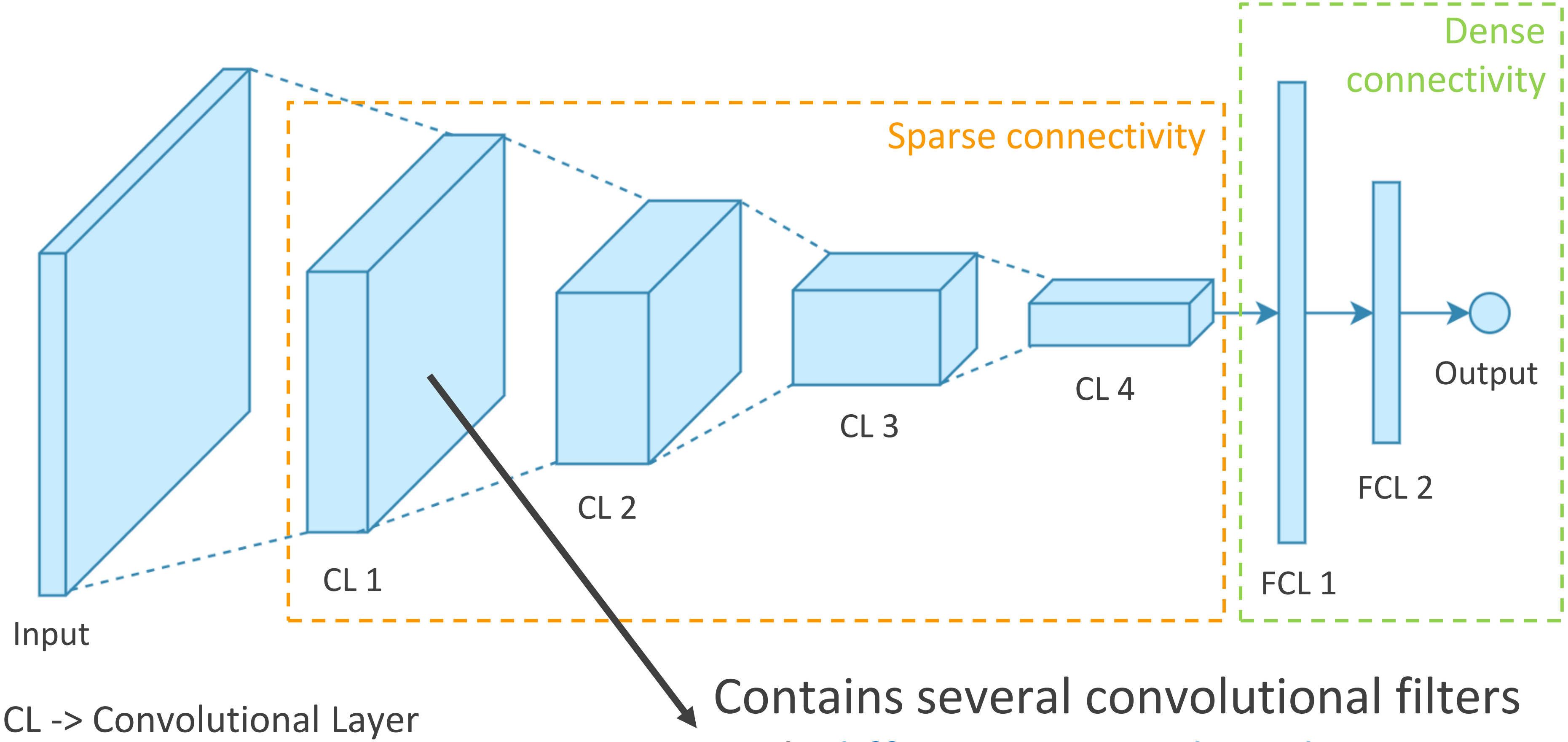
The Convolutional Architecture



- An architecture made by a hierarchical composition of the basic elements
- Convolution layer is an abstraction for the composition of the 3 basic operations
- Network parameters are in the convolutional component

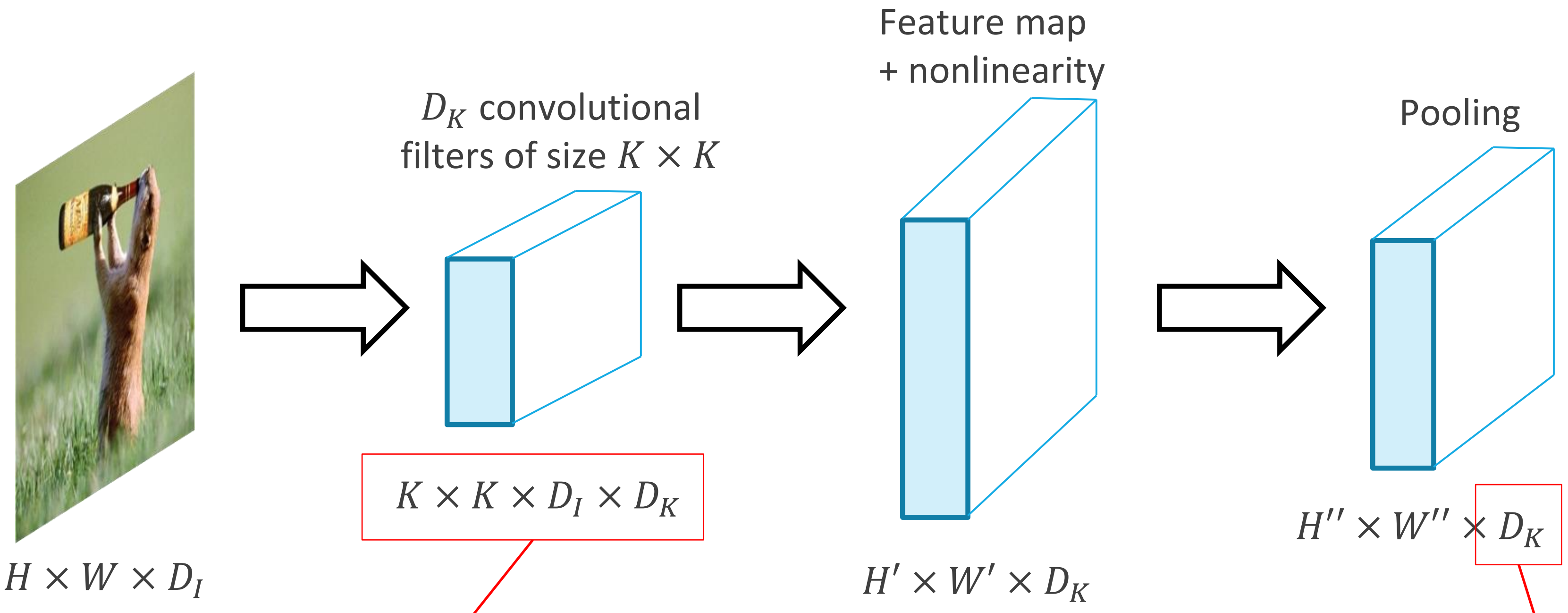
A Bigger Picture



CL -> Convolutional Layer
FCL -> Fully Connected Layer

Contains several convolutional filters with different size and stride

Convolutional Filter Banks



Number of model parameters due to this convolution element (add D_K bias terms)

Pooling is often (not always) applied independently on the D_K convolutions

Specifying CNN in Code (Keras)

Number of convolution filters D_k

Define input size (only first hidden layer)

```
model = Sequential()
model.add(Conv2D(32, kernel_size=(5, 5), strides=(1, 1),
                 activation='relu',
                 input_shape=input_shape))
model.add(MaxPooling2D(pool_size=(2, 2), strides=(2, 2)))
model.add(Conv2D(64, (5, 5))
model.add(Activation='relu'))
model.add(MaxPooling2D(pool_size=(2, 2)))
model.add(Flatten())
model.add(Dense(1000, activation='relu'))
model.add(Dense(num_classes, activation='softmax'))
```

Does for you all the calculations to determine the final size to the dense layer

A (Final?) Note on Convolution

- We know that discrete convolution between an image I and a filter/kernel K is

$$(I * K)(i,j) = \sum_m \sum_n I(i-m, j-n) K(m,n)$$

and it is commutative.

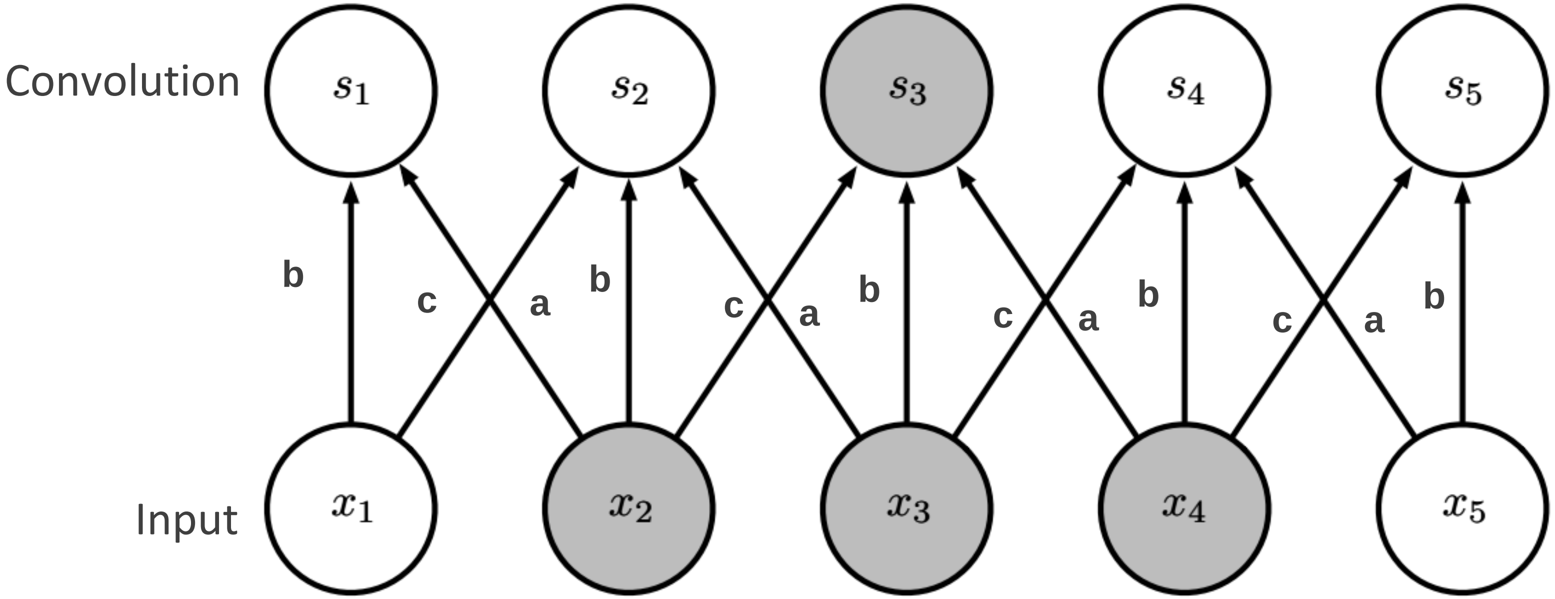
- In practice, convolution implementation in DL libraries does not flip the kernel

$$(I * K)(i,j) = \sum_m \sum_n I(i+m, i+n) K(m,n)$$

Which is cross-correlation and it is not commutative.

CNN as a Sparse Neural Network

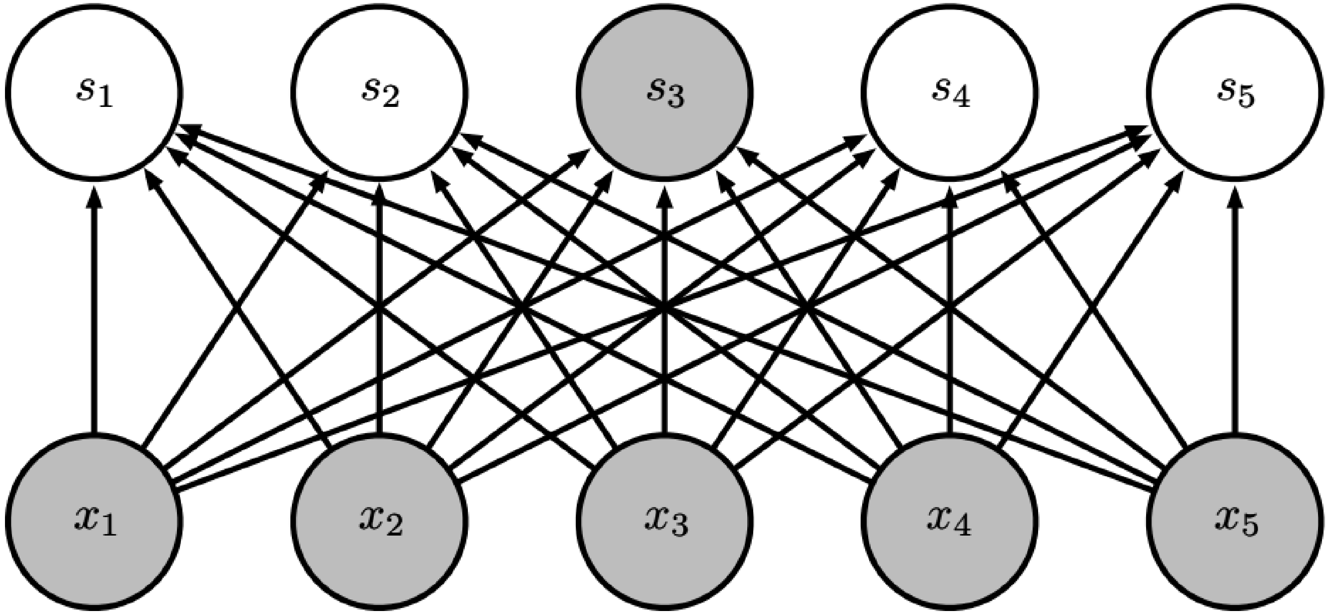
Let us take a 1-D input (sequence) to ease graphics



Convolution amounts to sparse connectivity (reduce parameters) with parameter sharing (enforces invariance)

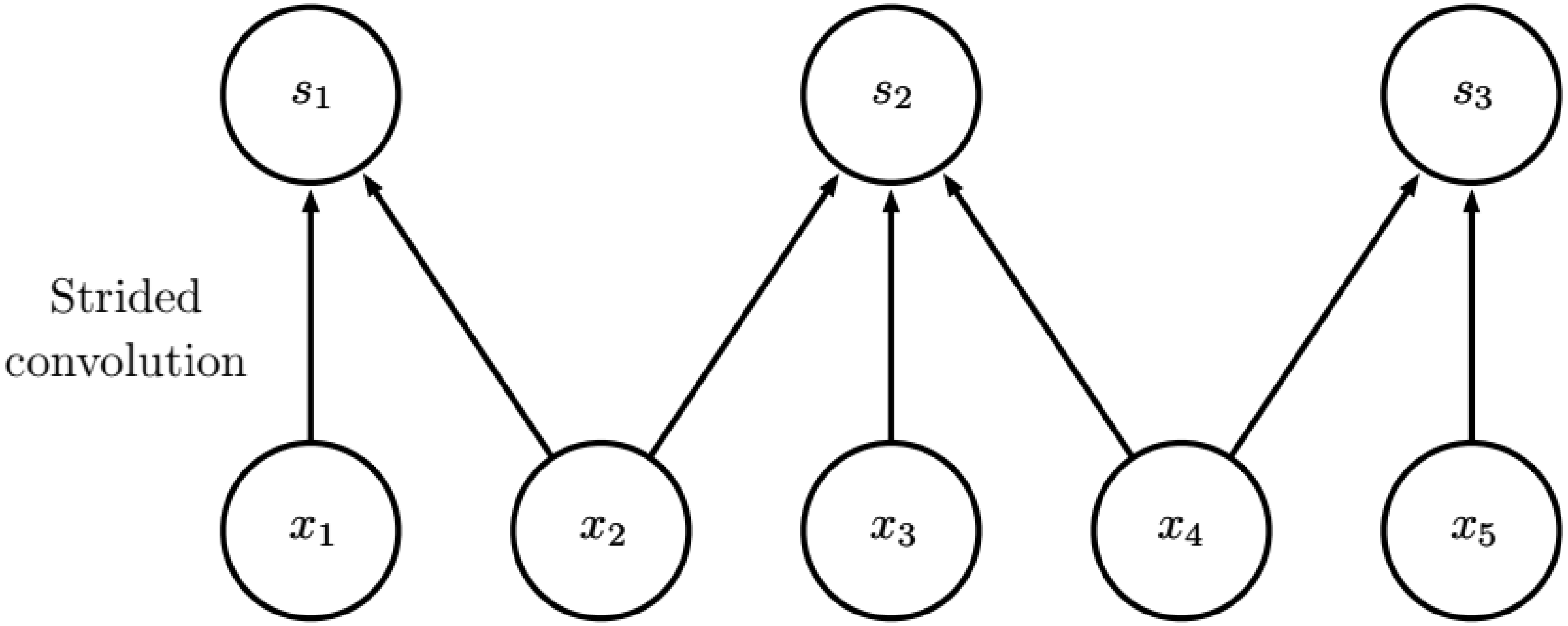
Dense Network

The dense counterpart would look like this



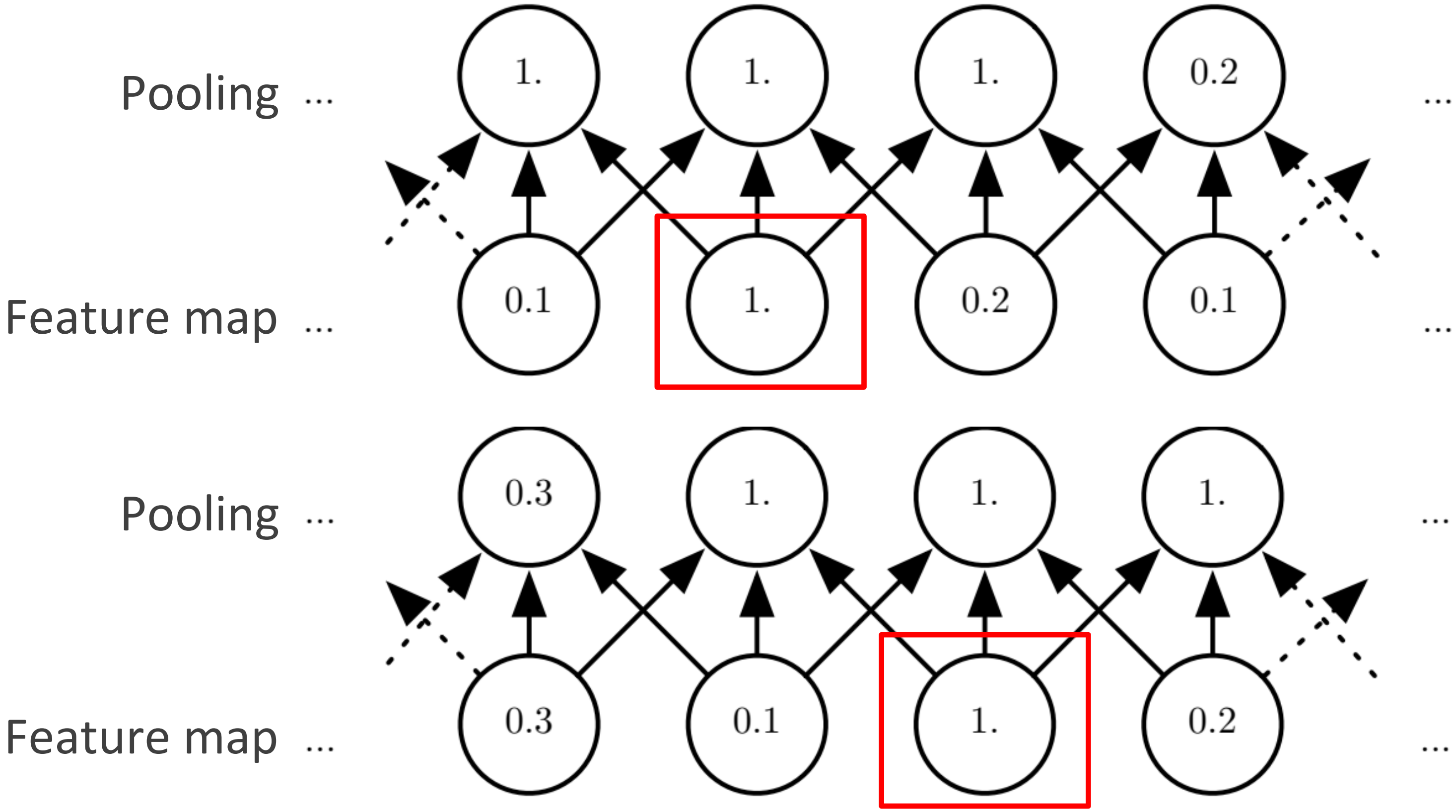
Strided Convolution

Make connectivity sparser

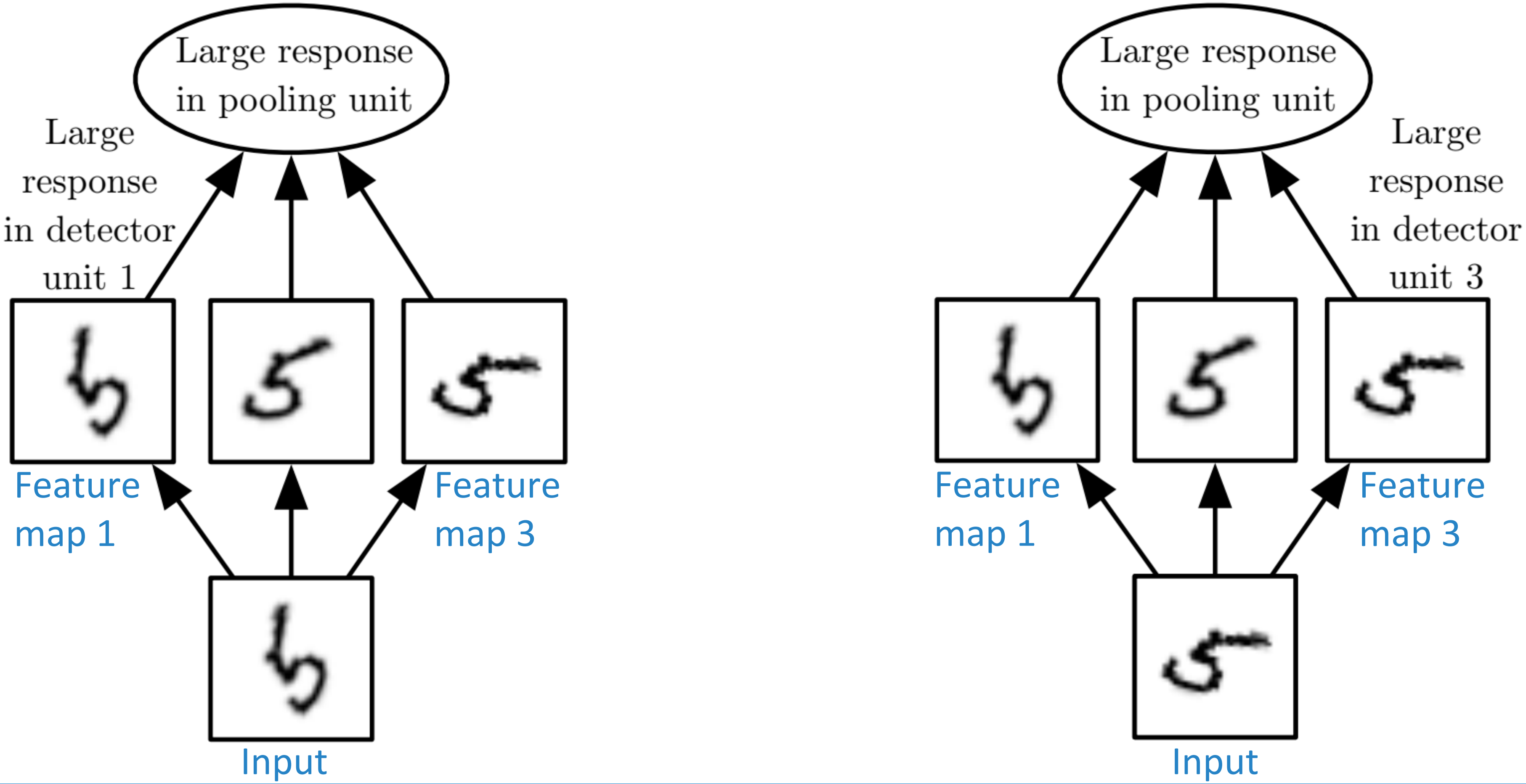


Max-Pooling and Spatial Invariance

A feature is detected even if it is spatially translated

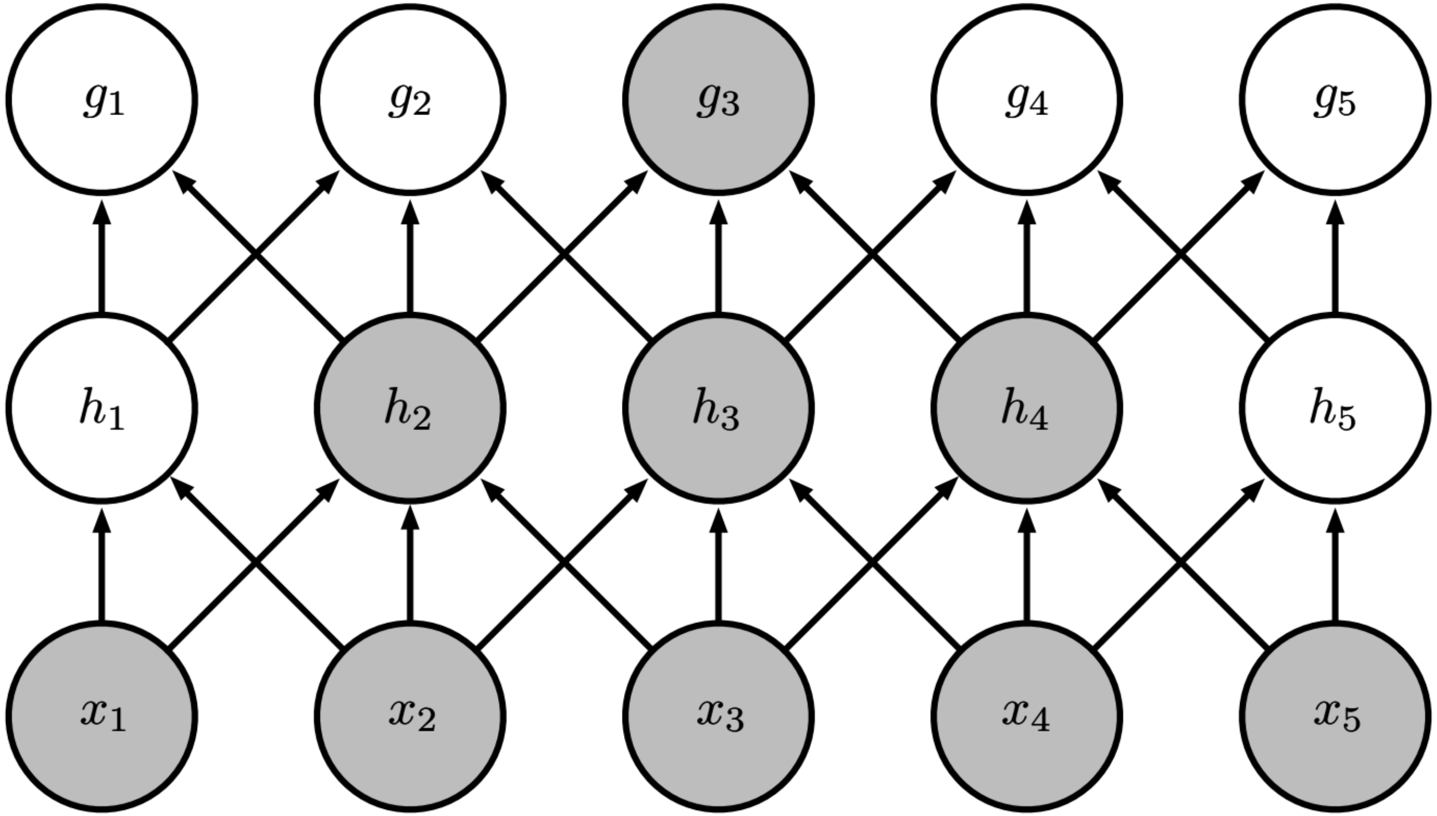


Cross Channel Pooling and Spatial Invariance

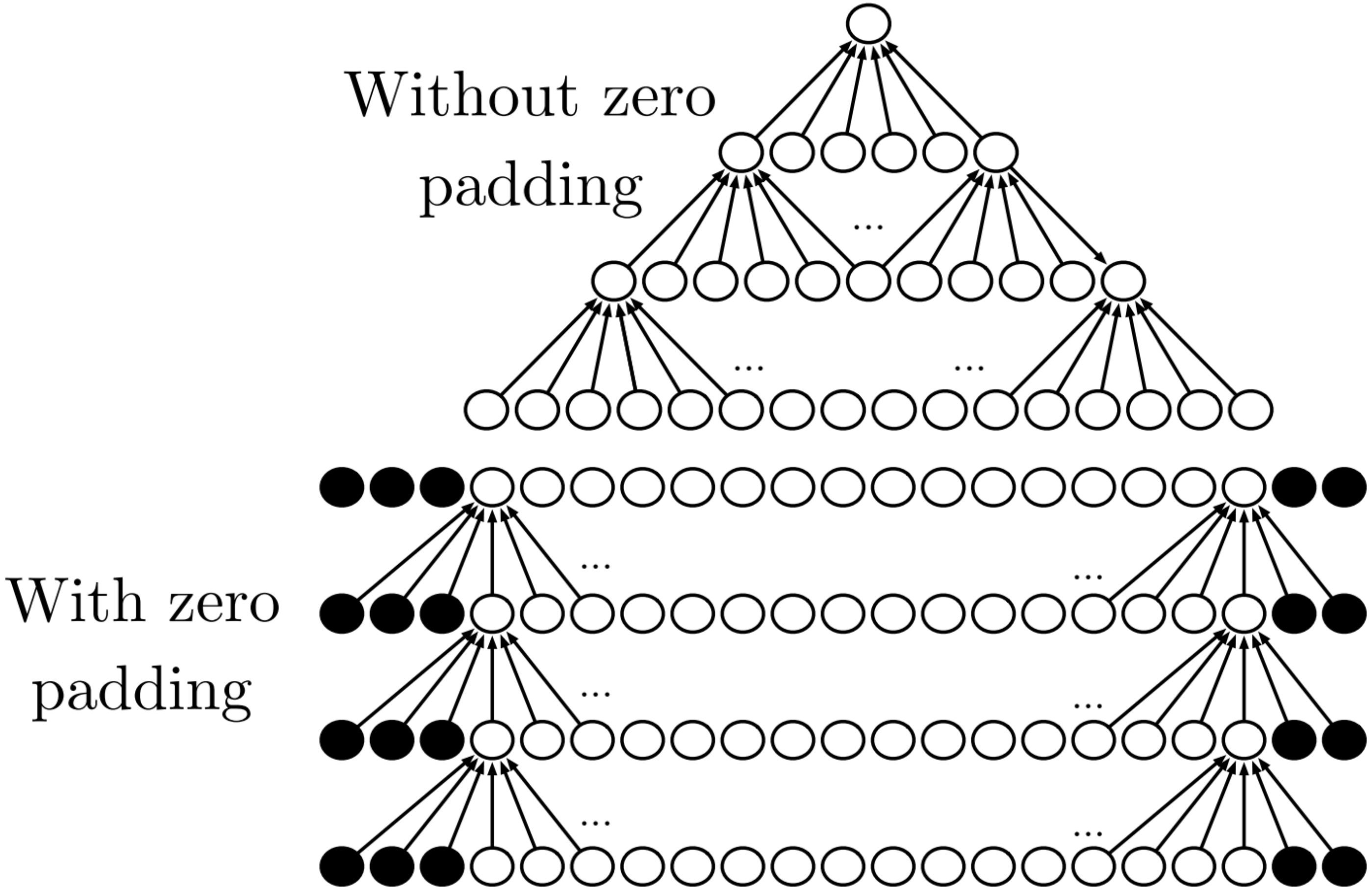


Hierarchical Feature Organization

The deeper the larger the receptive field of a unit



Zero-Padding Effect

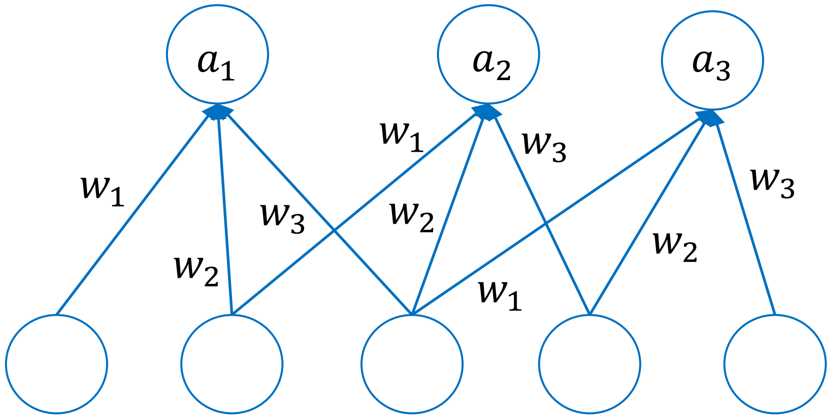


Assuming
no pooling

CNN Lecture – Part II

CNN Training

Variants of the standard backpropagation that account for the fact that connections share weights (convolution parameters)

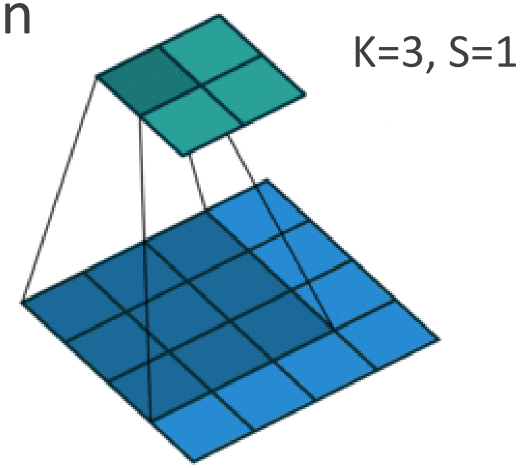


The gradient Δw_i is obtained by summing the contributions from all connections sharing the weight

Backpropagating gradients from convolutional layer N to N-1 is not as simple as transposing the weight matrix (need deconvolution with zero padding)

Backpropagating on Convolution

Convolution



Input is a 4x4 image
Output is a 2x2 image

Backpropagation step requires going back from the 2x2 to the 4x4 representation

Can write convolution as dense multiplication with shared weights

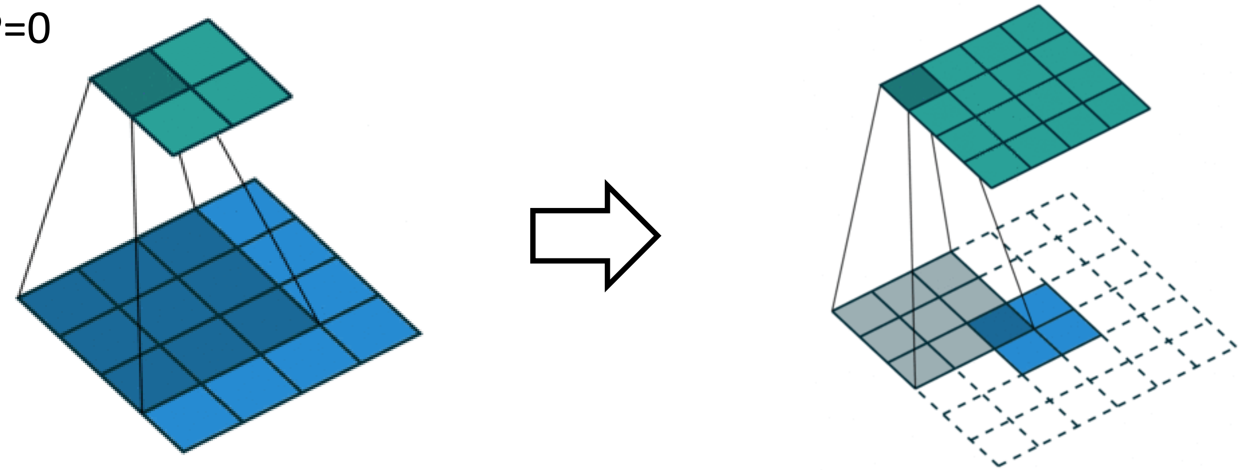
$$\begin{pmatrix} w_{0,0} & w_{0,1} & w_{0,2} & 0 & w_{1,0} & w_{1,1} & w_{1,2} & 0 & w_{2,0} & w_{2,1} & w_{2,2} & 0 & 0 & 0 & 0 & 0 \\ 0 & w_{0,0} & w_{0,1} & w_{0,2} & 0 & w_{1,0} & w_{1,1} & w_{1,2} & 0 & w_{2,0} & w_{2,1} & w_{2,2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & w_{0,0} & w_{0,1} & w_{0,2} & 0 & w_{1,0} & w_{1,1} & w_{1,2} & 0 & w_{2,0} & w_{2,1} & w_{2,2} & 0 \\ 0 & 0 & 0 & 0 & 0 & w_{0,0} & w_{0,1} & w_{0,2} & 0 & w_{1,0} & w_{1,1} & w_{1,2} & 0 & w_{2,0} & w_{2,1} & w_{2,2} \end{pmatrix}$$

Backpropagation is performed by multiplying the 4x1 representation to the transpose of this matrix

Deconvolution (Transposed Convolution)

We can obtain the transposed convolution using the same logic of the forward convolution

K=3, S=1, P=0



If you had no padding in the forward convolution, you need to pad much when performing transposed convolution

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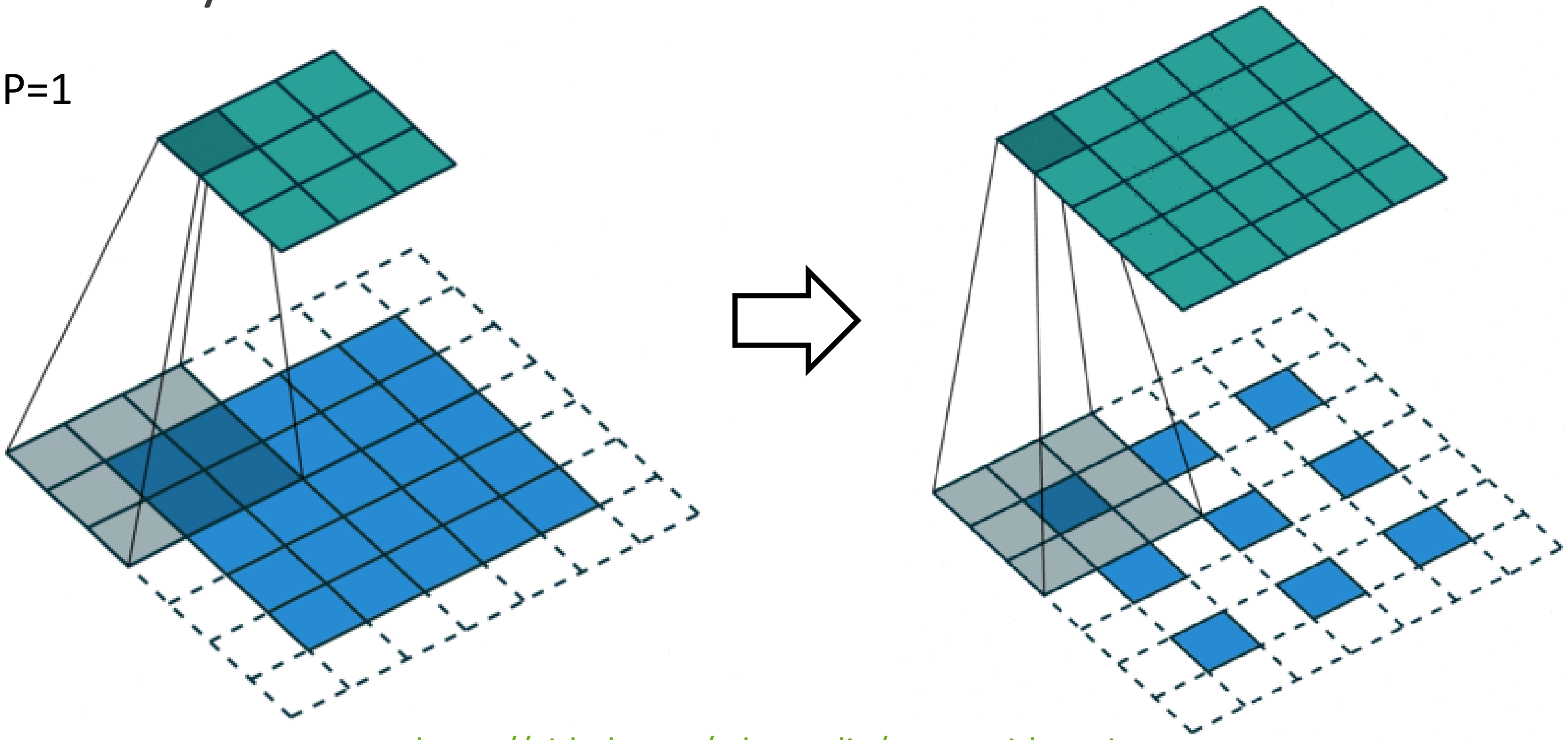
Deconvolution (Transposed Convolution)

If you have striding, you need to fill in the convolution map with zeroes to obtain a correctly sized deconvolution

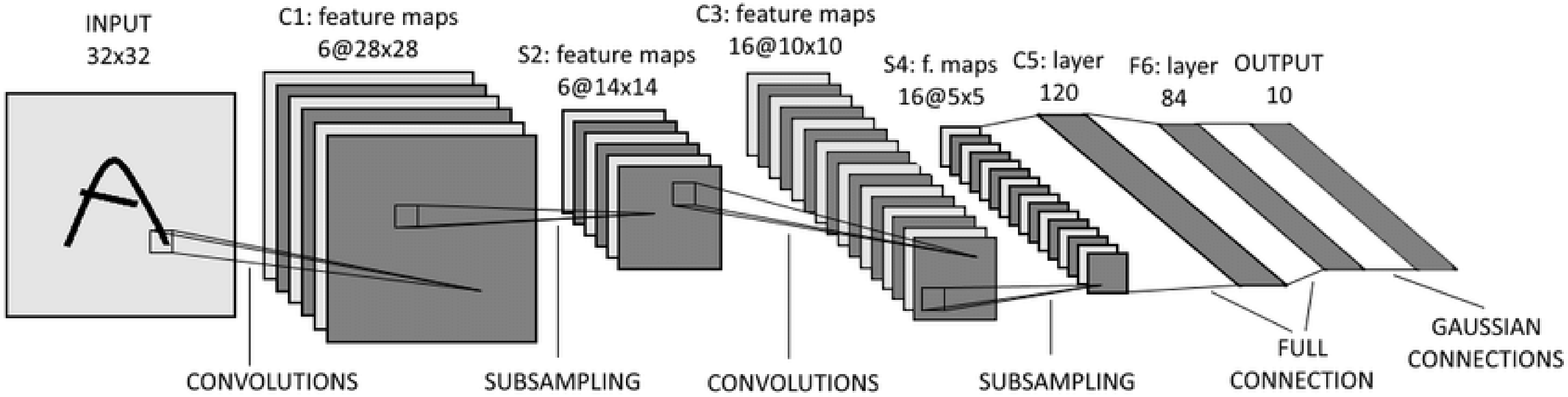
K=3, S=2, P=1



https://github.com/vdumoulin/conv_arithmetic

IN SUPREMÆ DIGNITATIS 1343 UNIVERSITÀ DI PISA

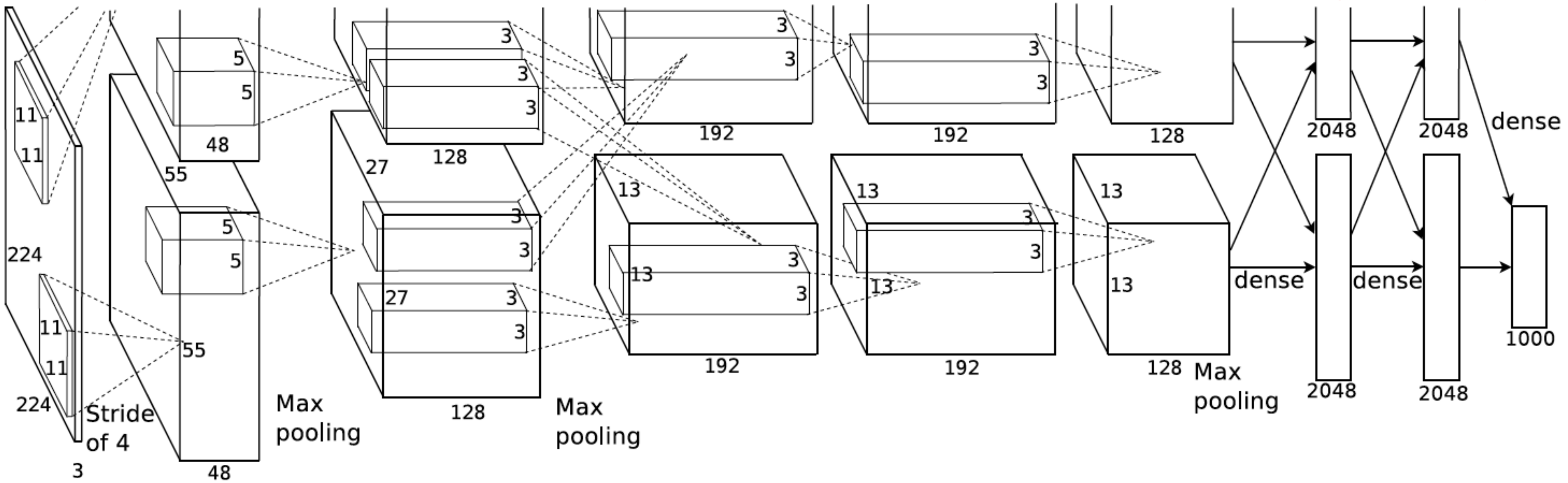
LeNet-5 (1989)



- Grayscale images
- Filters are 5x5 with stride 1 (sigmoid nonlinearity)
- Pooling is 2x2 with stride 2
- No zero padding

AlexNet (2012) - Architecture

ImageNet Top-5 : 15.4%



- RGB images 227x227x3
- 5 convolutional layers + 3 fully connected layers
- Split into two parts (top/bottom) each on 1 GPU

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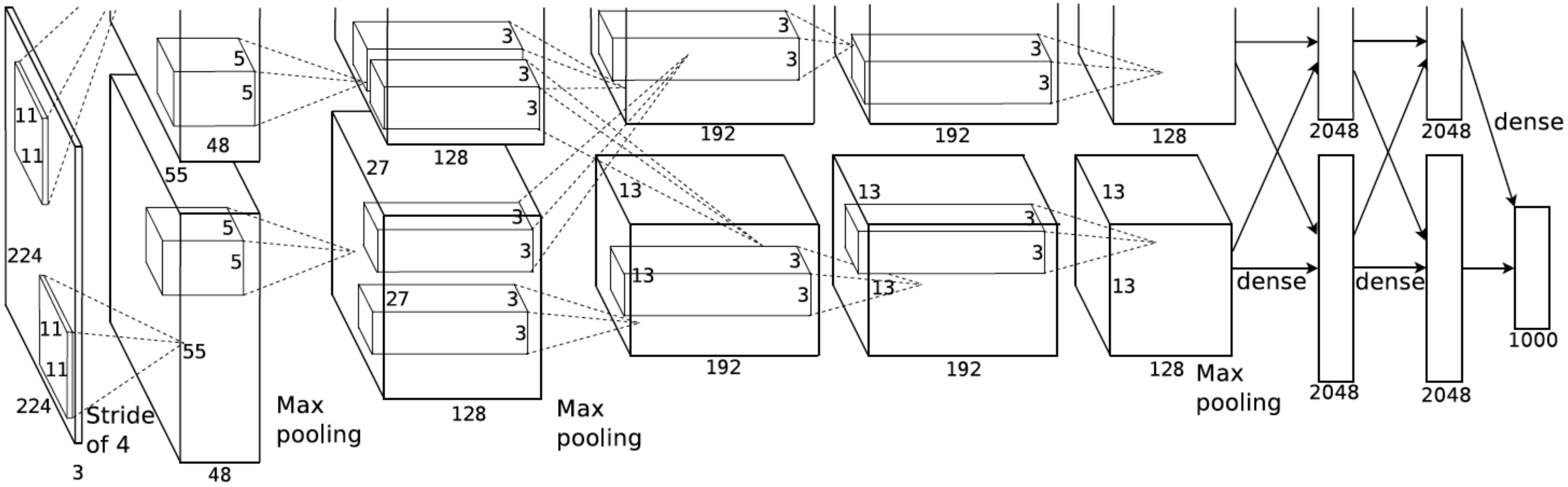
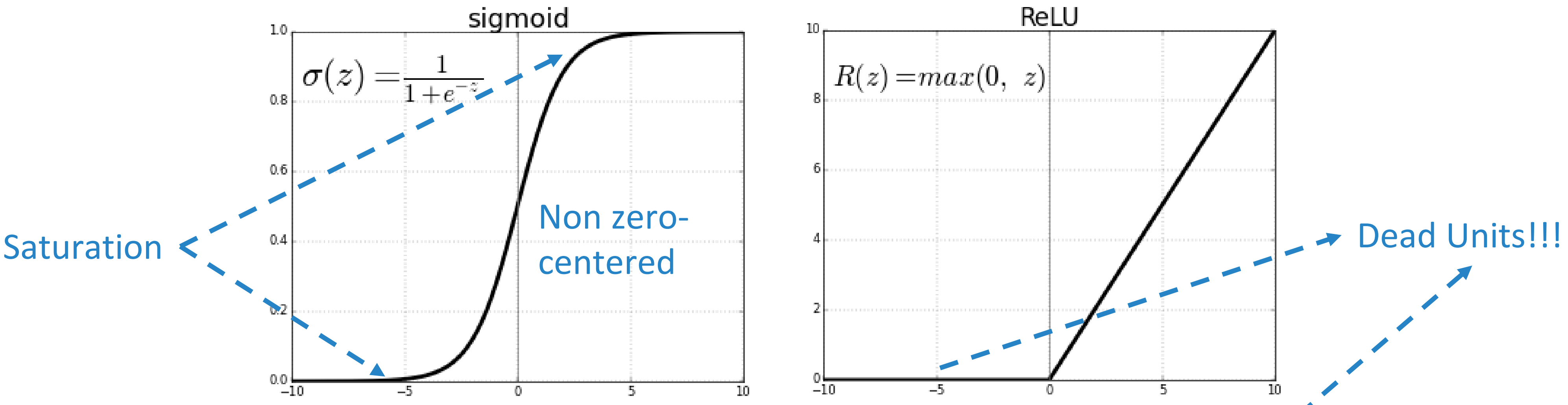
AlexNet - Innovations



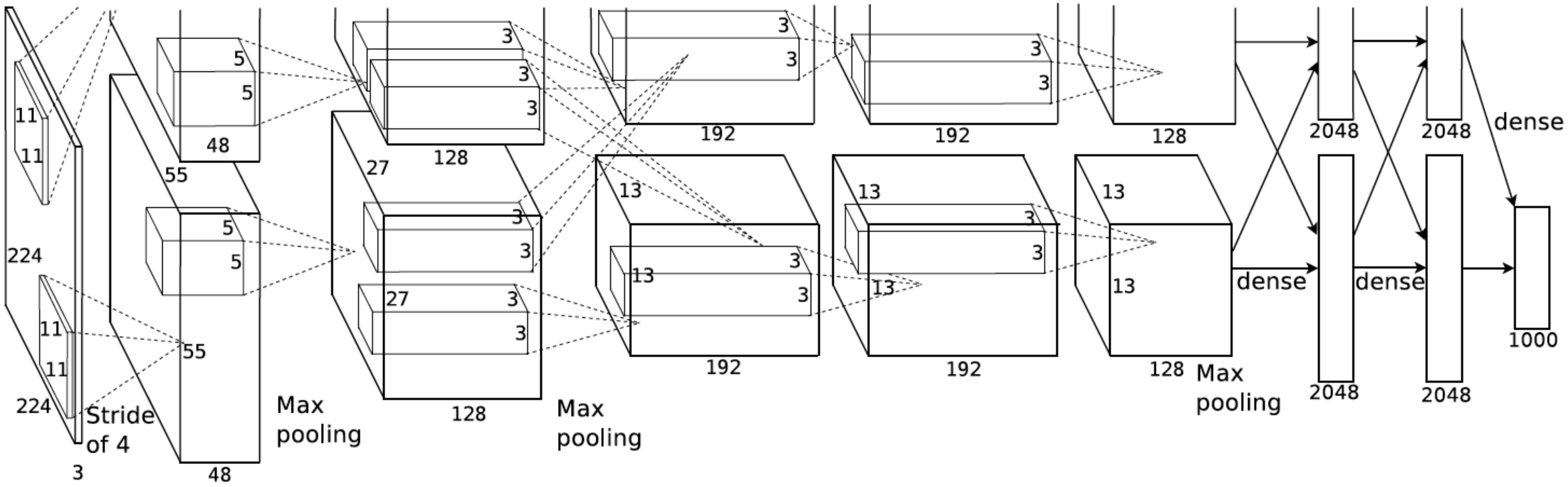
- Use heavy data augmentation (rotations, random crops, etc.)
- Introduced the use of ReLu
- Dense layers regularized by dropout

ReLU Nonlinearity



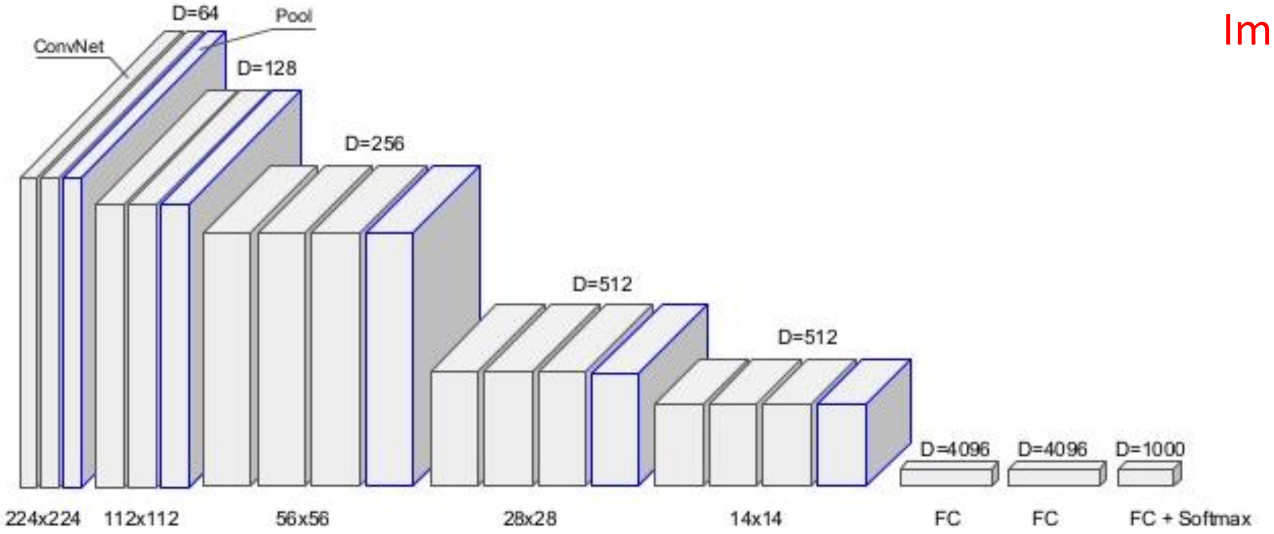
- ReLu help counteract gradient vanish
  - Sigmod first derivative vanishes as we increase or decrease z
  - ReLu first derivative is 1 when unit is active and 0 elsewhere
  - ReLu second derivative is 0 (no second order effects)
- Easy to compute (zero thresholding)
- Favors sparsity

AlexNet - Parameters



- 62.3 millions of parameters (6% in convolutions)
- 5-6 days to train on two GTX 580 GPUs (95% time in convolutions)

VGGNet – VGG16 (2014)

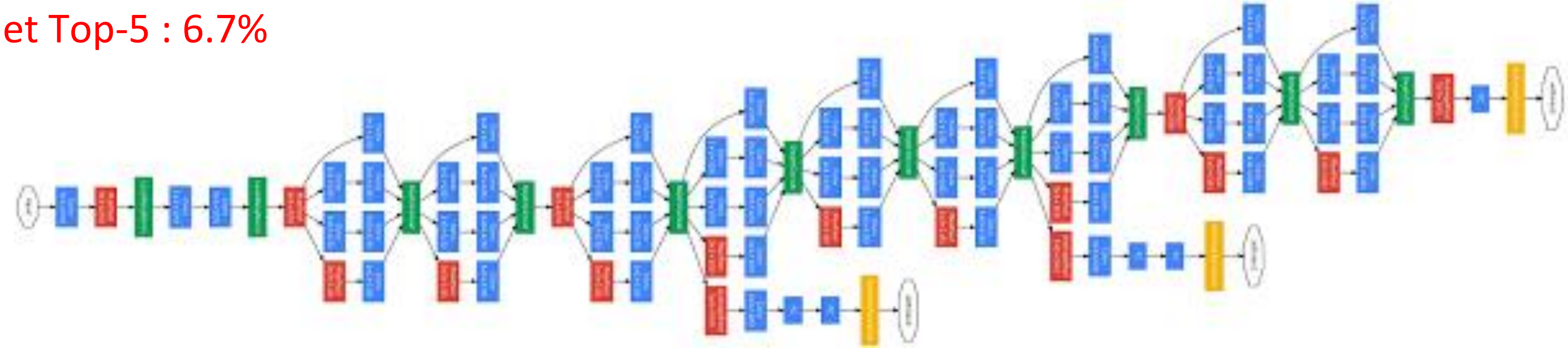


ImageNet Top-5 : 7.3%

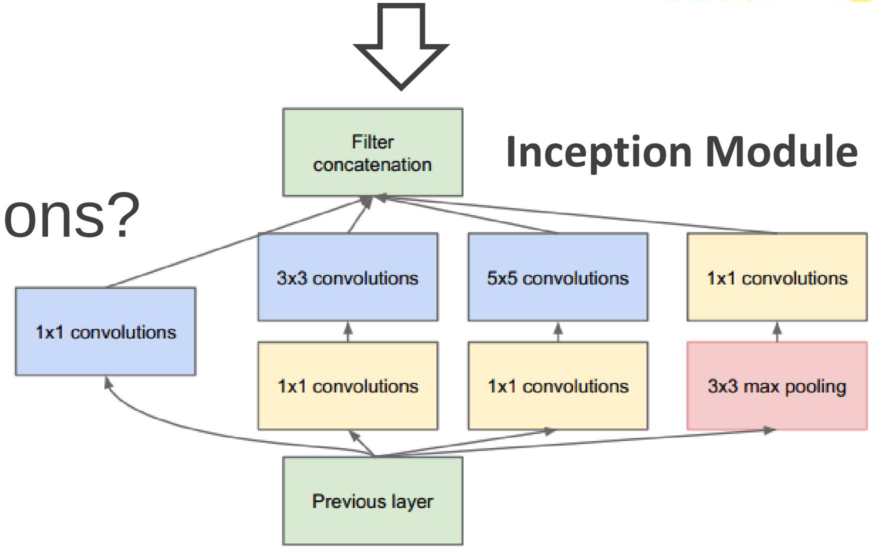
- Standardized convolutional layer
  - 3x3 convolutions with stride 1
  - 2x2 max pooling with stride 2 (not after every convolution)
- Various configuration analysed, but best has
  - 16 Convolutional + 3 Fully Connected layers
  - About 140 millions parameters (85% in FC)

GoogLeNet (2015)

ImageNet Top-5 : 6.7%



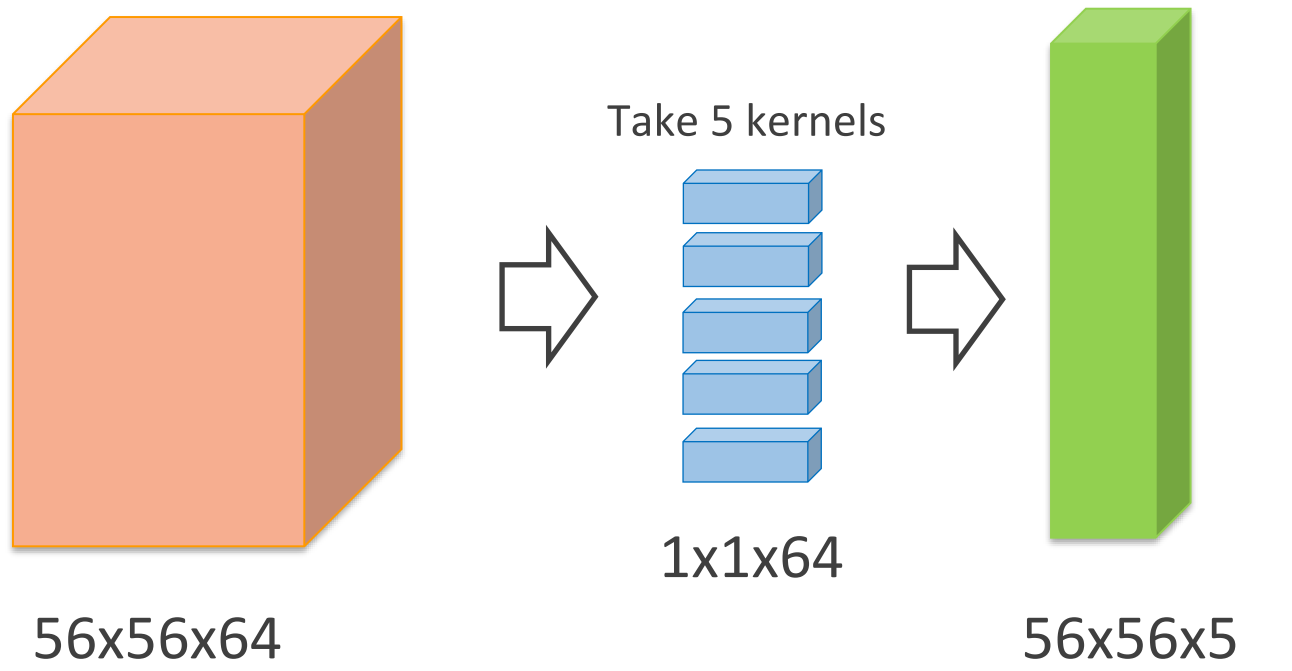
Why 1x1 convolutions?



Inception Module

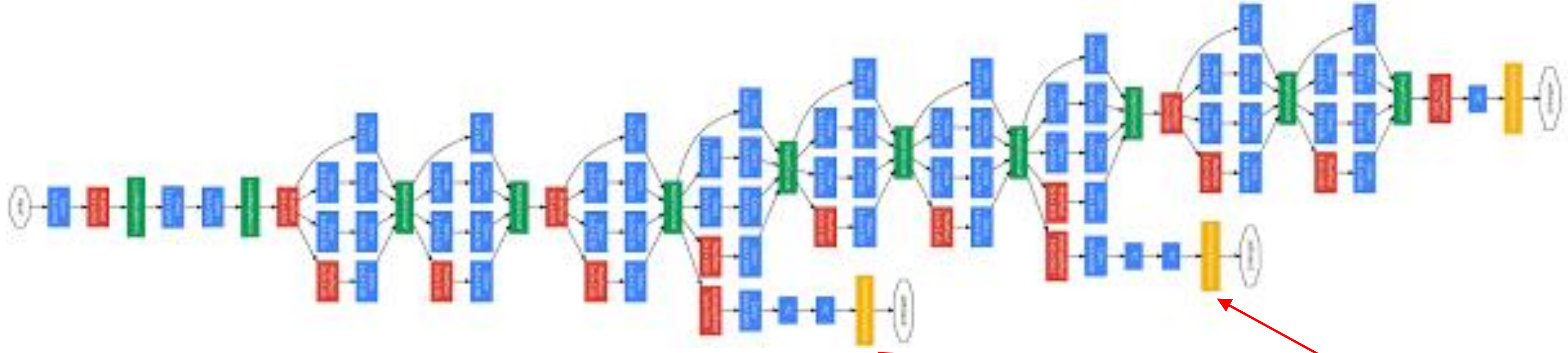
- Kernels of different size to capture details at varied scale
- Aggregated before sending to next layer
- Average pooling
- No fully connected layers

1x1 Convolutions are Helpful



By placing 1x1 convolutions before larger kernels in the Inception module, the number of input channels is reduced, saving computations and parameters

Back on GoogLeNet



Auxiliary outputs to inject gradients at deeper layers

- Only 5 millions of parameters
- 12X less parameters than AlexNet
- Followed by v2, v3 and v4 of the Inception module
  - More filter factorization
  - Introduce heavy use of Batch Normalization

Batch Normalization

- Very deep neural network are subject to internal covariate shift
  - Distribution of inputs to a layer N might vary (shift) with different minibatches (due to adjustments of layer N-1)
  - Layer N can get confused by this
  - Solution is to normalize for mean and variance in each minibatch (bit more articulated than this actually)

$$\mu_b = \frac{1}{N_b}\sum_{i=1}^{N_b} x_i \qquad \hat{x}_i = \frac{x_i - \mu_b}{\sqrt{\sigma_b^2 + \epsilon}}$$

$$\sigma_b^2 = \frac{1}{N_b}\sum_{i=1}^{N_b} (x_i - \mu_b)^2$$

Normalization

$$y = \gamma \hat{x}_i + \beta$$

Scale and shift

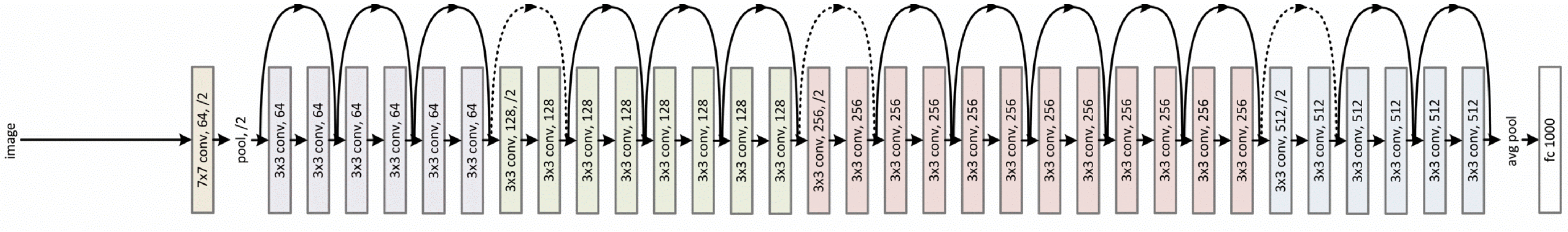
Trainable linear transform potentially allowing to cancel unwanted zero-centering effects (e.g. sigmoid)

Need to backpropagate through this!

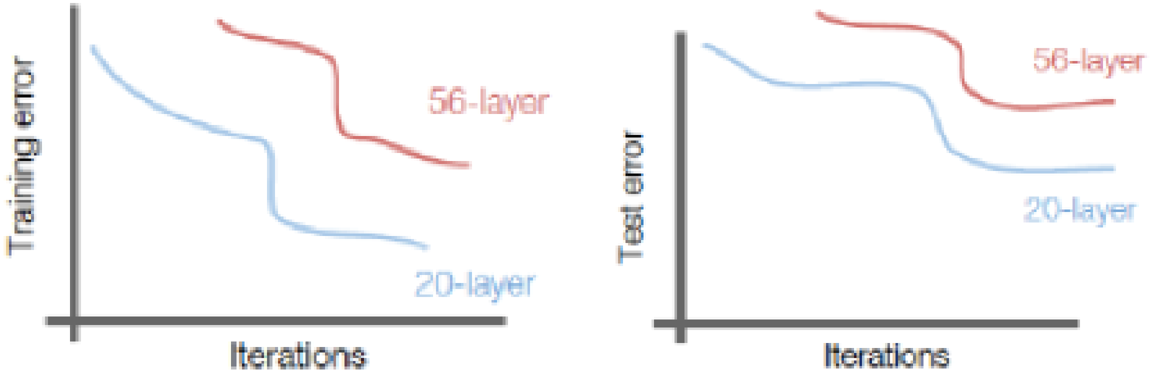
ResNet (2015)

Begin of the Ultra-Deep Network Era (152 Layers)

ImageNet Top-5 : 3.57%

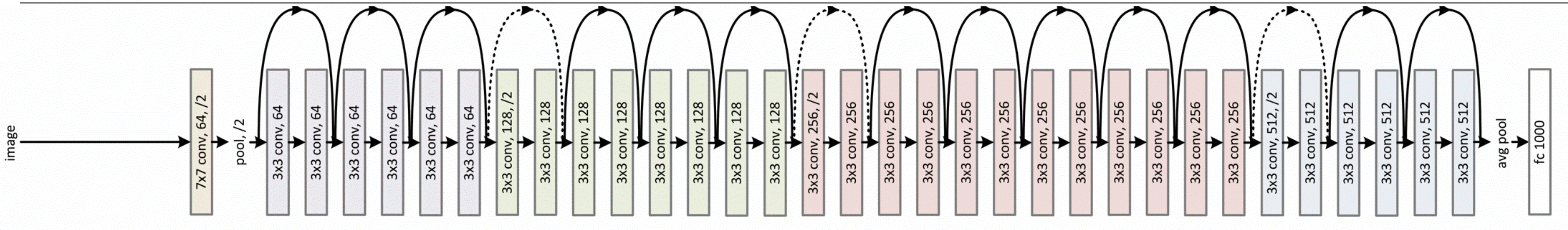


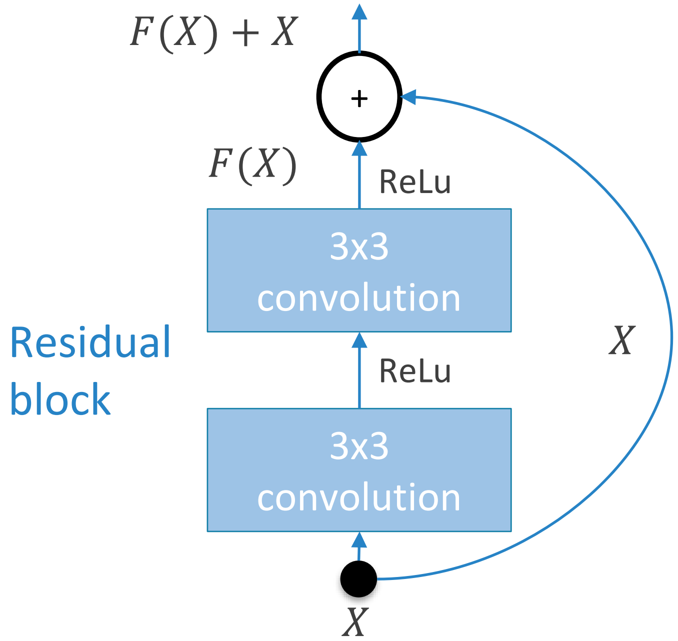
Why wasn't this working before?



Gradient vanishes when backpropagating too deep!

ResNet Trick

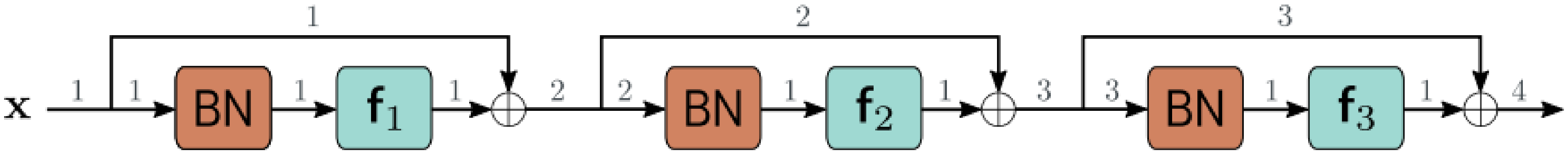




The input to the block X bypasses the convolution and is then combined with its residual $F(X)$ resulting from the convolutions

When backpropagating the gradient flows in full through these bypass connections

ResNet & Batch Norm



When connecting several Residual Blocks in series, one need to be careful about amplification/compounding of variance due to the residual connectivity

- Batch norm can alleviate this effect

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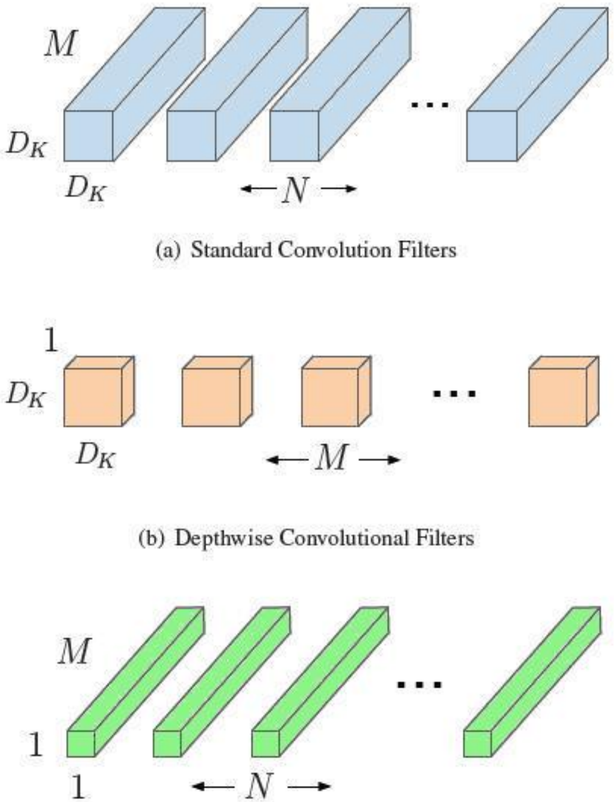
MobileNets



(a) Standard Convolution Filters

(b) Depthwise Convolutional Filters

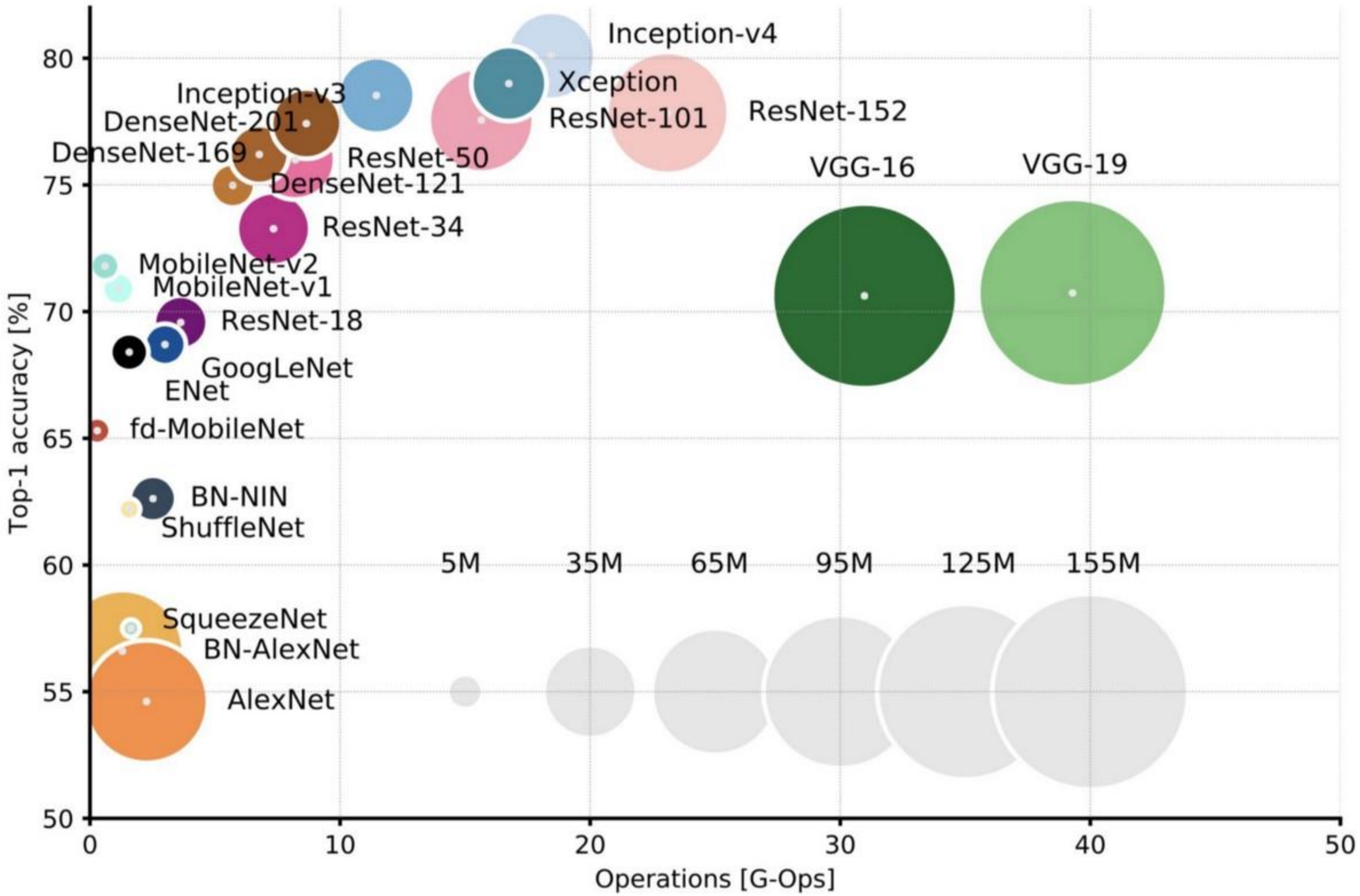
(c) 1×1 Convolutional Filters called Pointwise Convolution in the context of Depthwise Separable Convolution

arxiv.org/pdf/1704.04861.pdf

Making CNNs efficient to run on mobile devices by depthwise separable convolutions

Basically run channel-independent convolutions followed by 1x1 convolutions for cross-channel mixing

CNN Architecture Evolution



Understanding CNN Embedding

tSNE projection of AlexNet last hidden dense layer

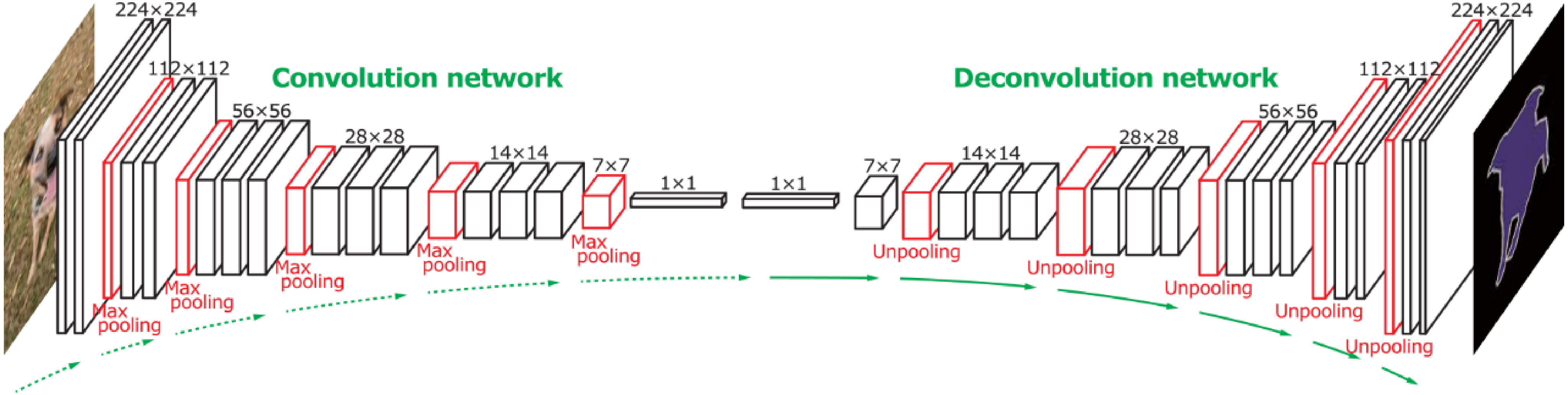
https://cs.stanford.edu/people/karpathy/cnnembed/

Interpreting Intermediate Levels

- What about the information captured in convolutional layers?
- Visualize kernel weights (filters)
  - Naïve approach
  - Works only for early convolutional layers
- Map the activation of the convolutional kernel back in pixel space
  - Requires to reverse convolution
  - Deconvolution

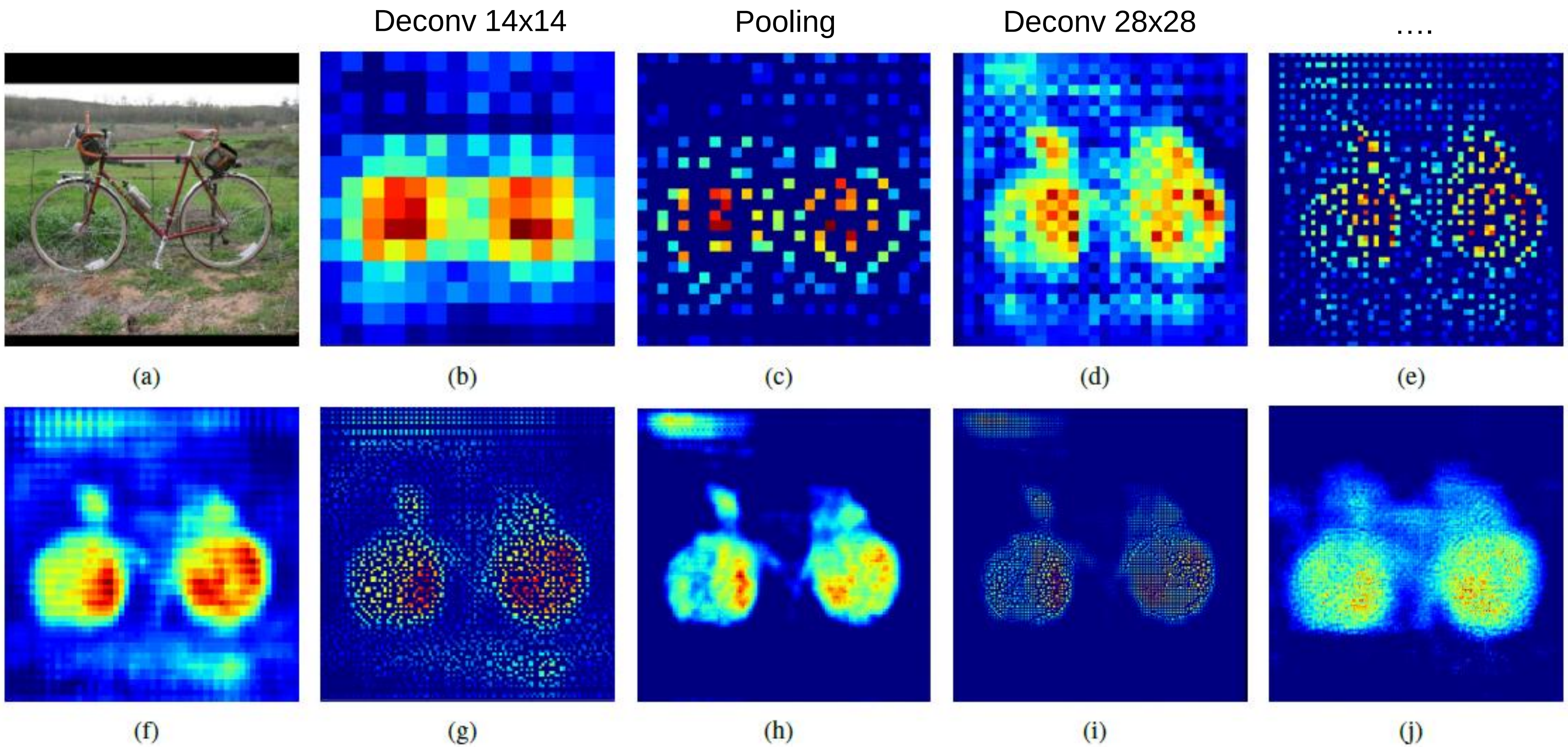
Zeiler&Fergus, Visualizing and Understanding Convolutional Networks, ICML 2013

Deconvolutional Network (DeConvNet)

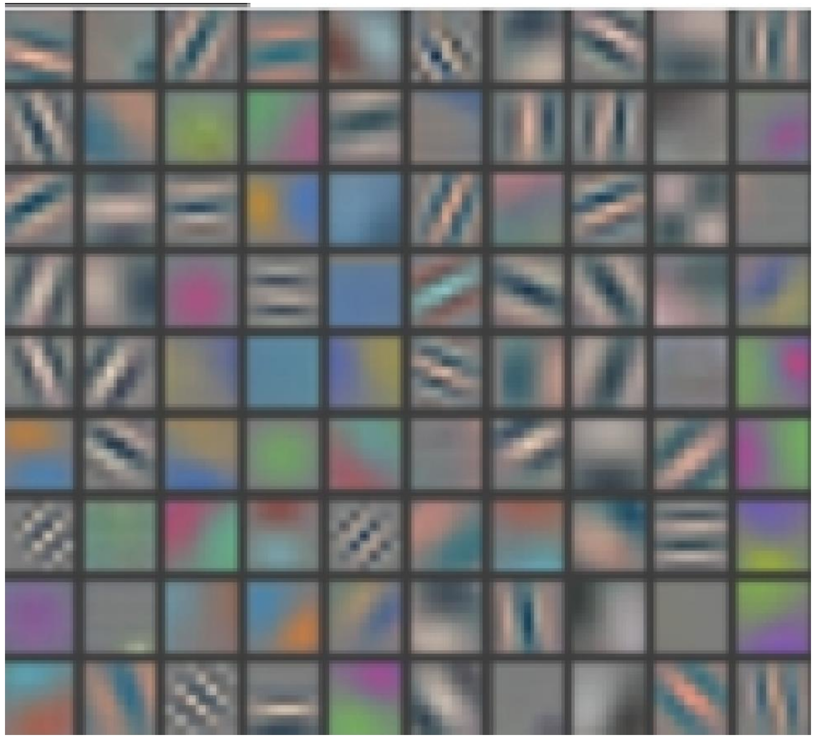


- Attach a DeConvNet to a target layer
- Plug an input and forward propagate activations until layer
- Zero activations of target neuron
- Backpropagate on the DeConvNet and see what parts of the reconstructed image are affected

Inspect Deconvolution Layers



Filters & Patches – Layer 1

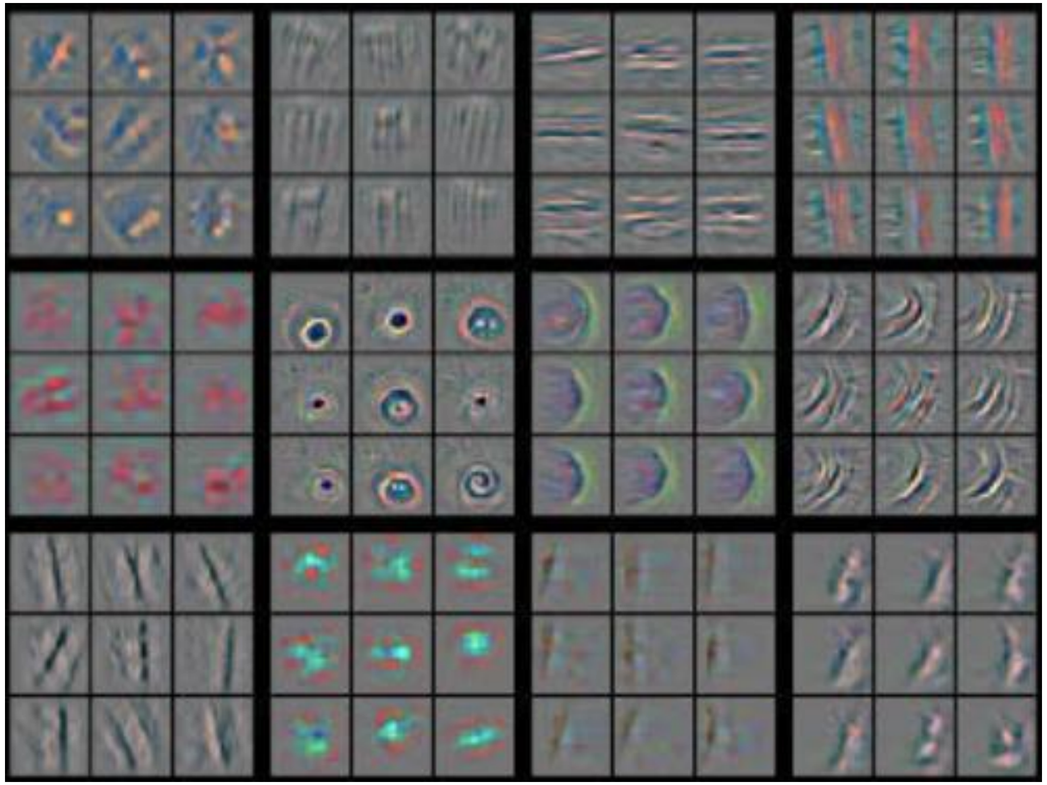


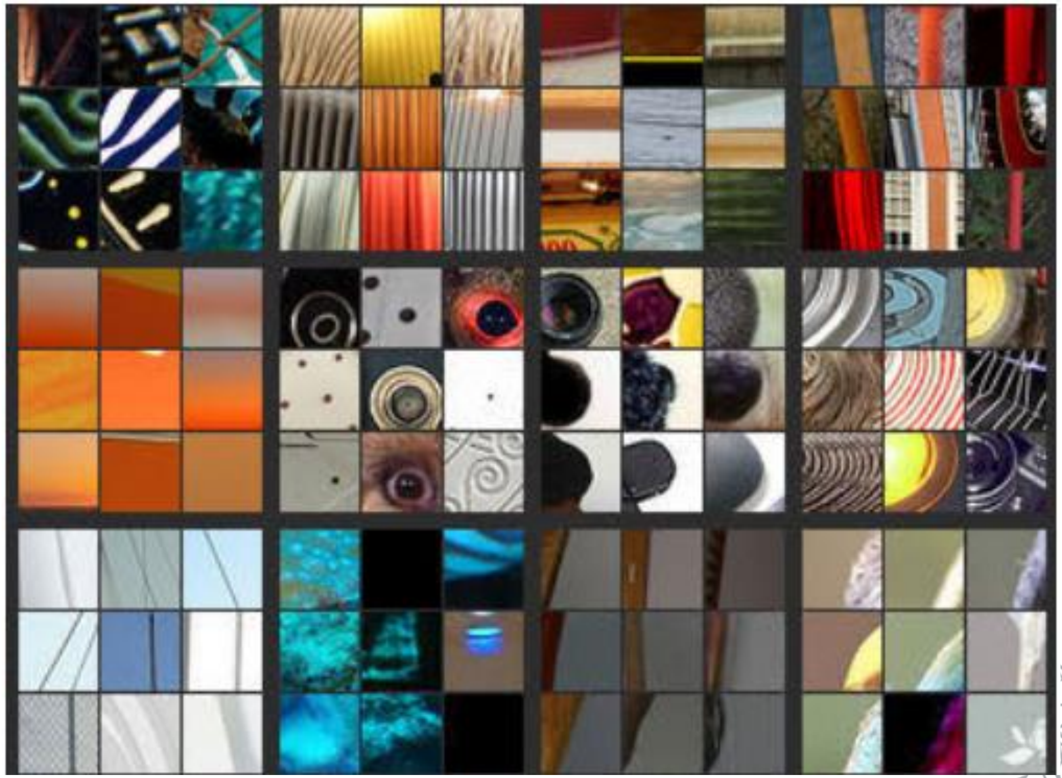
Reconstructed filters in pixel space

Corresponding top-9 image patches

Zeiler&Fergus, Visualizing and Understanding Convolutional Networks, ICML 2013

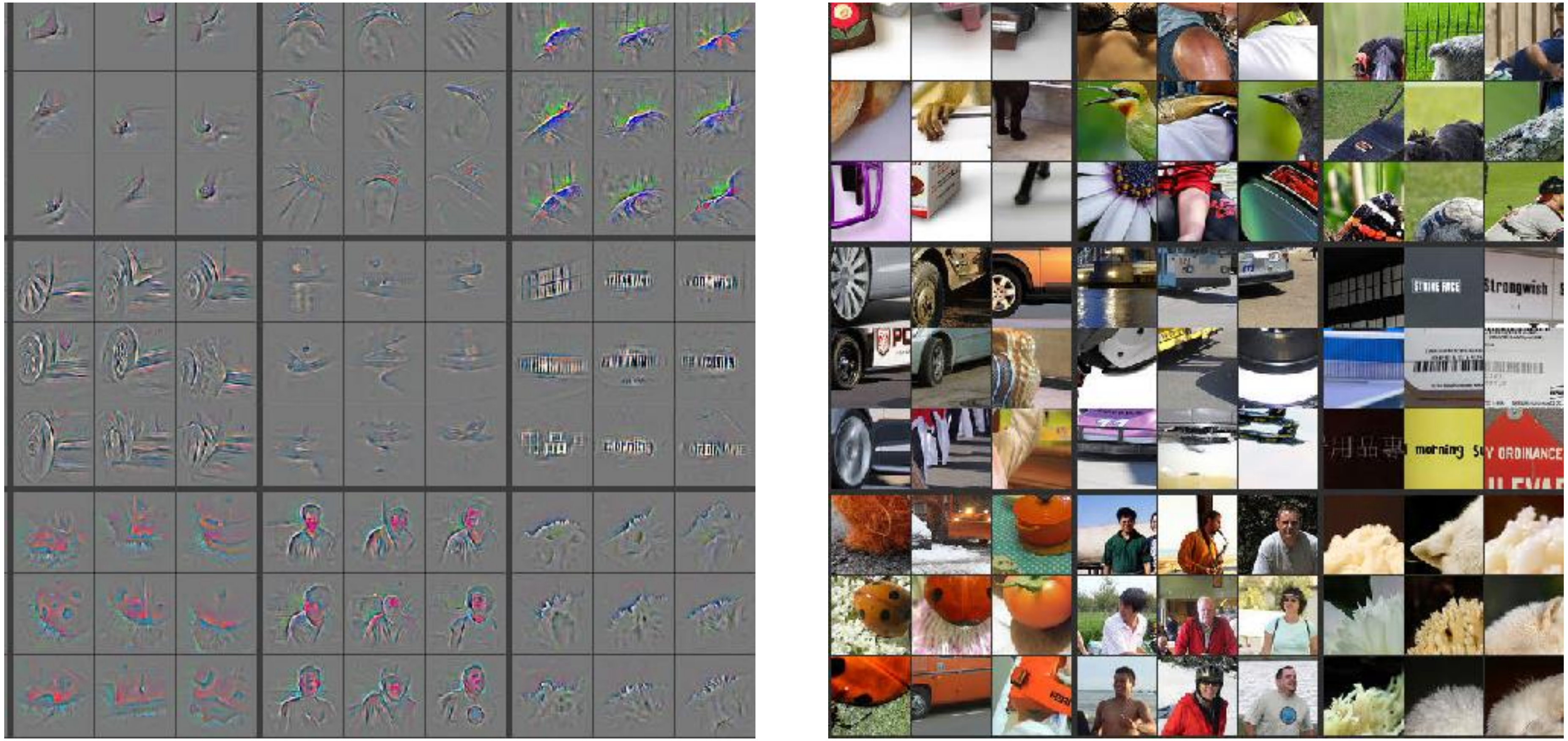
Filters & Patches – Layer 2





Zeiler&Fergus, Visualizing and Understanding Convolutional Networks, ICML 2013

Filters & Patches – Layer 3



Zeiler&Fergus, Visualizing and Understanding Convolutional Networks, ICML 2013

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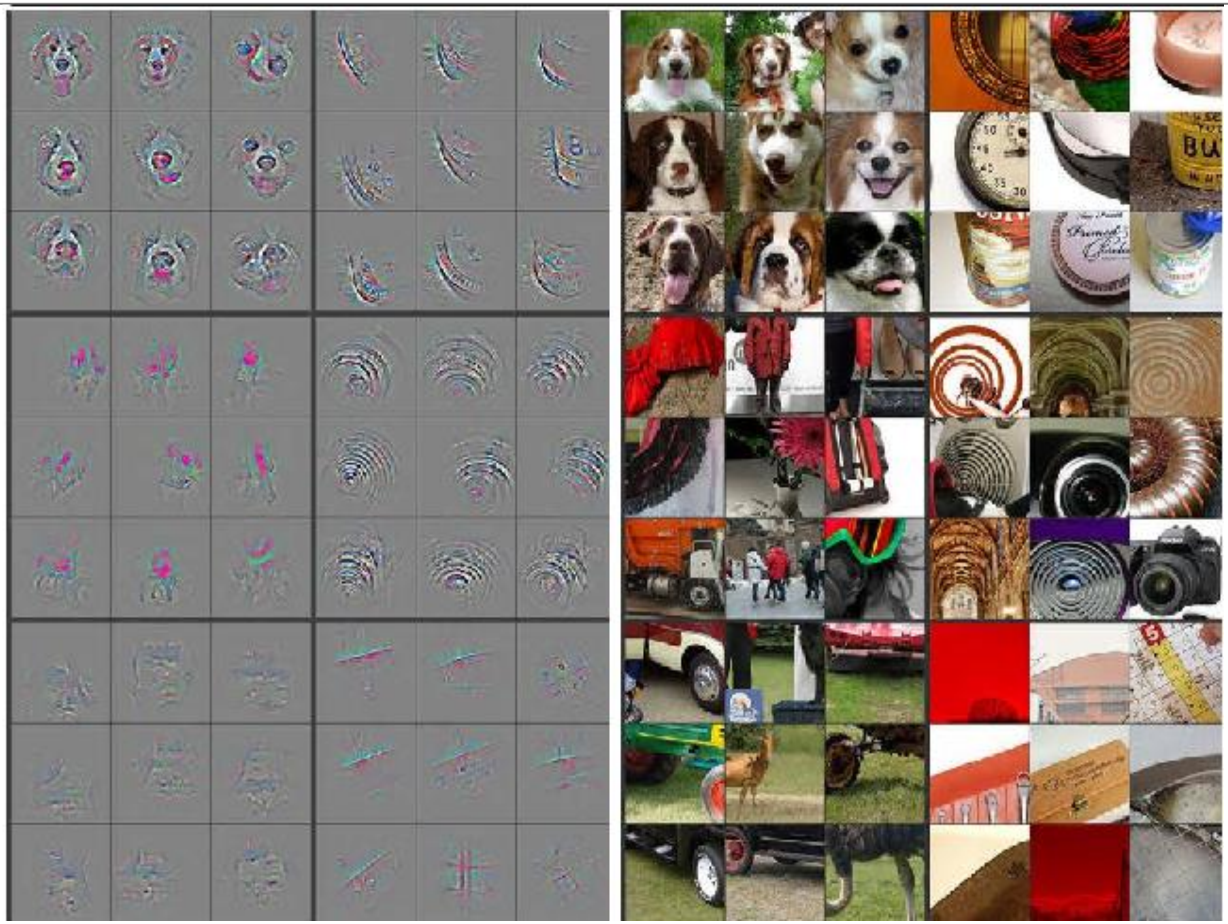
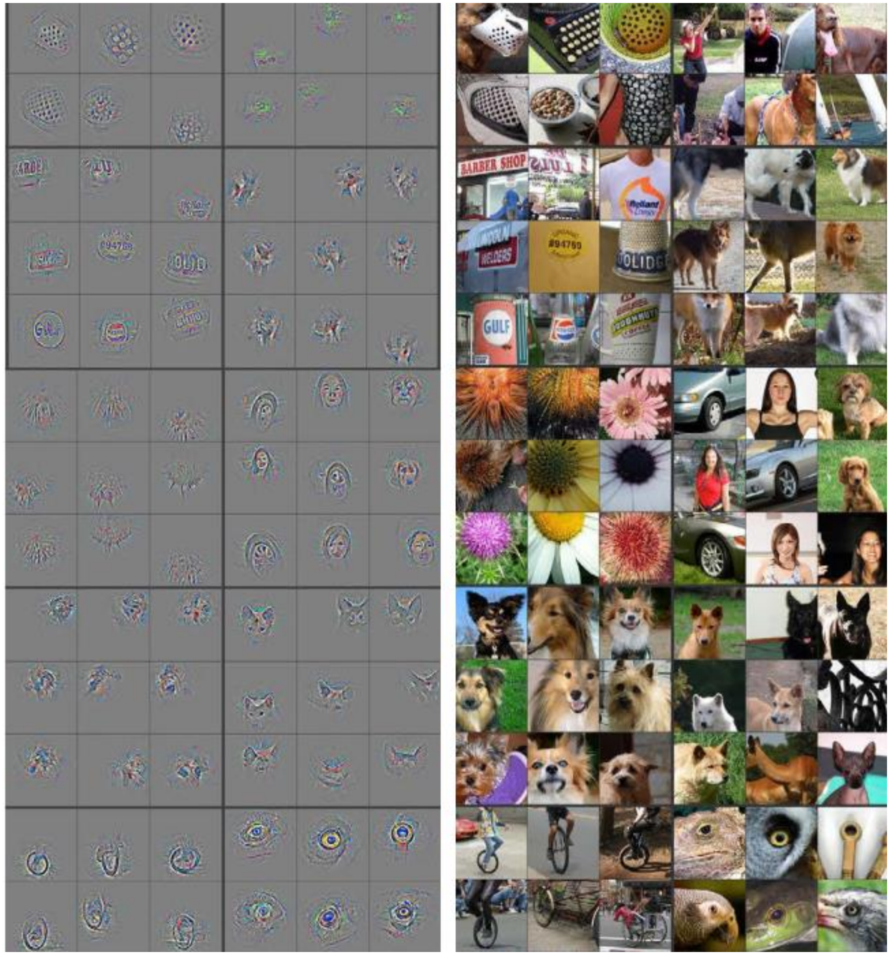
Filters & Patches – Layer 4



Zeiler&Fergus, Visualizing and Understanding Convolutional Networks, ICML 2013

Filters & Patches – Layer 5

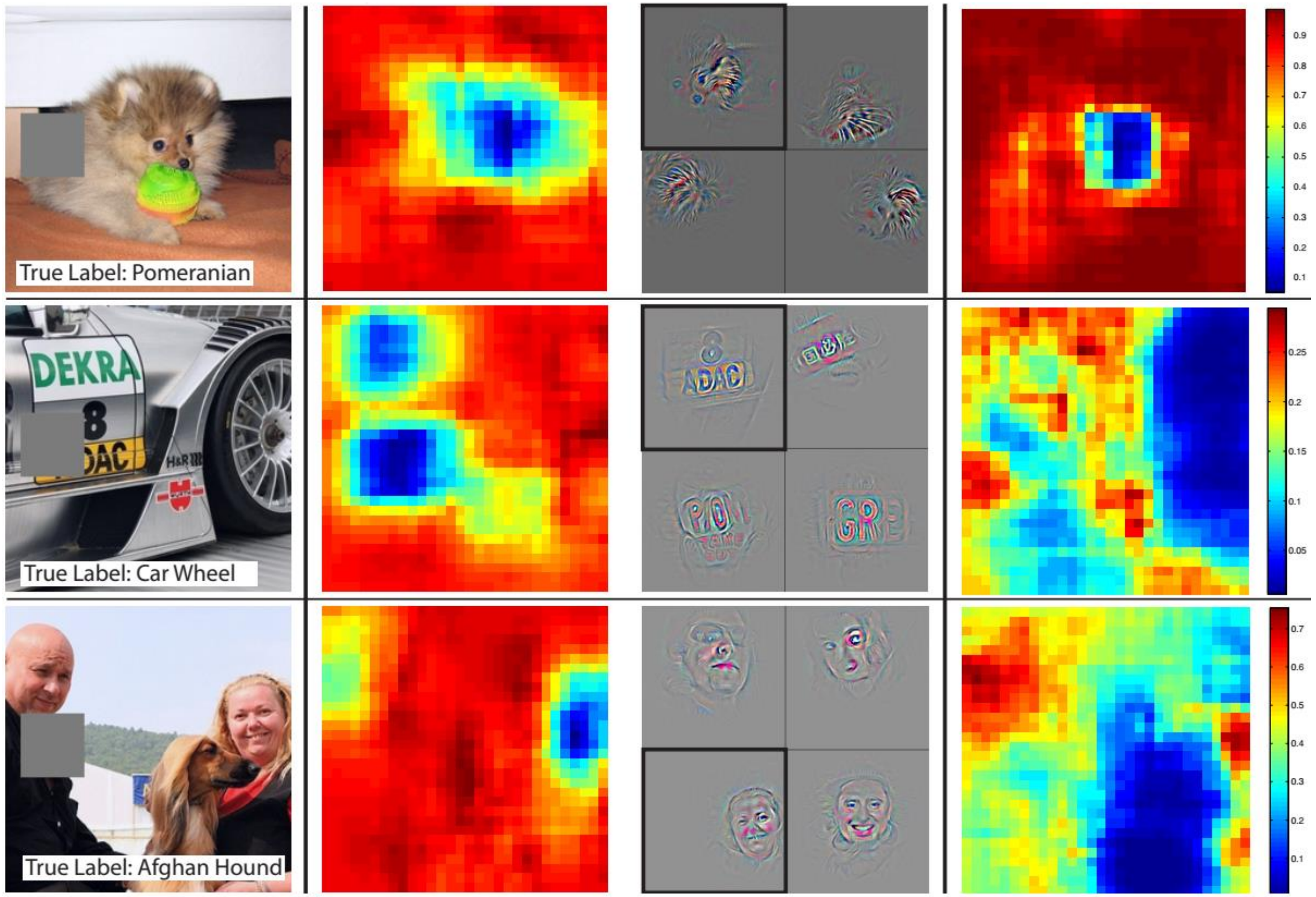


Zeiler&Fergus, Visualizing and Understanding Convolutional Networks, ICML 2013

Occlusions

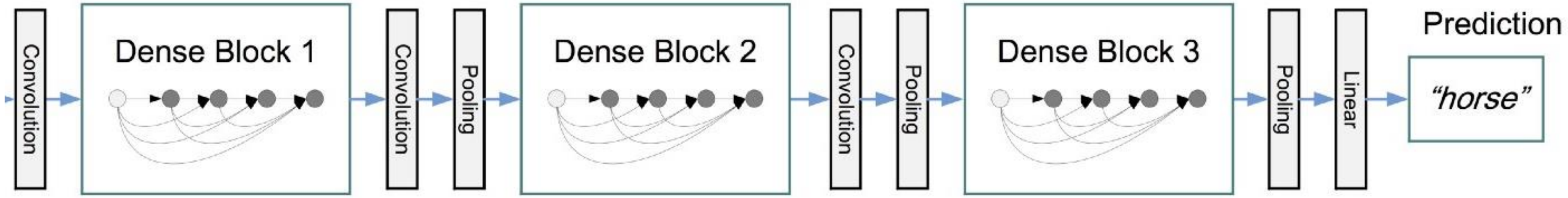
- Measure what happens to feature maps and object classification if we occlude part of the image
- Slide a grey mask on the image and project back the response of the best filters using deconvolution

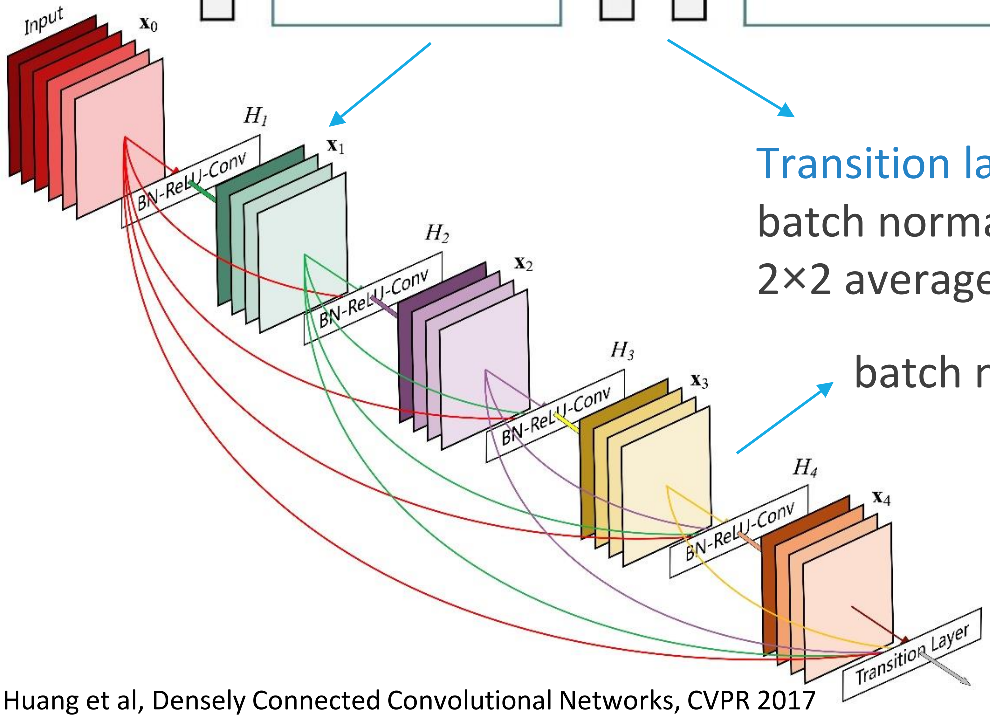
Occlusions



Zeiler&Fergus, Visualizing and Understanding Convolutional Networks, ICML 2013

Dense CNN





Transition layers
batch normalization + 1×1 convolutional + 2×2 average pooling layer

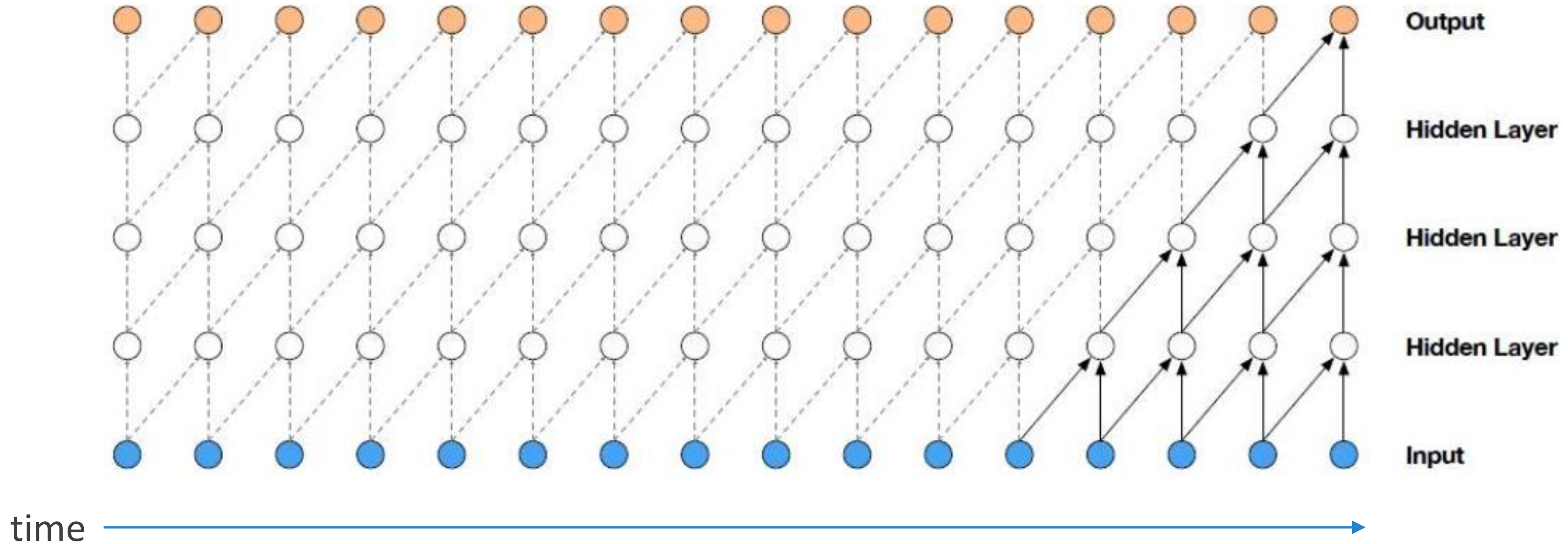
batch normalization + ReLU + 3x3 conv

- Gradient flows well in bypass connections
- Each layer in the dense block has access to all information from previous layers

Huang et al, Densely Connected Convolutional Networks, CVPR 2017

Causal Convolutions

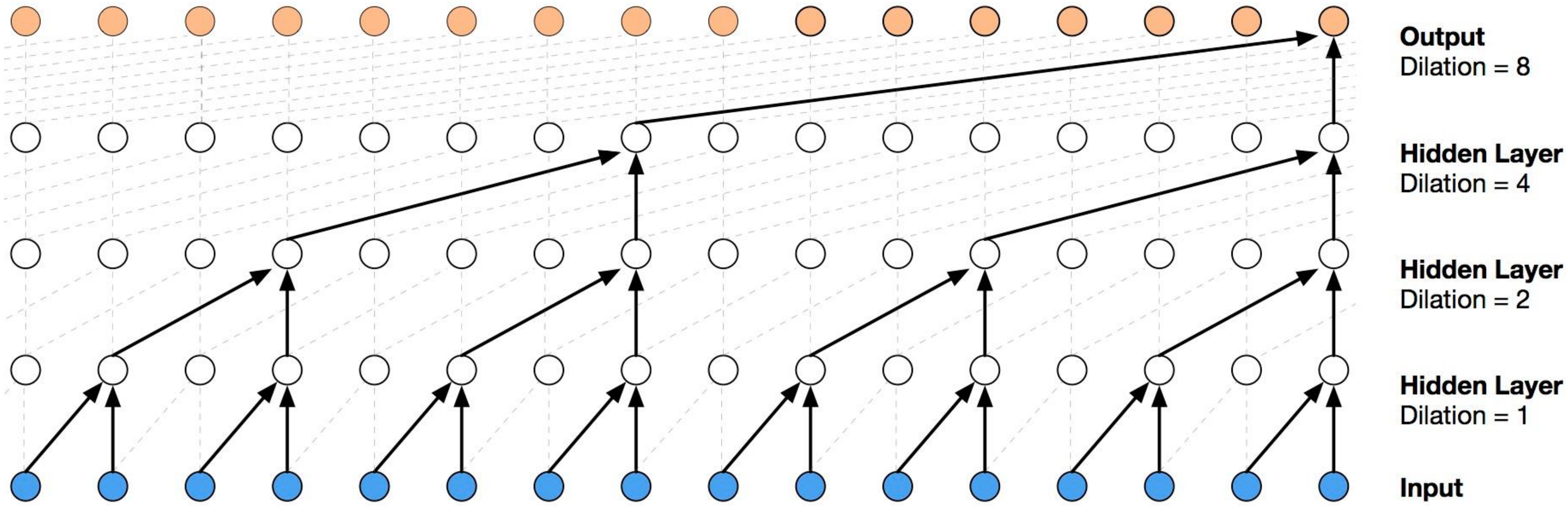
Preventing a convolution from allowing to see into the future…



Problem is the context size grows slow with depth

Causal & Dilated Convolutions

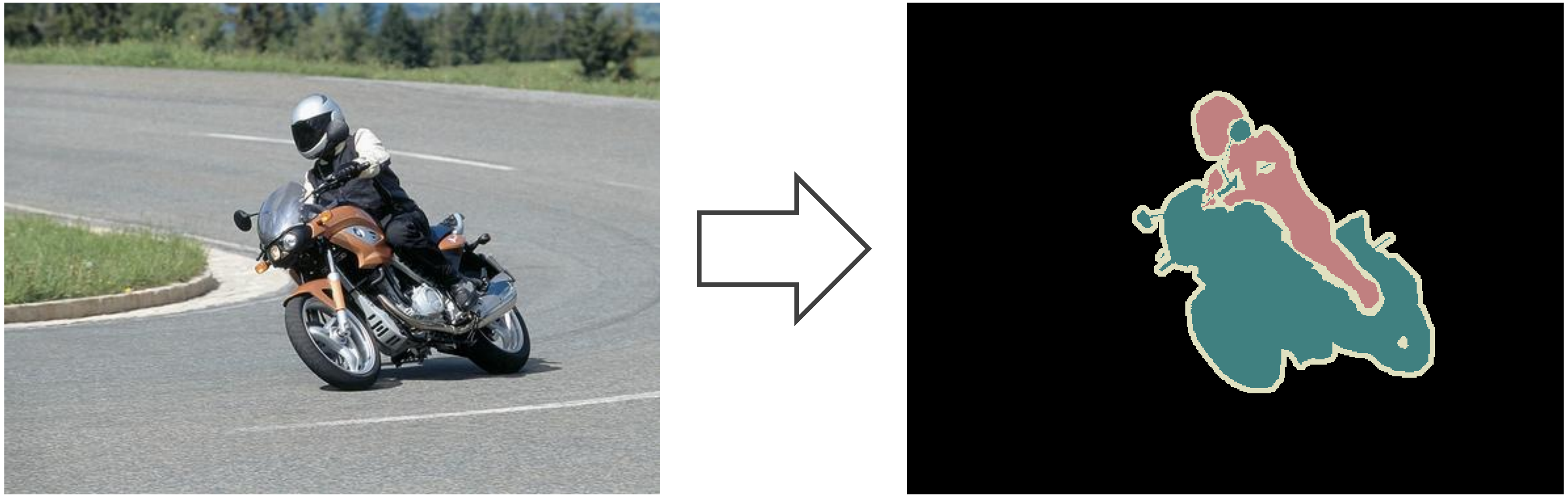
$$(I * K)(i,j) = \sum_m \sum_n I(i - lm, i - ln)K(m,n)$$



Similar to striding, but size is preserved

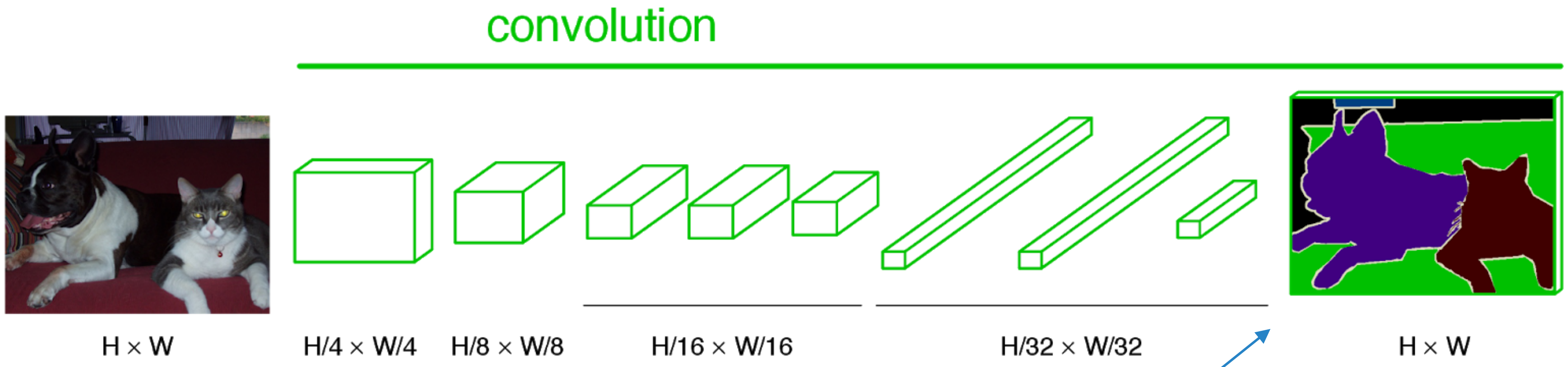
Oord et al, WaveNet: A Generative Model for Raw Audio, ICLR 2016

Semantic Segmentation



Traditional CNN cannot be used for this task due to the downsampling of the striding and pooling operations

Fully Convolutional Networks (FCN)



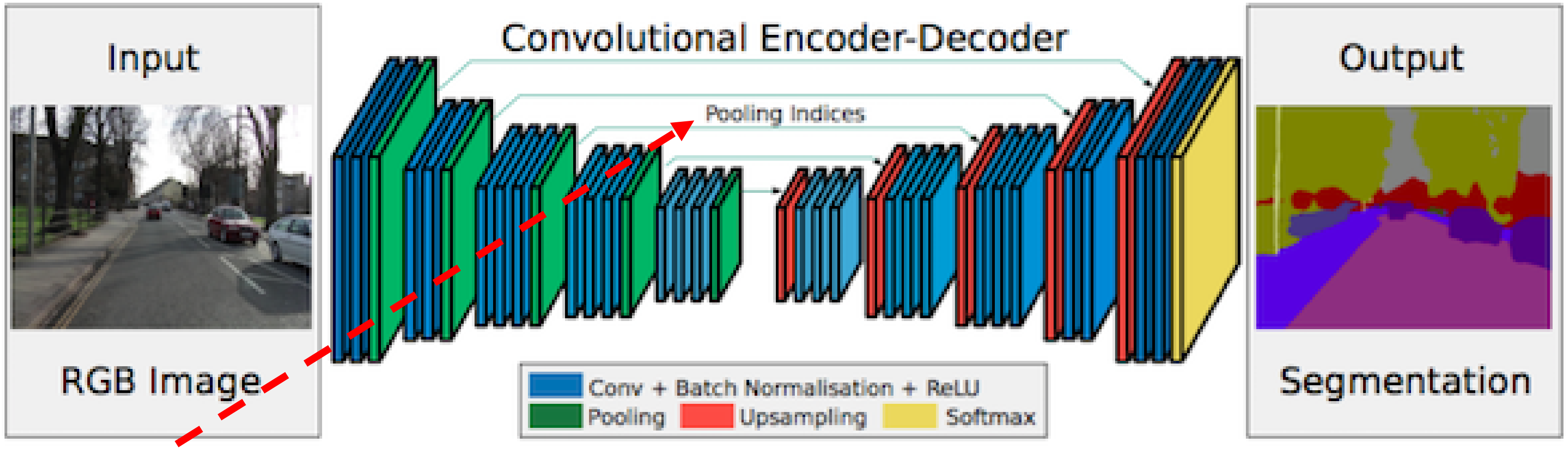
Convolutional part to extract interesting features at various scales

Learn an upsampling function of the fused map to generate the semantic segmentation map

Fuse information from feature maps of different scale

Shelhamer et at, Fully Convolutional Networks for Semantic Segmentation, PAMI 2016

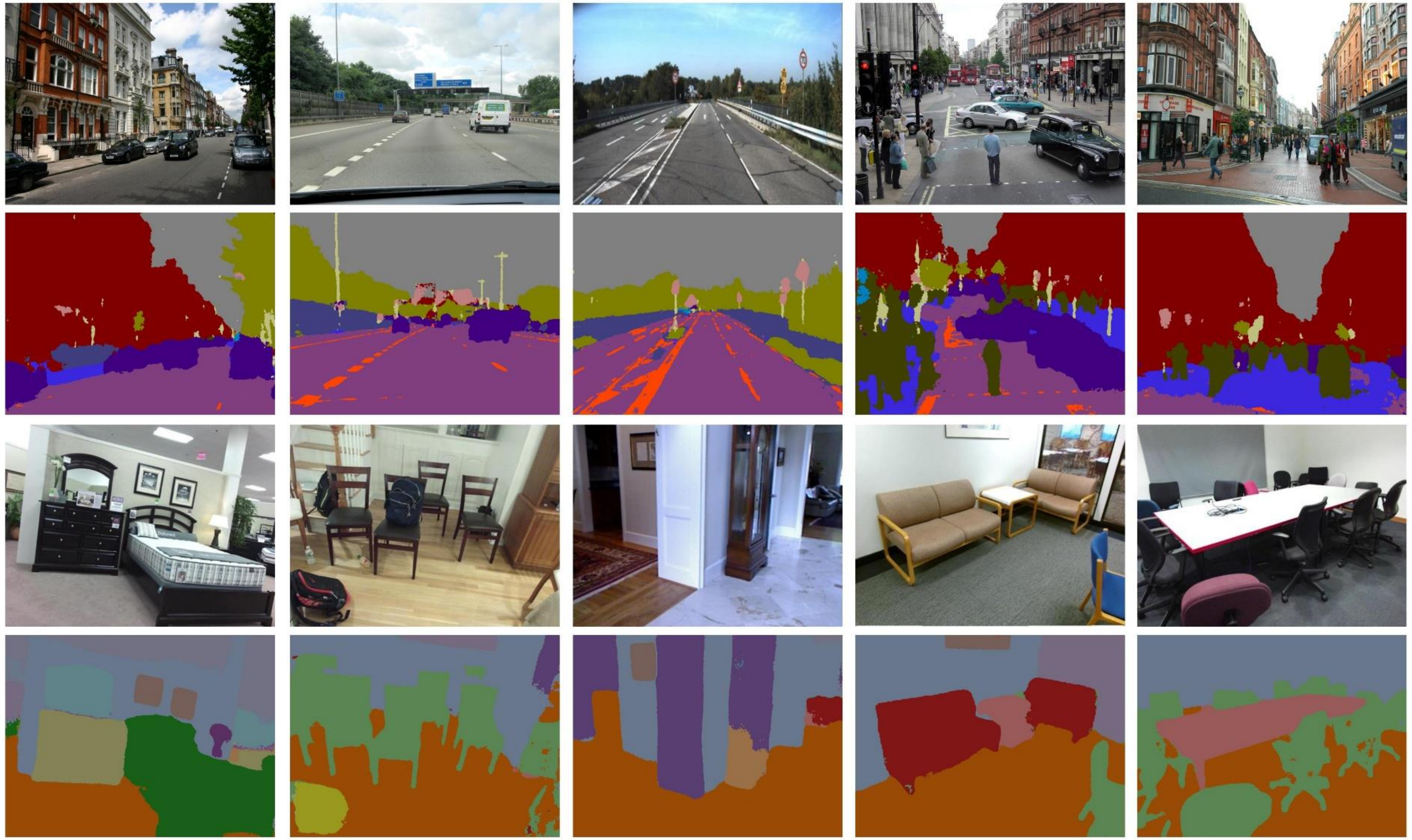
Deconvolution Architecture



Maxpooling indices transferred to decoder to improve the segmentation resolution.

Badrinarayanan et al, SegNet: A Deep Convolutional Encoder-Decoder Architecture for Image Segmentation, PAMI 2017

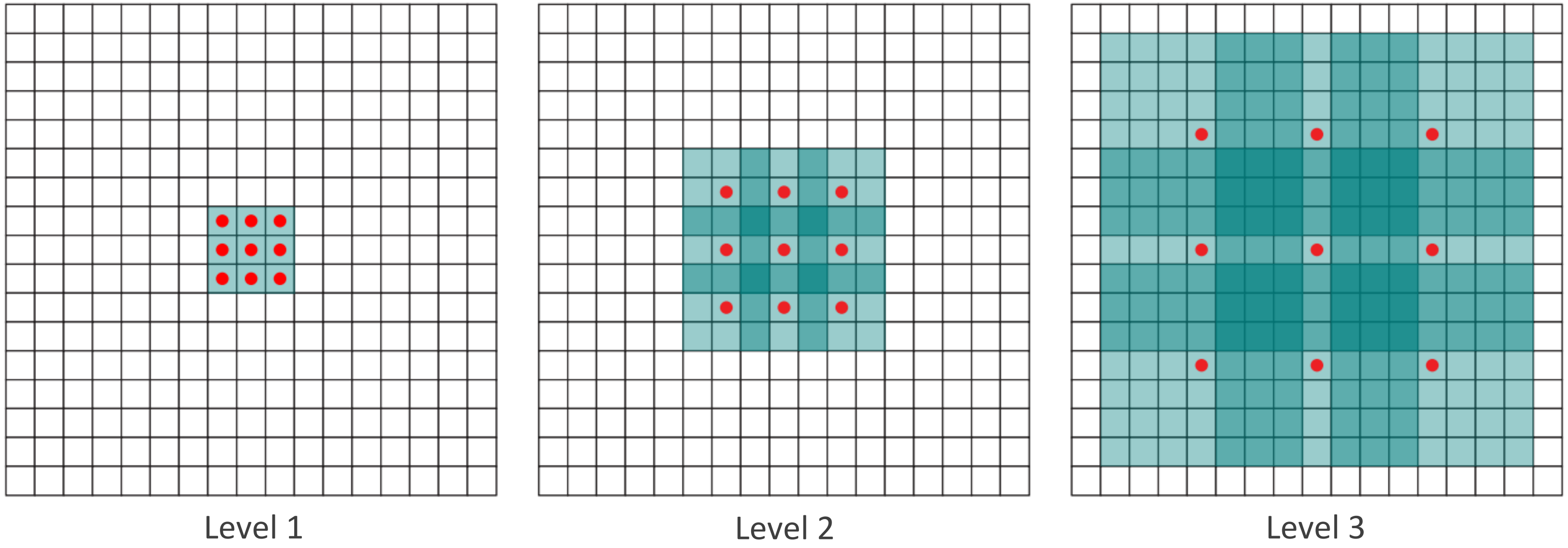
SegNet Segmentation



Demo here: http://mi.eng.cam.ac.uk/projects/segnet/

Use Dilated Convolutions

Always perform 3x3 convolutions with no pooling at each level



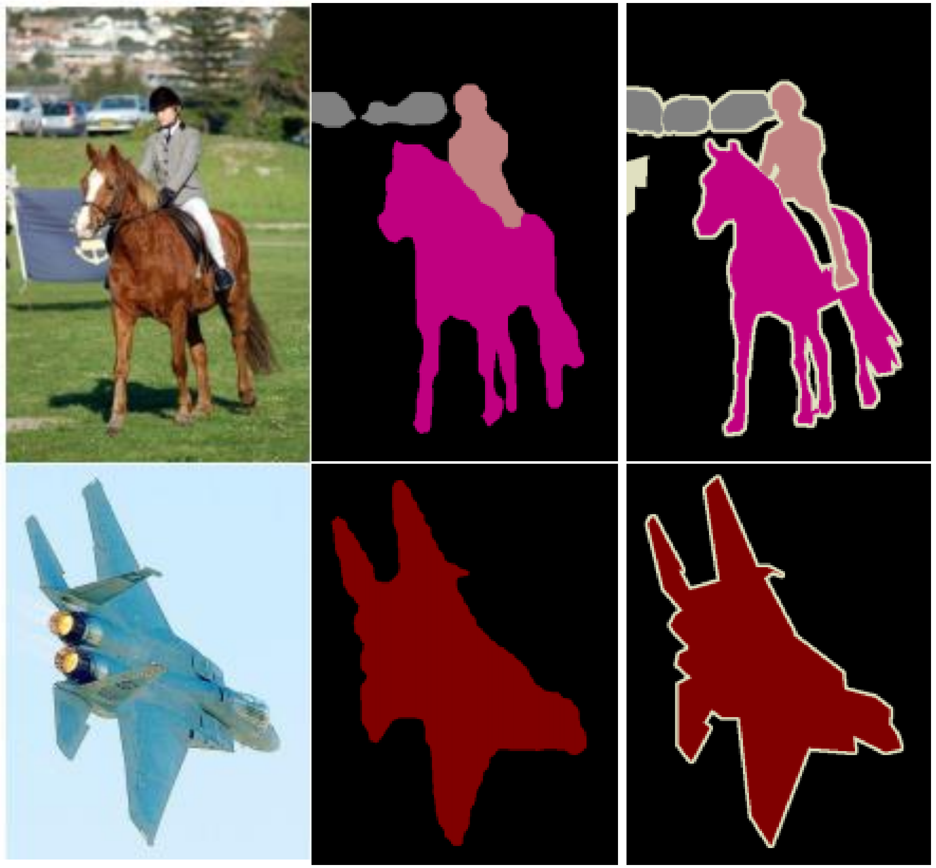
Context increases without

- Pooling (changes map size)
- Increasing computational complexity

Yu et al, Multi-Scale Context Aggregation by Dilated Convolutions, ICLR 2016

Segmentation by Dilated CNN

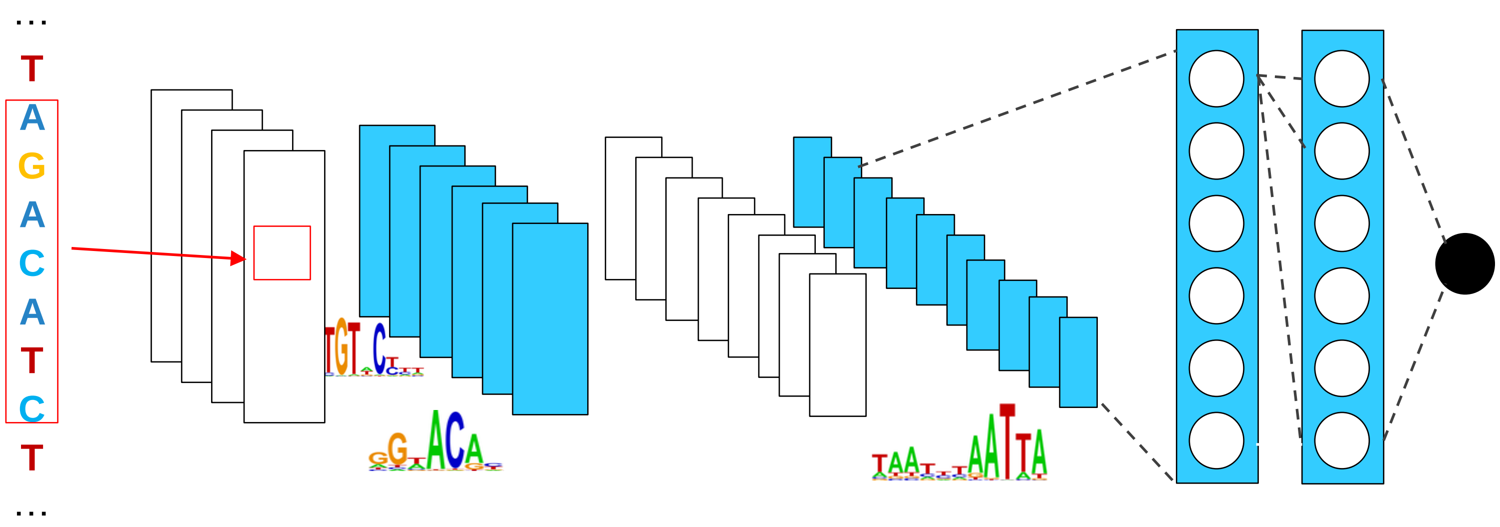
Dilated CNN GT



Dilated CNN GT

Yu et al, Multi-Scale Context Aggregation by Dilated Convolutions, ICLR 2016

CNN & Genomic Sequences



1D convolutions throughout the input sequence

- Trained to respond to task-specific motifs
- Applied to small sequence regions

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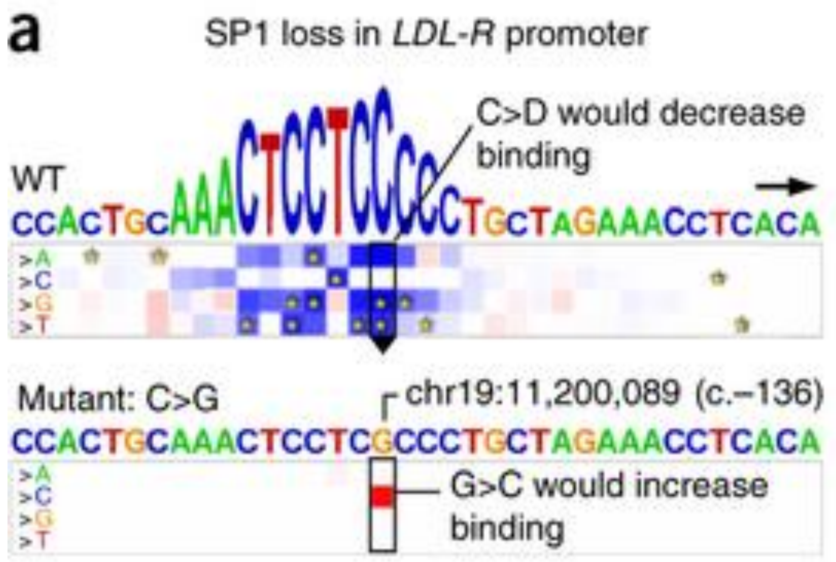
DeepBind

- 927 CNN models predicting a binding score for transcription factors and RNA-binding proteins
  - Score new sequences
  - Assess mutations that deplete/increase binding score
- Use convolution visualization to interpret results of CNN training

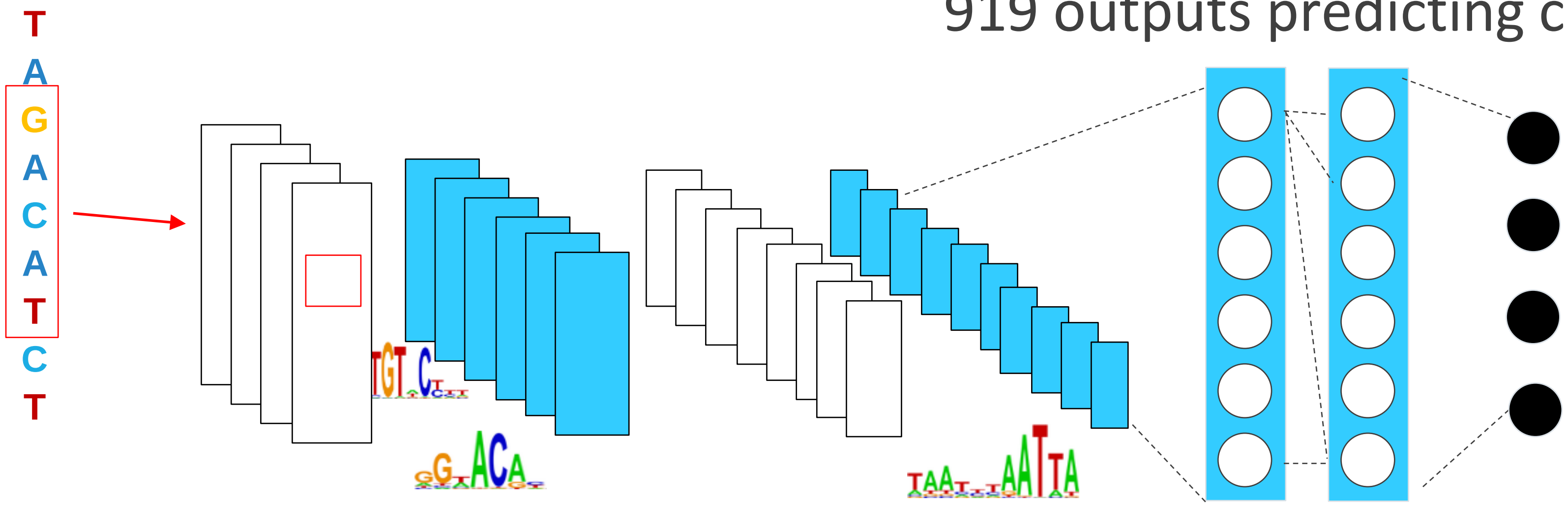


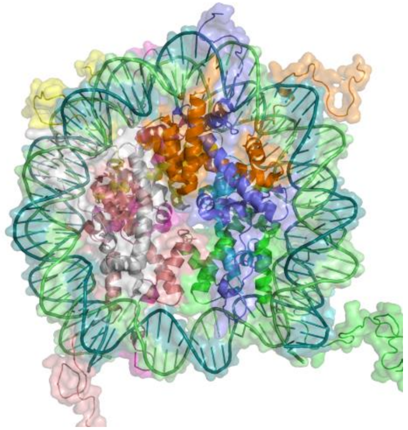
Mutation Maps

Alipanahi et al. "Predicting the sequence specificities of DNA-and RNA-binding proteins by deep learning." *Nature biotechnology* 2015 - http://tools.genes.toronto.edu/deepbind/

DeepSea

919 outputs predicting chromatin features





The feature detectors in the deeper layers are shared between the predictive tasks

Alipanahi et al. "Predicting the sequence specificities of DNA-and RNA-binding proteins by deep learning." Nature biotechnology 2015 - http://tools.genes.toronto.edu/deepbind/

Software

- CNN are supported by any deep learning framework (Keras-TF, Pytorch, MS Cognitive TK, Intel OpenVino, …)
- Caffe was one of the initiators and basically built around CNN
  - Introduced protobuffer network specification
  - ModelZoo of pretrained models (LeNet, AlexNet, …)
  - Support for GPU
- Caffe2 is Facebook's extensions to Caffe
  - Less CNN oriented
  - Support from large scale to mobile nets
  - More production oriented than other frameworks

Caffe Protobuffer

```
name: "LeNet"
layer {
  name: "data"
  type: "Input"
  …
  input_param { shape: { dim: 64 dim: 1 dim: 28 dim: 28 } }
}
layer {
  name: "conv1"
  type: "Convolution"
  bottom: "data"
  …
  convolution_param {
    num_output: 20
    kernel_size: 5
    stride: 1
    weight_filler {
      type: "xavier"
    }
```

Other Software

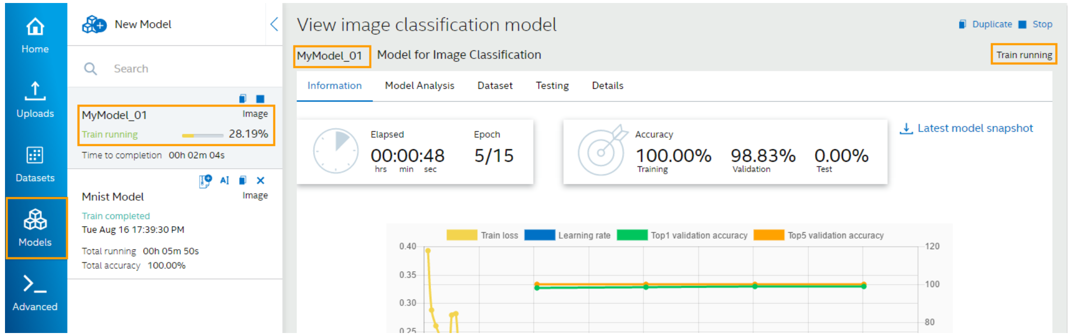
- Matlab distributes its Neural Network Toolbox which allows importing pretrained models from Caffe and Keras-TF
- Matconvnet is an unofficial Matlab library specialized for CNN development (GPU, modelzoo, …)
- Want to have a CNN in your browser?
  - Try ConvNetJS (https://cs.stanford.edu/people/karpathy/convnetjs/)

GUIs

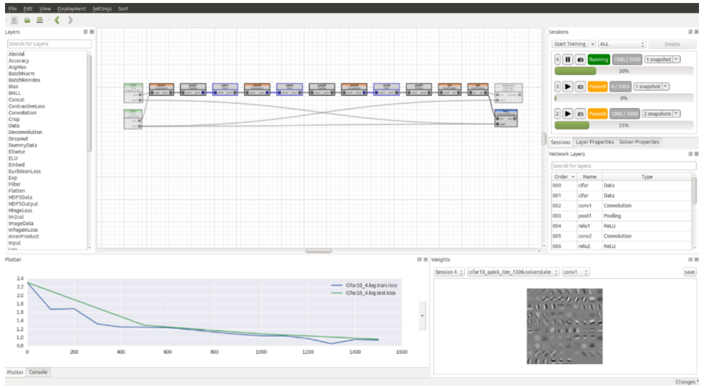
Major hardware producers have GUI and toolkits wrapping Caffe, Keras and TF to play with CNNs

NVIDIA Digits

Intel OpenVino



Barista



Plus others...

Take Home Messages

- Key things
  - Convolutions in place of dense multiplications allow sparse connectivity and weight sharing
  - Pooling enforces invariance and allows to change resolution but shrinks data size
  - Full connectivity compress information from all convolutions but accounts for 90% of model complexity
- Lessons learned
  - ReLU are efficient and counteract gradient vanish
  - 1x1 convolutions are useful
  - Need batch normalization
  - Bypass connections allow to go deeper
- Dilated (à trous) convolutions
- You can use CNN outside of machine vision

Next Lecture

Deep Autoencoders

- Autoencoders and dimensionality reduction
- Neural autoencoders (sparse, denoising contractive)
- Deep neural autoencoders and pretraining
- Deep generative-based autoencoders
- Visualization and multi-modal data fusion with autoencoders

Next Week Lectures

- Wednesday h. 16-18
- Thursday h. 14-16
- Friday h. 16-18 – Room E

Happy Easter Break!