Statistical Machine Learning (BE4M33SSU) Lecture 8: Deep Neural Networks

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Overview



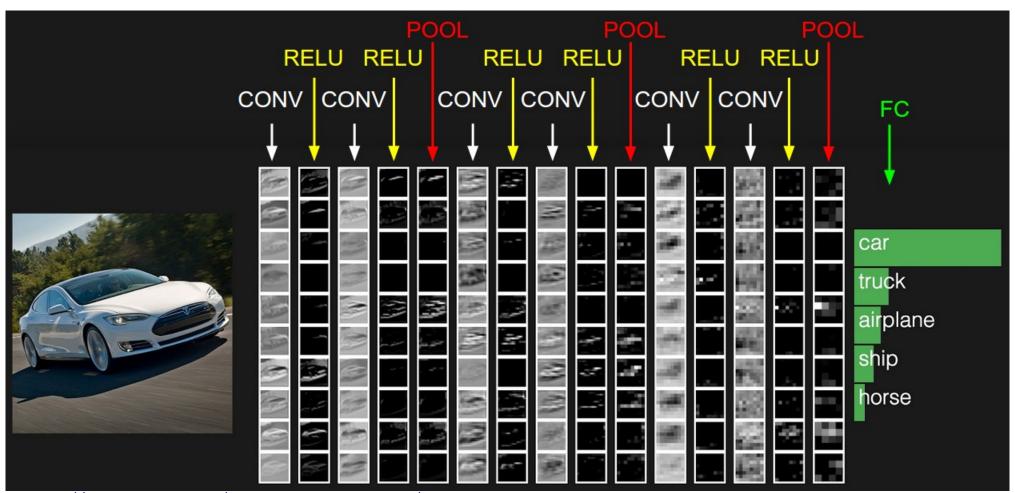
Topics covered in the lecture:

- Deep Architectures
- Convolutional Neural Networks (CNNs)
- Transfer learning
- Weight initialization
- Autoencoders and unsupervised pre-training

- We know that deep architectures evolved in Nature (e.g., cortex)
- Universal approximation theorem: one layer is enough so why to bother with more layers?
- Poggio et al: Why and When Can Deep but Not Shallow Networks Avoid the Curse of Dimensionality, 2016:
 - deep networks can be exponentially better (have less units) than shallow networks for learning compositional functions
- Handcrafted features vs. automatic extraction
- Gradually increasing complexity, intermediate representations: each successive layer brings higher abstraction

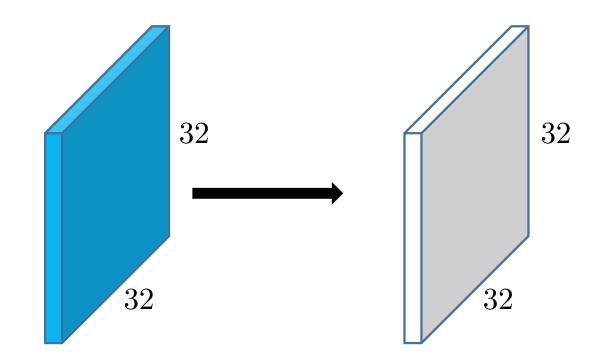
Convolutional Neural Networks (CNNs)





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

- Topographical mapping in the visual cortex nearby cells represent nearby regions in the visual field
- Input: grayscale image 32×32 pixels
- lack Output: layer of 32×32 features
- How many parameters do we need when input and output is fully connected?

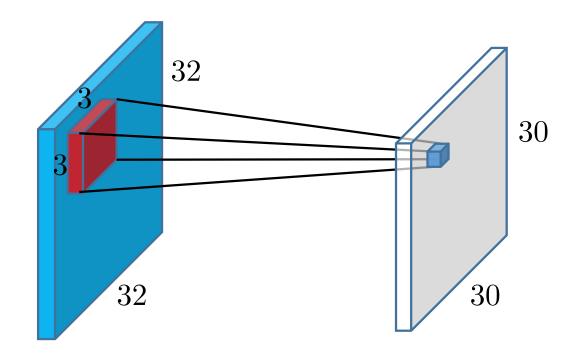


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 $32^2\times (32^2+1)\approx 1\text{M}$ outputs 32 32 32 32

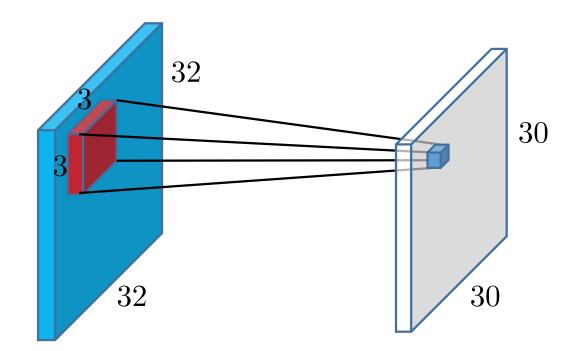
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- Each neuron has a **receptive field** of 3×3 pixels
- It is fully connected only to the corresponding set of 9 inputs
- How many parameters do we need now?

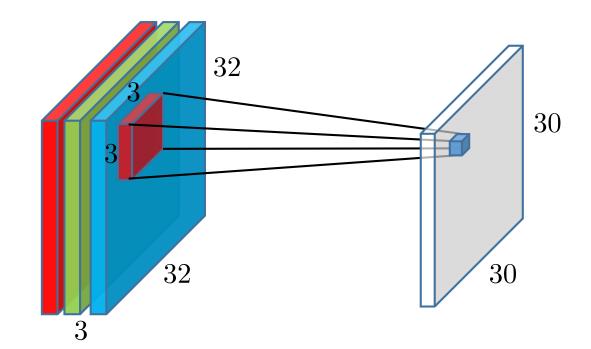


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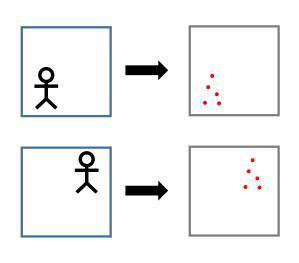
$$30^2 \times (3^2 + 1) = 9 \mathrm{k}$$
 outputs

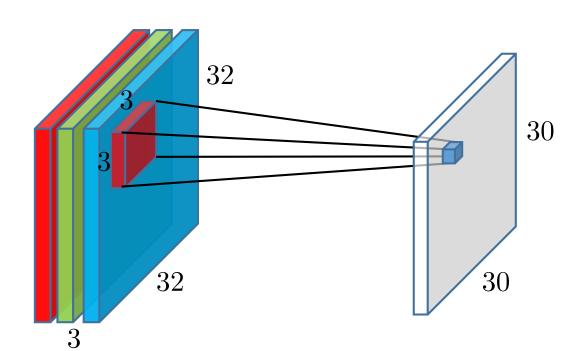


- We can have more input channels, e.g., colors
- ullet Now the input is defined by width, height and depth: $32 \times 32 \times 3$
- \bullet The number of parameters is $30^2\times(3\times3^2+1)\approx25\text{k}$

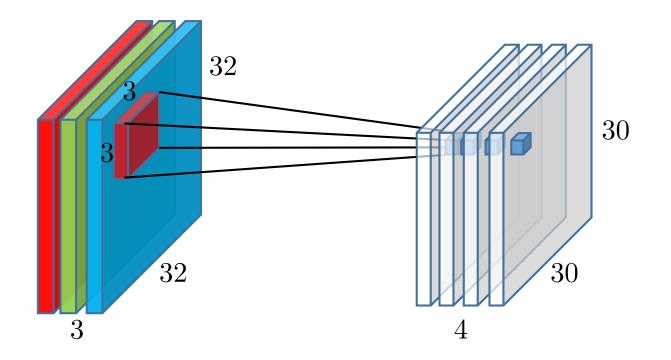


- We can further reduce the number of parameters by sharing weights
- Use the same set of weights and bias for all outputs, define a filter
- lacktriangle The number of parameters drops to $3\times 3^2 + 1_{\rm bias} = 28$
- Translation equivariance





- Extract multiple different of features
- Use multiple filters to get more feature maps
- \bullet For 4 filters we have $\underset{\text{filters}}{4}\times(3\times3^2+1)=112$ parameters
- This is the convolutional layer
- Processes volume into volume

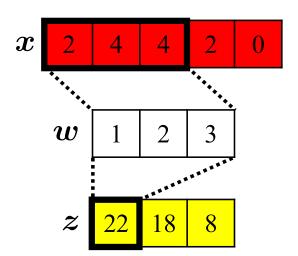


Convolution

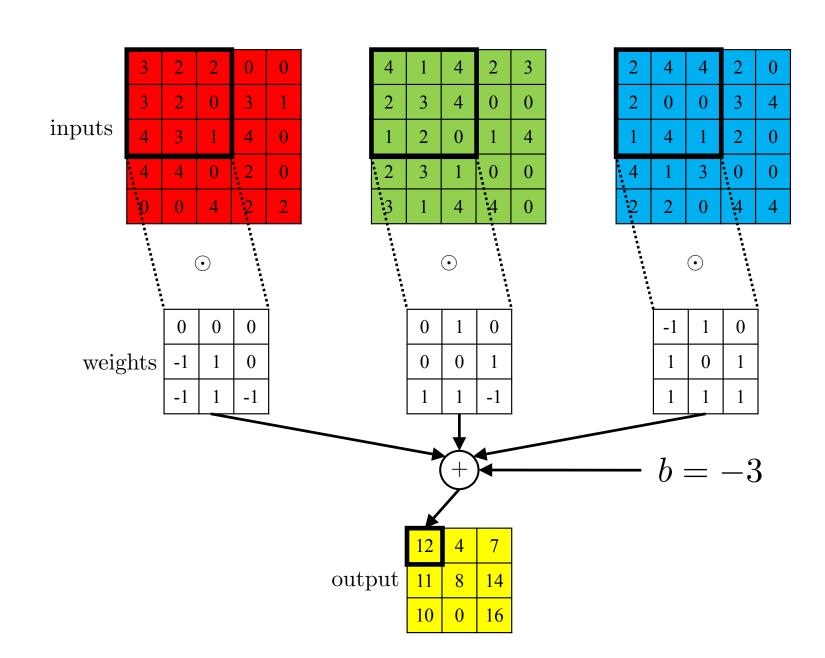
lacktriangle 1D convolution with no bias, single input channel and filter size F:

$$z_{i'} = \sum_{i=1}^F w_i x_{i'+(i-1)}$$
 correlations (similarity) $z_{i'} = \sum_{i=1}^F ar{w}_i x_{i'-(i-F)}$ convolution

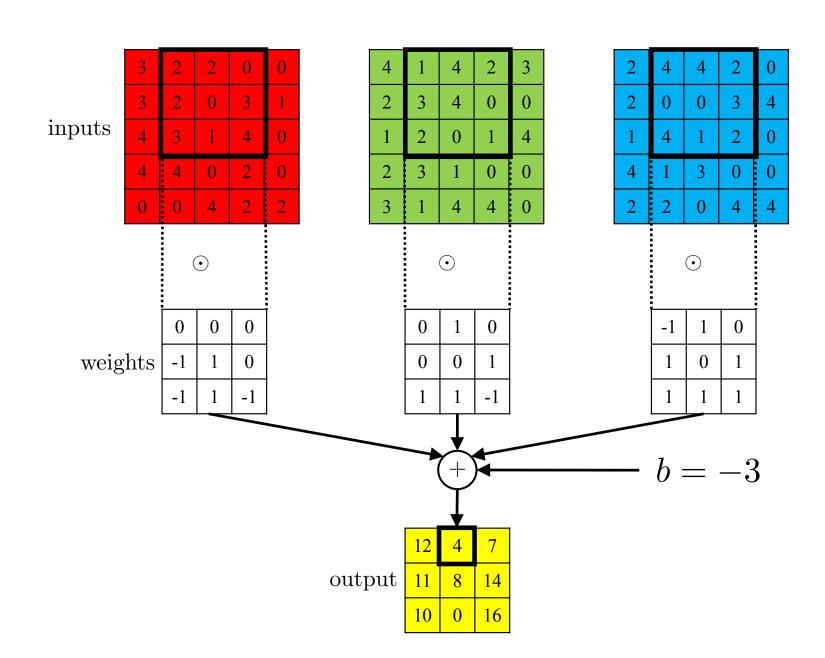
where $\bar{\boldsymbol{w}}$ is a reverse of \boldsymbol{w} ($\bar{w}_i = w_{F-i+1}$) and $i \in \{1, \dots, N-F+1\}$ for the input size N



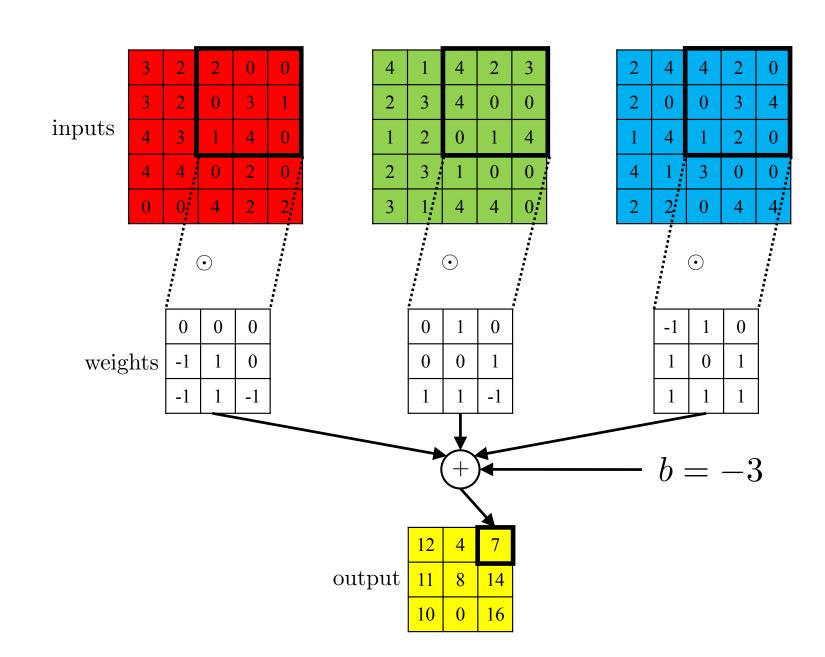




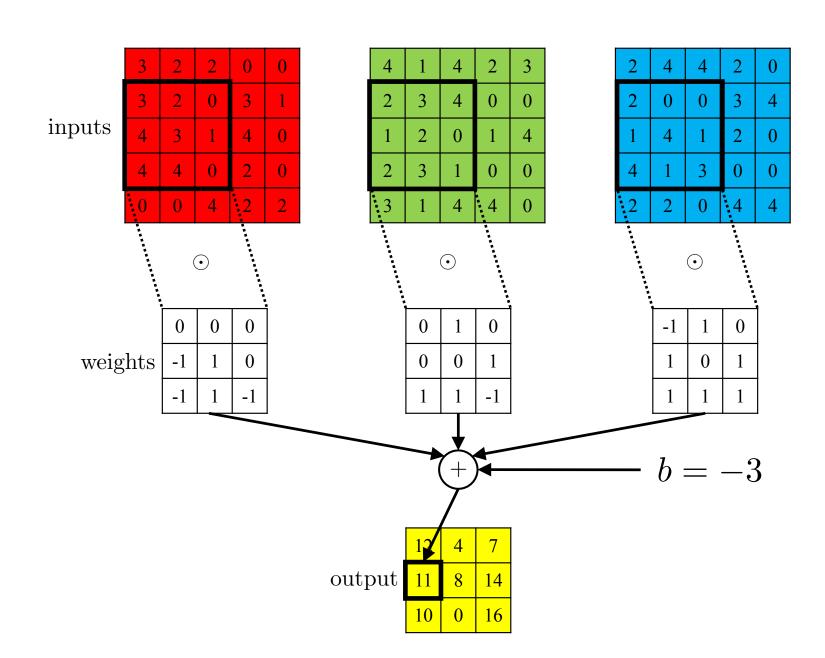






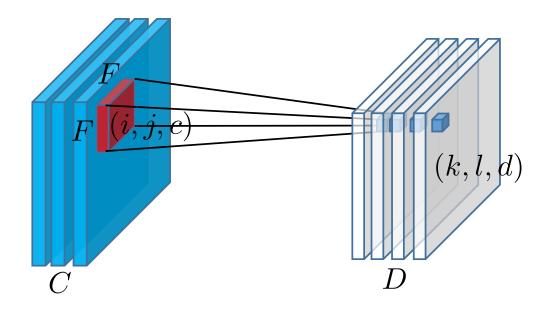






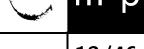
Convolution in 2D: Forward Message

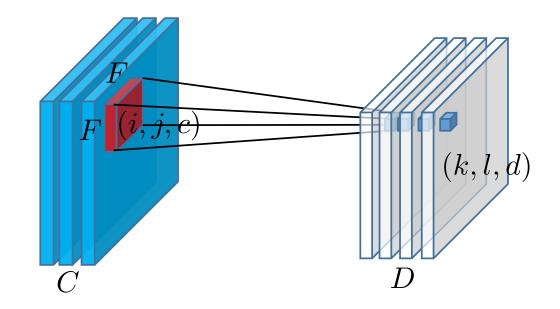




$$z_{kld} = f_{kld}(\boldsymbol{x}, \boldsymbol{w}, \boldsymbol{b}) = b_d + \sum_{i=1}^{F} \sum_{j=1}^{F} \sum_{c=1}^{C} x_{k+i-1, l+j-1, c} w_{ijcd}$$

Convolution in 2D: Parameter Gradient

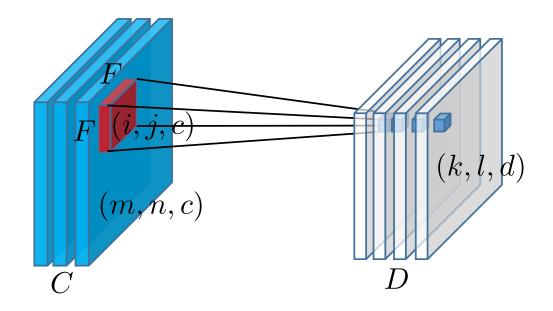




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$$\frac{\partial \mathcal{L}}{\partial w_{ijcd}} = \sum_{k',l',d'} \frac{\partial \mathcal{L}}{\partial f_{k',l',d'}} \frac{\partial f_{k',l',d'}}{\partial w_{ijcd}} = \sum_{k',l',d'} \delta_{k',l',d'}^{l+1} \frac{\partial f_{k',l',d'}}{\partial w_{ijcd}} = \sum_{k',l'} \delta_{k',l',d'}^{l+1} \frac{\partial f_{k',l',d'}}{\partial w_{ijcd}} = \sum_{k',l'} \delta_{k',l',d}^{l+1} x_{k'+i-1,l'+j-1,c}$$

Convolution in 2D: Backward Message

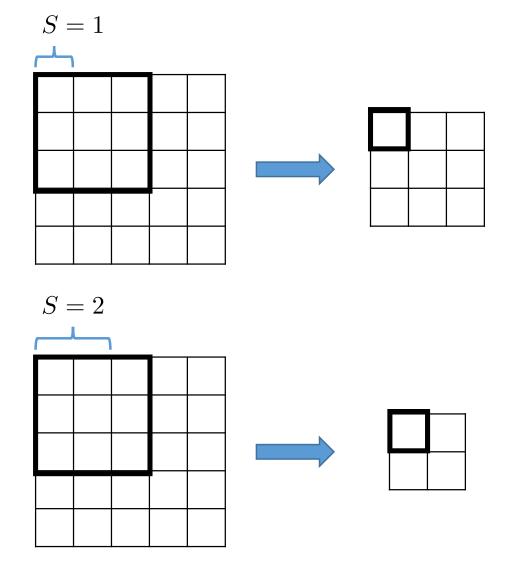


$$z_{kld} = f_{kld}(\boldsymbol{x}, \boldsymbol{w}, \boldsymbol{b}) = b_d + \sum_{i=1}^{F} \sum_{j=1}^{F} \sum_{c=1}^{C} x_{k+i-1, l+j-1, c} w_{ijcd}$$

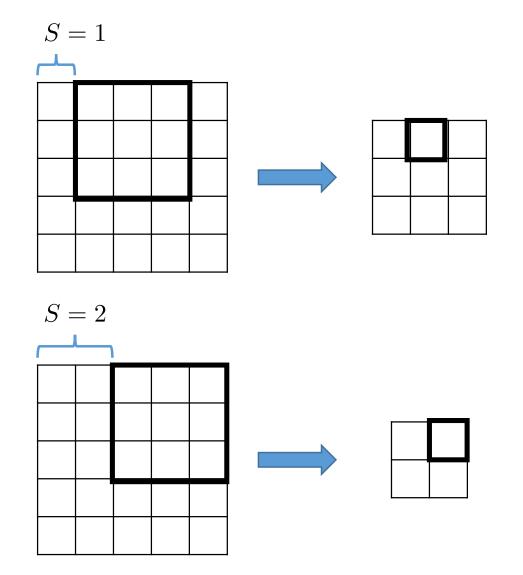
Substitute m = k + i - 1 and n = l + j - 1

$$\delta_{mnc}^{l} = \frac{\partial \mathcal{L}}{\partial x_{mnc}} = \sum_{k',l',d'} \delta_{k',l',d'}^{l+1} \frac{\partial f_{k',l',d'}}{\partial x_{mnc}}$$
$$= \sum_{k',l',d'} \delta_{k',l',d'}^{l+1} w_{m-k'+1,n-l'+1,c,d'}$$

- Stride hyper parameter, typically $S \in \{1, 2\}$
- Higher stride produces smaller output volumes spatially



- lacktriangle Stride hyper parameter, typically $S \in \{1,2\}$
- Higher stride produces smaller output volumes spatially



Zero Padding

- Convolutional layer reduces the spatial size of the output w.r.t. the input
- For many layers this might be a problem
- This is often fixed by zero padding the input
- lacktriangle The size of the zero padding is denote P

$$P = 1, S = 1$$

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

- Input volume: $W_{\mathsf{input}} \times H_{\mathsf{input}} \times C$
- Output volume: $W_{\text{output}} \times H_{\text{output}} \times D$
- lacktriangle Having D filters:
 - ullet receptive field of $F \times F$ units,
 - \bullet stride S
 - ullet zero padding P

$$W_{\text{output}} = (W_{\text{input}} - F + 2P)/S + 1$$
$$H_{\text{output}} = (H_{\text{input}} - F + 2P)/S + 1$$

- lacktriangle Needs F^2CD weights and D biases
- The number of activations and δ s to store: $W_{\text{output}} \times H_{\text{output}} \times D$

Convolution Applied to an Image



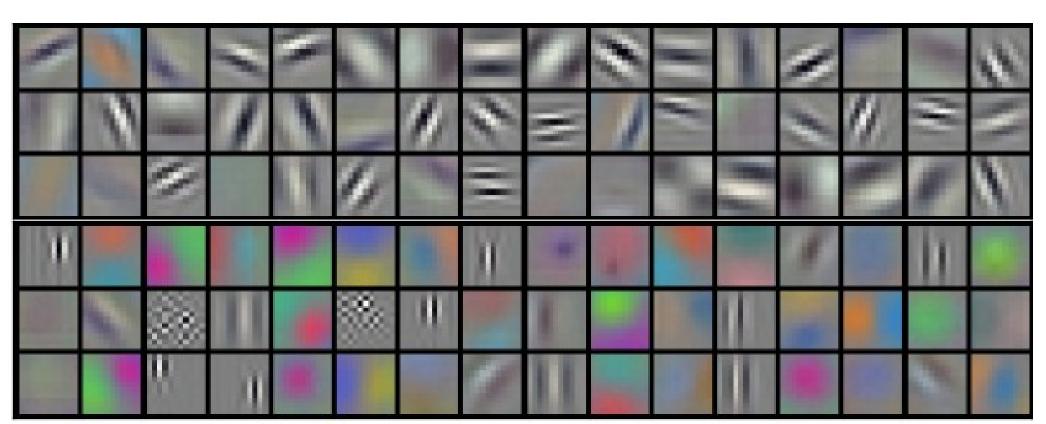
Identity	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	Sharpen	$\begin{bmatrix} 0 & -1 & 0 \\ -1 & 5 & -1 \\ 0 & -1 & 0 \end{bmatrix}$	
	$\begin{bmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{bmatrix}$	Box blur (normalized) Gaussian blur (approximation)	$\frac{1}{9} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$	
Edge detection	$\begin{bmatrix} 0 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & 0 \end{bmatrix}$		9 [1 1 1]	
	$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$		$\frac{1}{16} \begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix}$	

https://en.wikipedia.org/wiki/Kernel_(image_processing)

Convolution: Weights Visualization



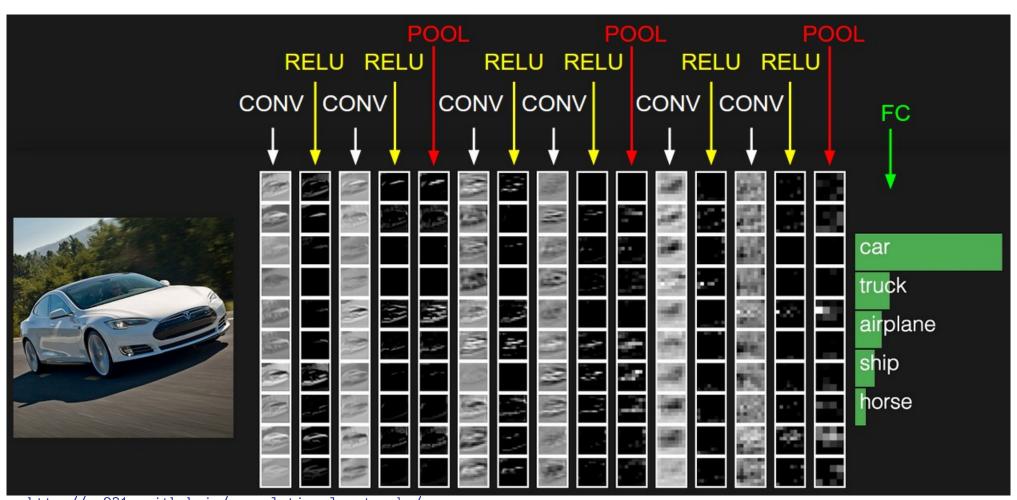
Filters of the first layer



Krizhevsky, Sutskever, Hinton: ImageNet Classification with Deep Convolutional Neural Networks, 2012

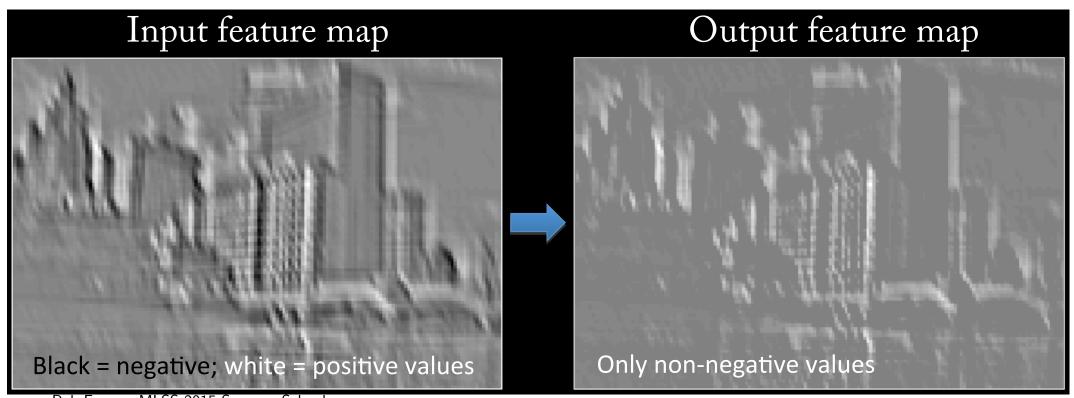
Convolution: Feature Map Visualization





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

- In most cases a nonlinearity (sigmoid, tanh, ReLU) is applied to the outputs of the convolutional layer
- Example: ReLU units



Rob Fergus: MLSS 2015 Summer School

- lacktriangle Reduces spatial resolution ightarrow less parameters ightarrow helps with overfitting
- Introduces translation invariance
- Depth is not affected

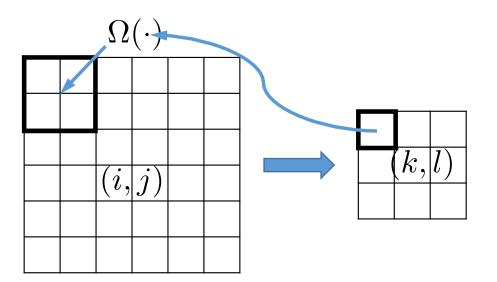
F = 2, S = 2												
2	2	0	4	3	4							
0	0	5	0	4	1		2	5				
4	5	2	5	1	4		2		4 			
5	2	1	0	2	1		5	5				
2	3	3	3	5	3		3	4	5			
0	3	0	4	0	1							

Max Pooling Gradient

- No changes to the depth
- Forward message: $z_{kl} = f_{kl}(\boldsymbol{x}) = \max_{(i,j) \in \Omega(k,l)} x_{ij}$
- Backward message:

$$\delta_{ij}^{l} = \sum_{k',l'} \delta_{k'l'}^{l+1} \frac{\partial f_{k'l'}}{\partial x_{ij}} = \sum_{k',l'} \delta_{k'l'}^{l+1} \mathbb{I} \left\{ (i,j) = \underset{(i',j') \in \Omega(k',l')}{\operatorname{argmax}} x_{i'j'} \right\}$$

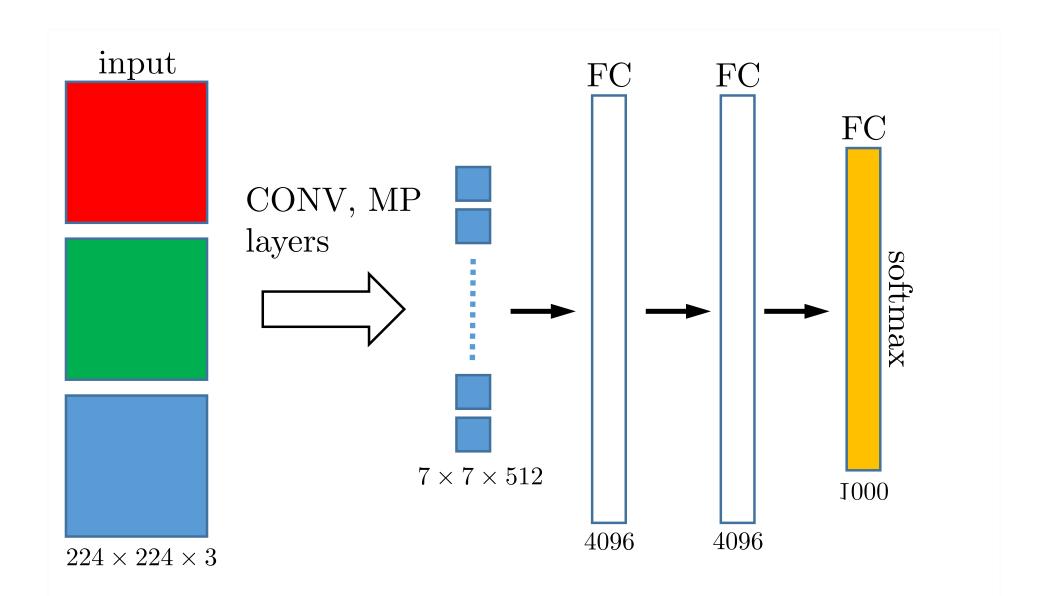
Backward message propagates only for the selected max unit



- lackbox Convolutional layer can be simply transformed to a Fully-connected layer \rightarrow sparse weight matrix
- ♦ The other direction is also possible: FC layer of D units following a $F \times F \times C$ convolutional layer can be replaced by a $1 \times 1 \times D$ convolutional layer using $F \times F$ filters (P = 0, S = 1)

Fully-Connected Layer to Convolutional Example

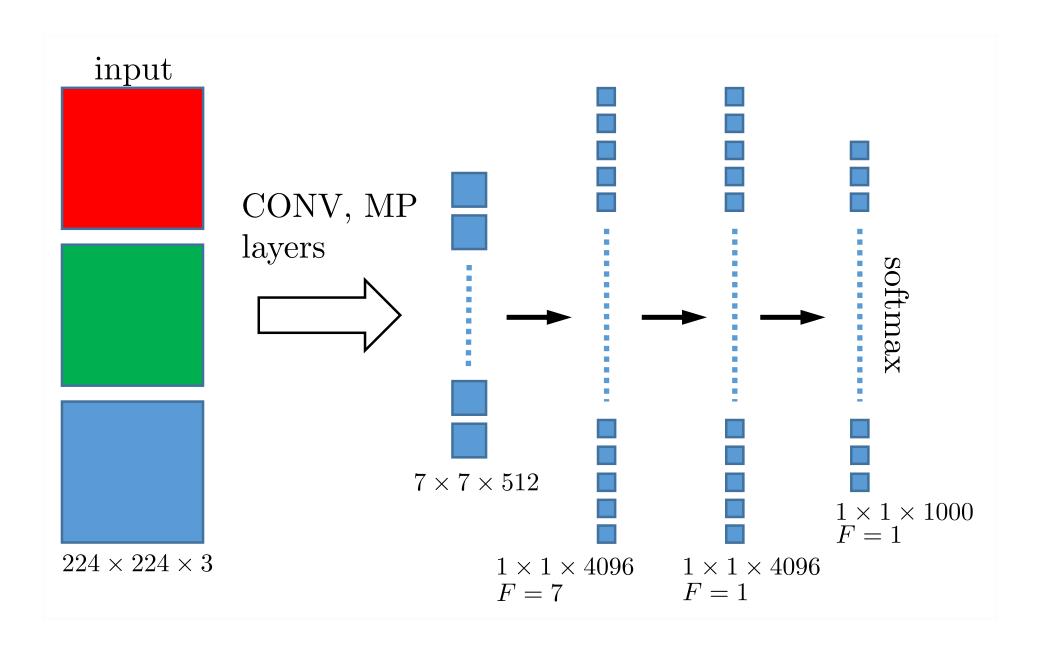




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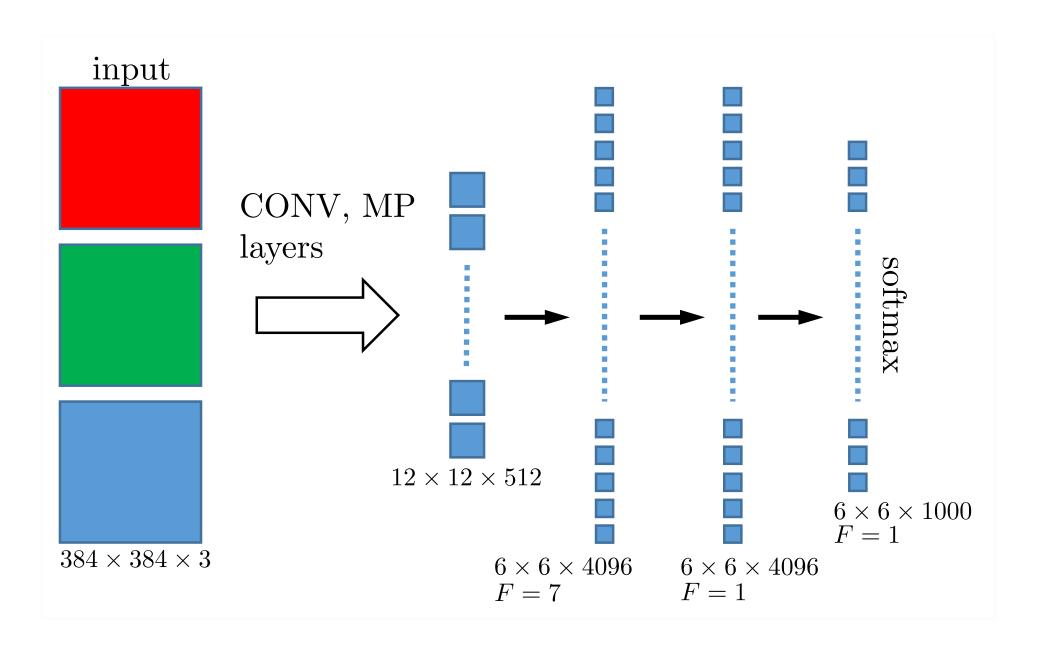
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Fully-Connected Layer to Convolutional Example



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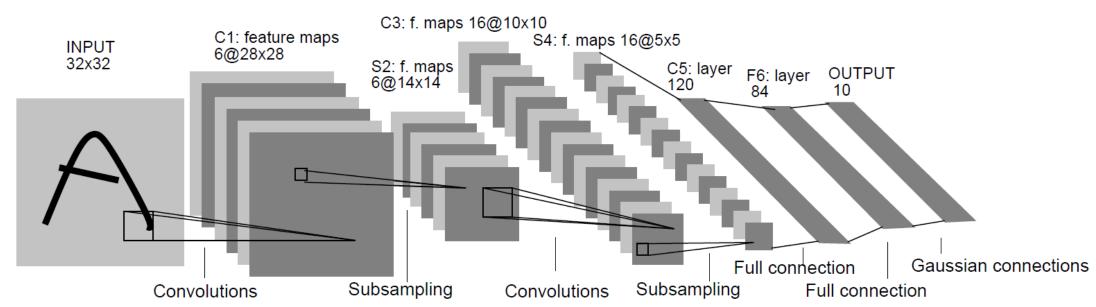


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- Use zero padding to preserve the spatial resolution
- Reduce the resolution only by means of max pooling
- Prefer image size with factorization containing higher power of 2 for pooling with F=2 (e.g., $224=2^5\times 7$ for ImageNet networks)
- Set the number of filters to powers of 2 (optimization)
- Read Andrej Karpathy's blog and see his course on CNNs http://cs231n.stanford.edu/

LeNet-5 (1998)

- Yann LeCun
- CNN for written character recognition dataset MNIST
- \bullet Training set 60,000, testing set 10,000 examples



LeCun et al.: Gradient-based learning applied to document recognition, 1998

Errors by LeNet-5

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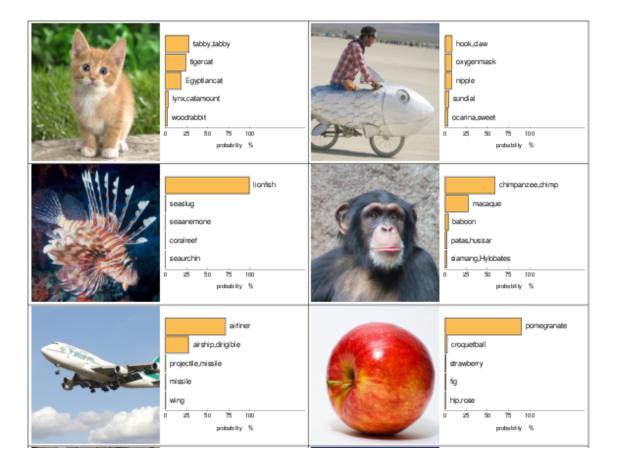
- \bullet 82 errors (current best 21)
- lacktriangle Human error expected to be between 20 to 30



LeCun et al.: Gradient-based learning applied to document recognition, 1998

ImageNet Dataset

- Dataset of high-resolution color images: 15M training examples, 22k classes
- ImageNet Large Scale Visual Recognition Challenge (ILSVRC) uses subset of the ImageNet: 1.3M training, 50k validation, 100k testing samples, 1000 classes







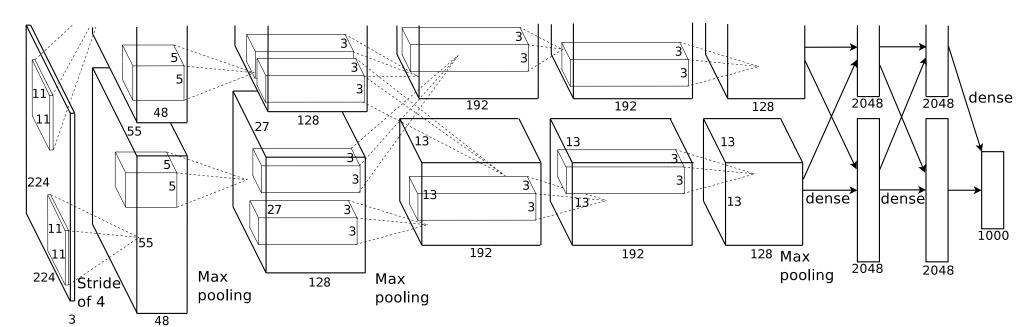
(a) Siberian husky

(b) Eskimo dog

Szegedy et al.: Going deeper with convolutions, 2014

AlexNet 2012

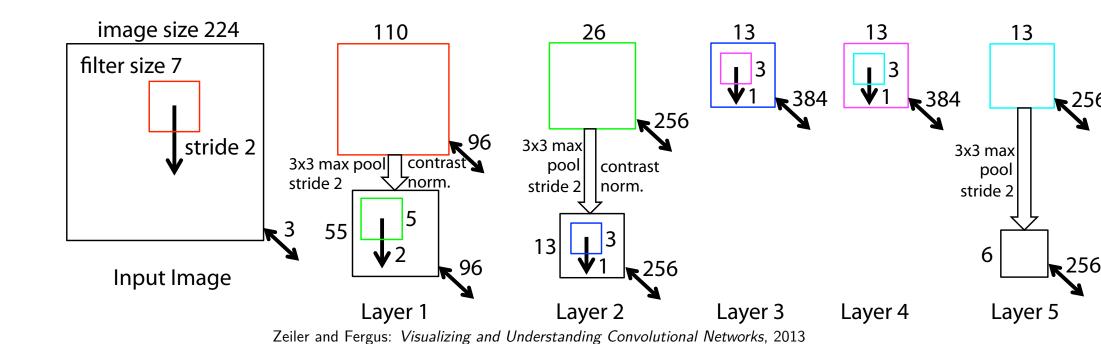
- Two separate streams for 2 GPUs, 60M parameters
- ullet Data augmentation (increasing dataset size): 224×224 patches (+ mirrored) of 256×256 original images, altering RGB intensities
- Uses ReLU and dropout
- ullet Top five error 18.2% for the basic net decreased to 15.4% for an ensemble of 7 CNNs, pre-CNN best was 25.6%



Krizhevsky et al.: ImageNet Classification with Deep Convolutional Neural Networks, 2012

ZFNet 2013

- Smaller filters for the first convolutional layer CONV1: 7×7 , S=2 instead of 11×11 , S=4
- CONV3-5: more depth
- \bullet Top five error 16.5%, 14.8% for an ensemble of 6 CNN



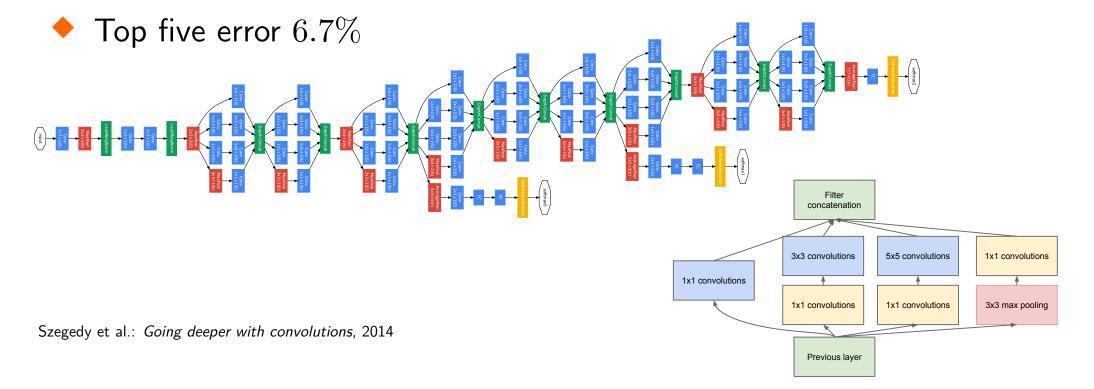
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- Simonyan, Zisserman: Very Deep Convolutional Networks for Large-Scale Image Recognition, 2014
- Simplification: lowering filter spatial resolution ($F=3,\ S=1,\ P=1$), increasing depth
- lacktriangle A sequence of 3×3 filters can emulate a single large one
- \bullet Top five error 7.3%, 6.8% for an ensemble of 2 CNNs



GoogLeNet 2014

- Use of inception layers instead of pure convolutional ones
- Fully connected output layer preceded by the global average pooling: the last layer before average pooling has $7 \times 7 \times 1024$ it is spatially reduced to $1 \times 1 \times 1024$
- Only 5M parameters (60M AlexNet)
- Auxiliary classifiers: their losses are added with discount weight



ResNet 2015

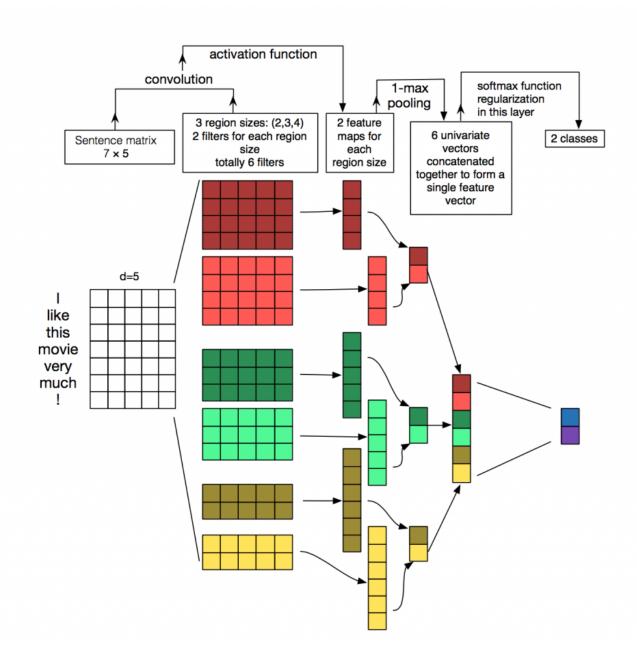


- He et al.: Deep Residual Learning for Image Recognition, 2015
- ◆ 152 layers (2-3 weeks on 8 GPUs)
- Using skip connections
- Batch normalization instead of dropout
- lacktriangle Top five error 3.6% (human performance 5.1% expected)

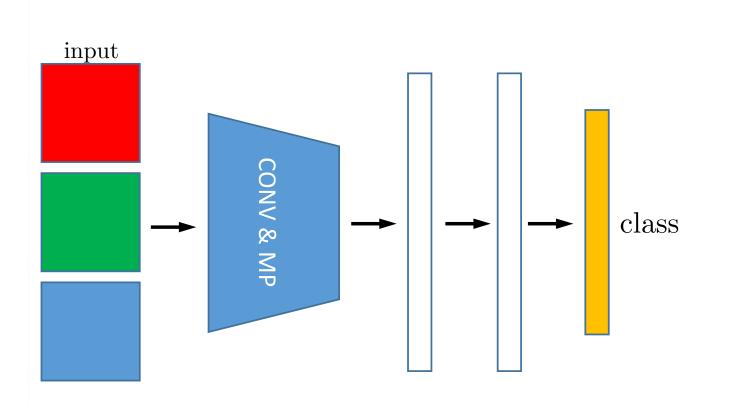
CNNs for Natural Language Processing (NLP)

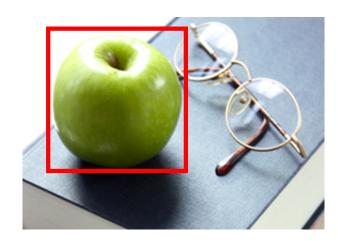


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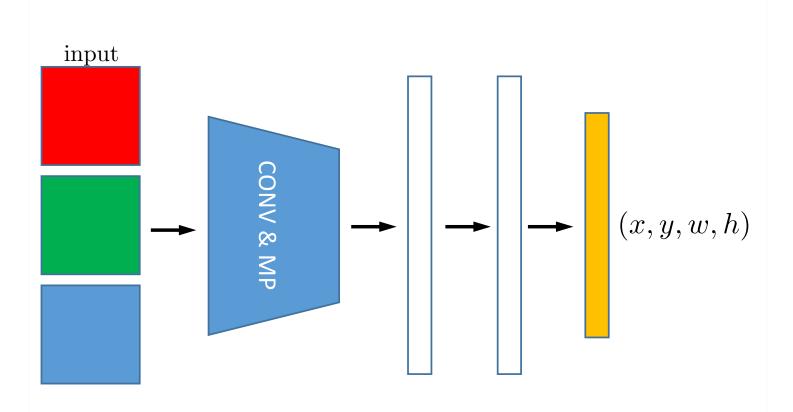


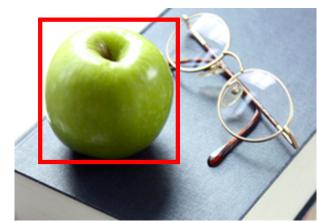
- Idea: use an existing model as a base to solve a similar problem
- Often used when not enough data available to solve the target problem directly
- Example: reuse an ImageNet network for object localization



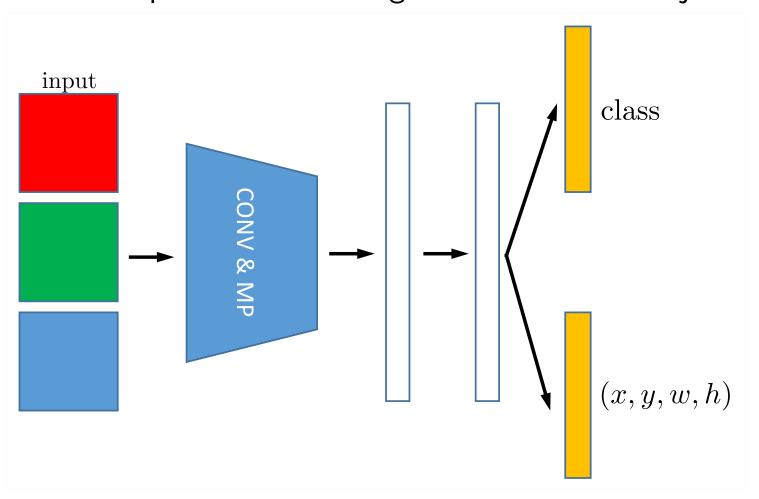


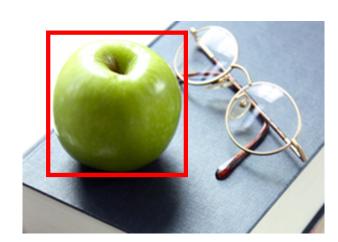
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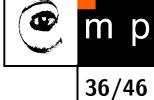


- ◆ Idea: use an existing model as a base to solve a similar problem
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Transfer Learning



- ◆ Idea: use an existing model as a base to solve a similar problem
- Often used when not enough data available to solve the target problem directly
- Example: reuse an ImageNet network for object localization
- You can:
 - cut the original network at various layers,
 - fix or not the weights of the original network or use different learning rates
 - use different type of model for the head, e.g., linear SVM

Parameter Initialization

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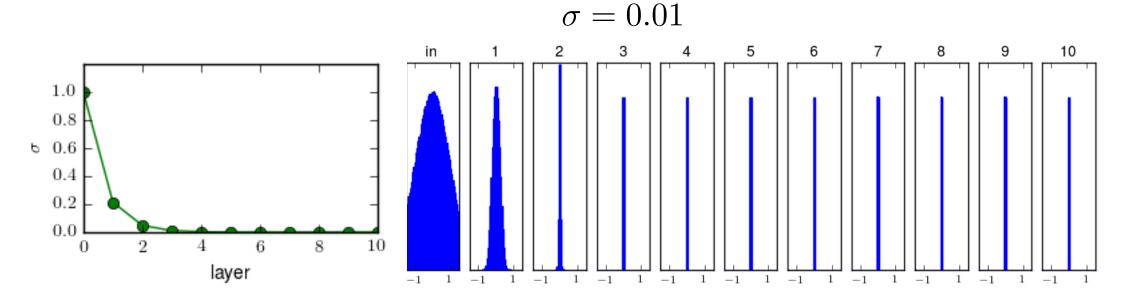
Is it a good idea to set all weights to zero?

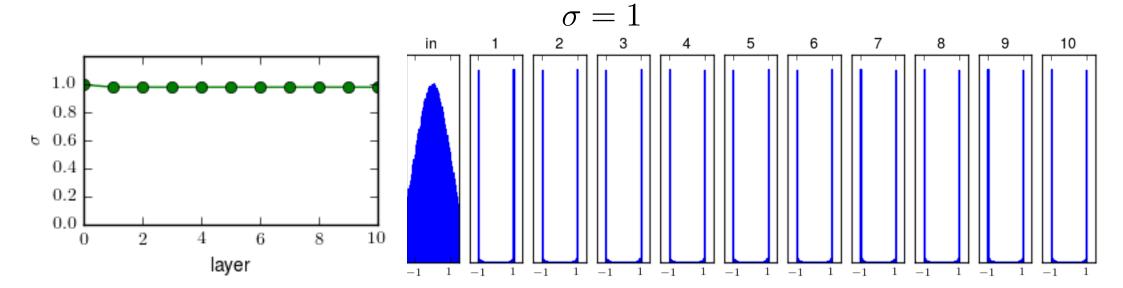
Parameter Initialization



- Is it a good idea to set all weights to zero?
- ullet No. All neurons would behave the same: the same δ s are backpropagated. We need to break the symmetry
- Use small numbers, e.g., sample from a Gaussian distribution with zero mean:
 - works well for shallow networks,
 - for deep networks it is not a good idea

- ullet MLP, ten anh layers, 500 units each. Each input fed with $\mathcal{N}(0,1)$
- Weights initialized to $\mathcal{N}(0, \sigma^2)$





- Glorot and Bengio: Understanding the difficulty of training deep feedforward neural networks, 2010
- For the linear neuron $s = \sum_i w_i x_i$, let w_i and x_i be independent random variables, w_i and x_i are i.i.d., $E(x_i) = E(w_i) = 0$:

$$Var(s) = Var\left(\sum_{i} w_{i}x_{i}\right) = \sum_{i} Var(w_{i}x_{i}) =$$

$$= \sum_{i} \left[\mathbb{E}(w_{i})\right]^{2} Var(x_{i}) + \left[\mathbb{E}(x_{i})\right]^{2} Var(w_{i}) + Var(x_{i}) Var(w_{i}) =$$

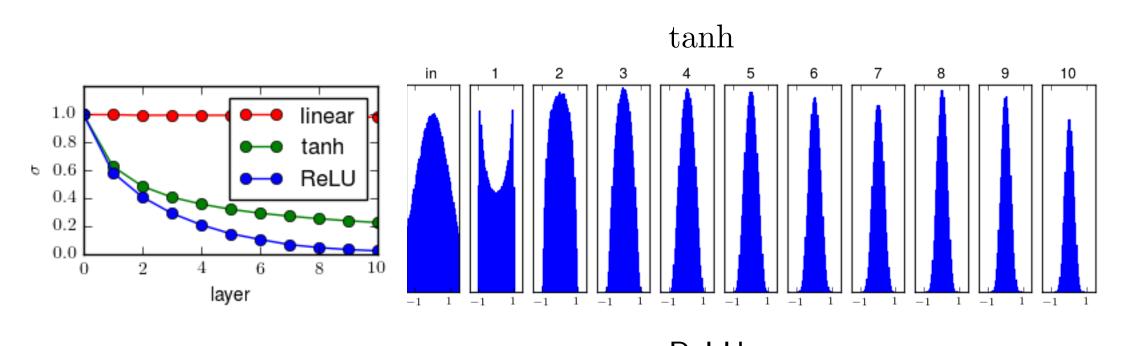
$$= \sum_{i} Var(x_{i}) Var(w_{i}) = n_{\mathsf{in}} Var(x) Var(w)$$

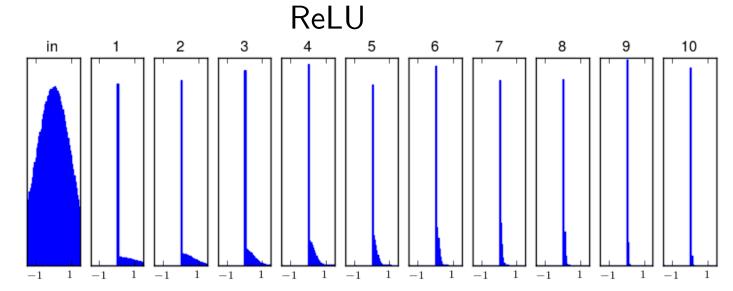
- We want Var(s) = Var(x), so choose $Var(w) = \frac{1}{n_{in}}$
- Similar analysis for the backpropagated signal: $Var(w) = \frac{2}{n_{in} + n_{out}}$
- Standardized inputs
- ♦ Works well for tanh as it is linear near zero

Xavier Initialization (contd.)

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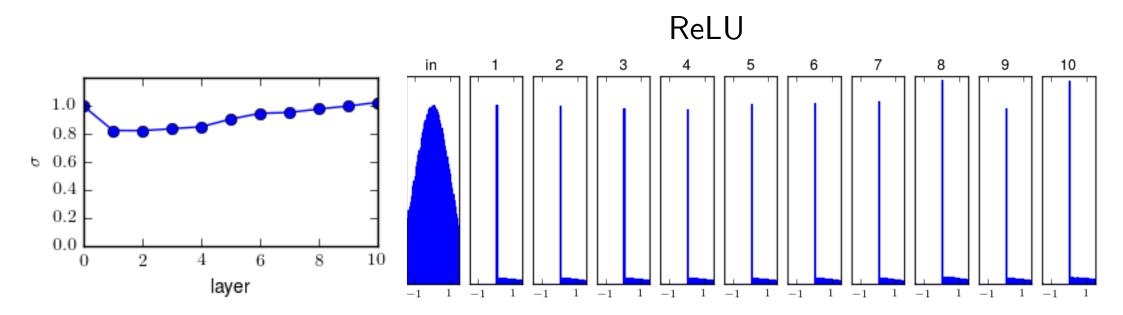
Xavier initialization does not work for ReLU





He Initialization

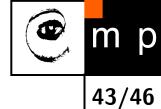
- He et al.: Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification, 2015
- Suggested ReLU initialization
- Uses $Var(w) = \frac{2}{n_{in}}$



Other Methods

- Recent data-driven techniques iteratively scaling weights in the network
- Batch normalization:
 - specialized layer which sets unit variance,
 - computes mean and variance estimates over batch,
 - normalizes but allow linear transformation (parameters) of the distribution to better deal with nonlinearities

Autoencoders



- lacktriangle Task: train the network for identity (same targets as inputs $\mathbf{Y} = \mathbf{X})$
- The number of hidden units is typically less than the number of inputs/outputs
- Compresses the input space
- lacktriangle May have tied weights $(\mathbf{W}' = \mathbf{W}^{\mathbf{T}})$
- Works as PCA for linear layers and squared loss: Bourlard and Kamp: Auto-Association by Multilayer Perceptrons and Singular Value Decomposition, 1988

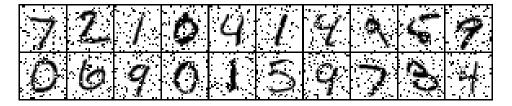
Denoising Autoencoders

Reconstruction from corrupted inputs

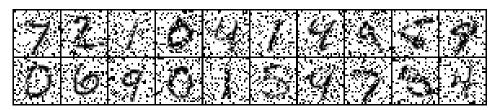
original

7	2	/	0	4	1	Ч	٩	1,8	9
0	S	9	0	j	U	9	7	Ф	4

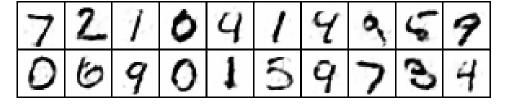
noise 5%



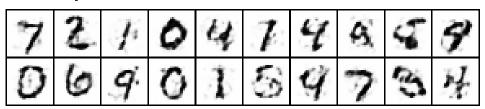
noise 10%



${\rm output}\ 5\%$

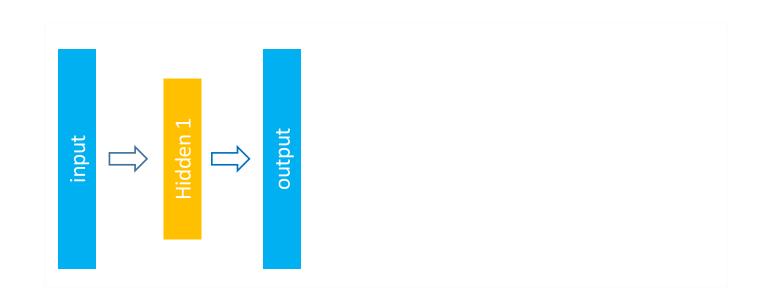


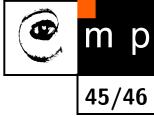
output 10%



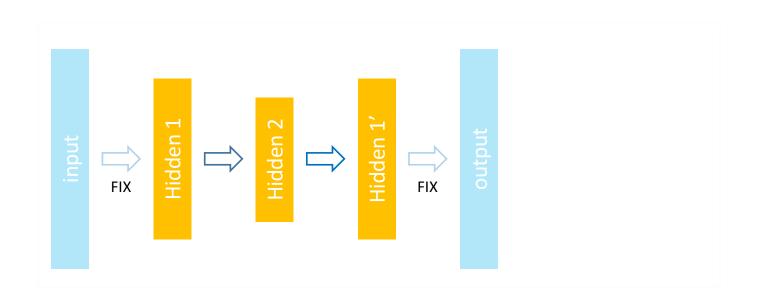
m p

1. Train the first layer as a shallow autoencoder



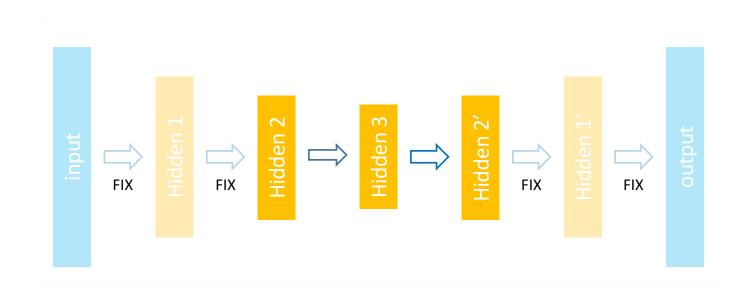


- 1. Train the first layer as a shallow autoencoder
- 2. Use its hidden units' activations to train another shallow autoencoder



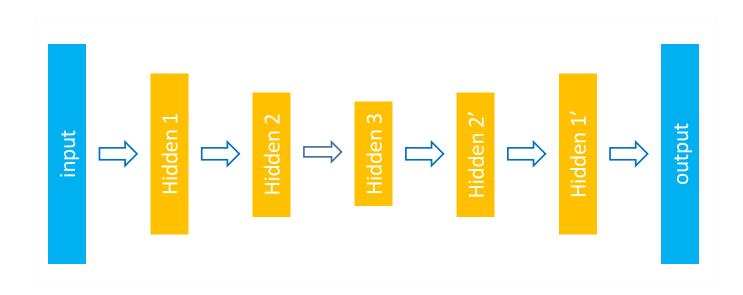


- 1. Train the first layer as a shallow autoencoder
- 2. Use its hidden units' activations to train another shallow autoencoder
- 3. Repeat (2) until the desired number of layers is reached





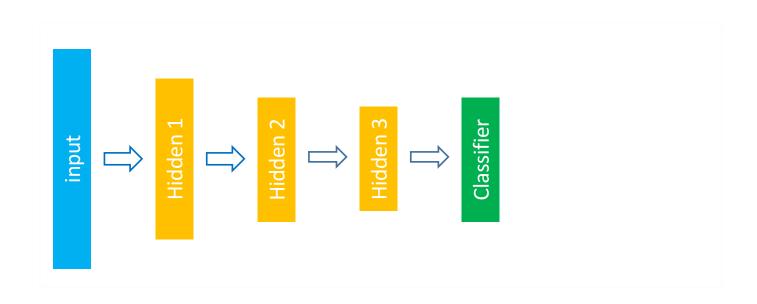
- 1. Train the first layer as a shallow autoencoder
- 2. Use its hidden units' activations to train another shallow autoencoder
- 3. Repeat (2) until the desired number of layers is reached
- 4. Fine-tune all parameters

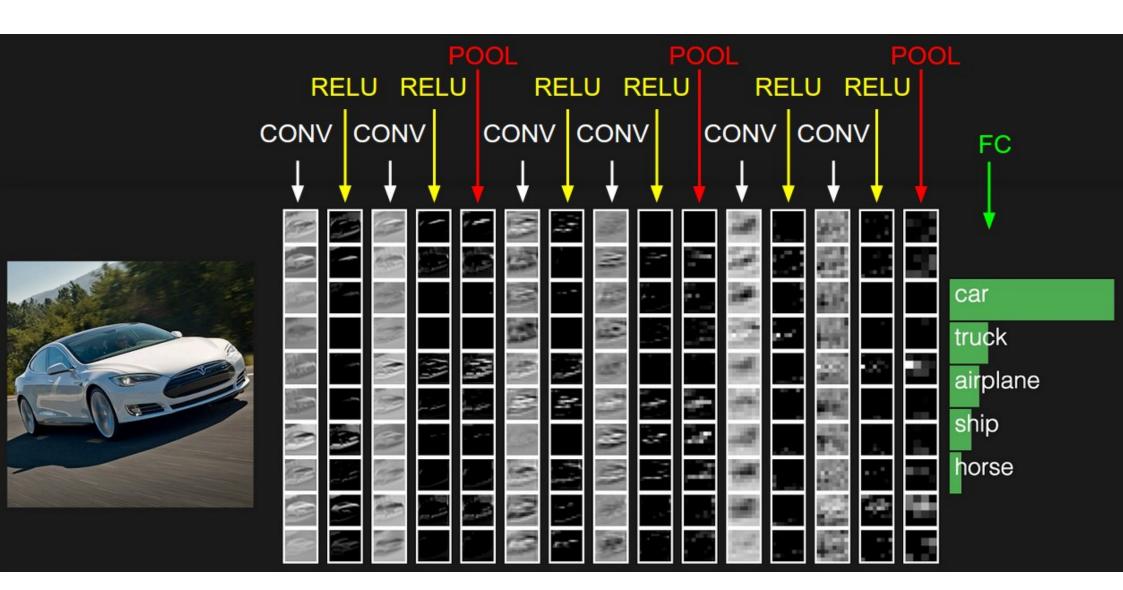


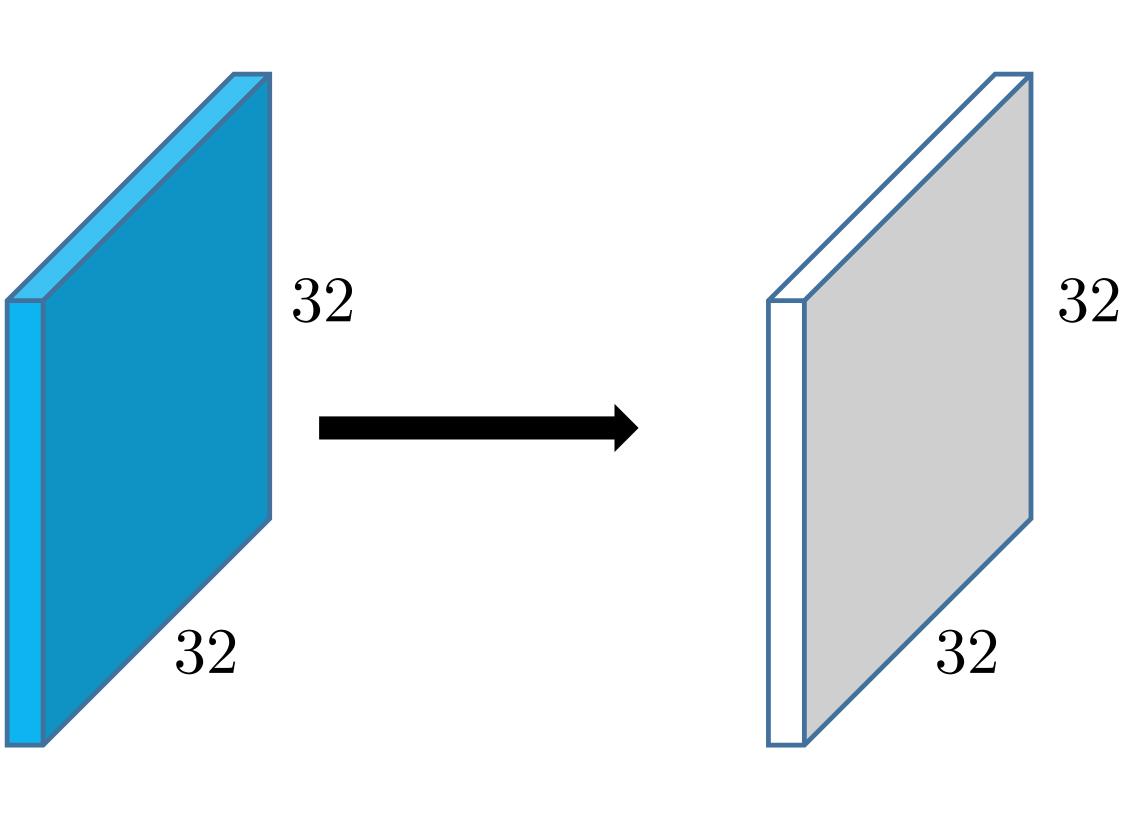
Unsupervised Pre-training

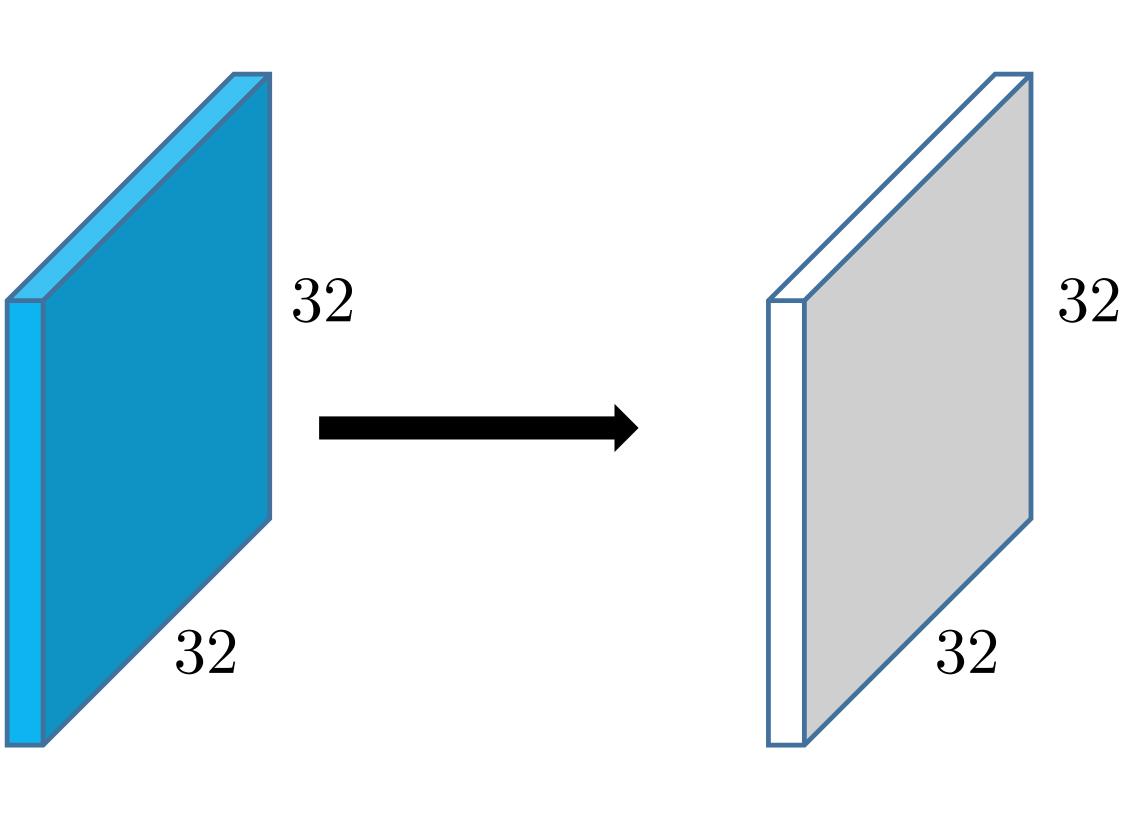


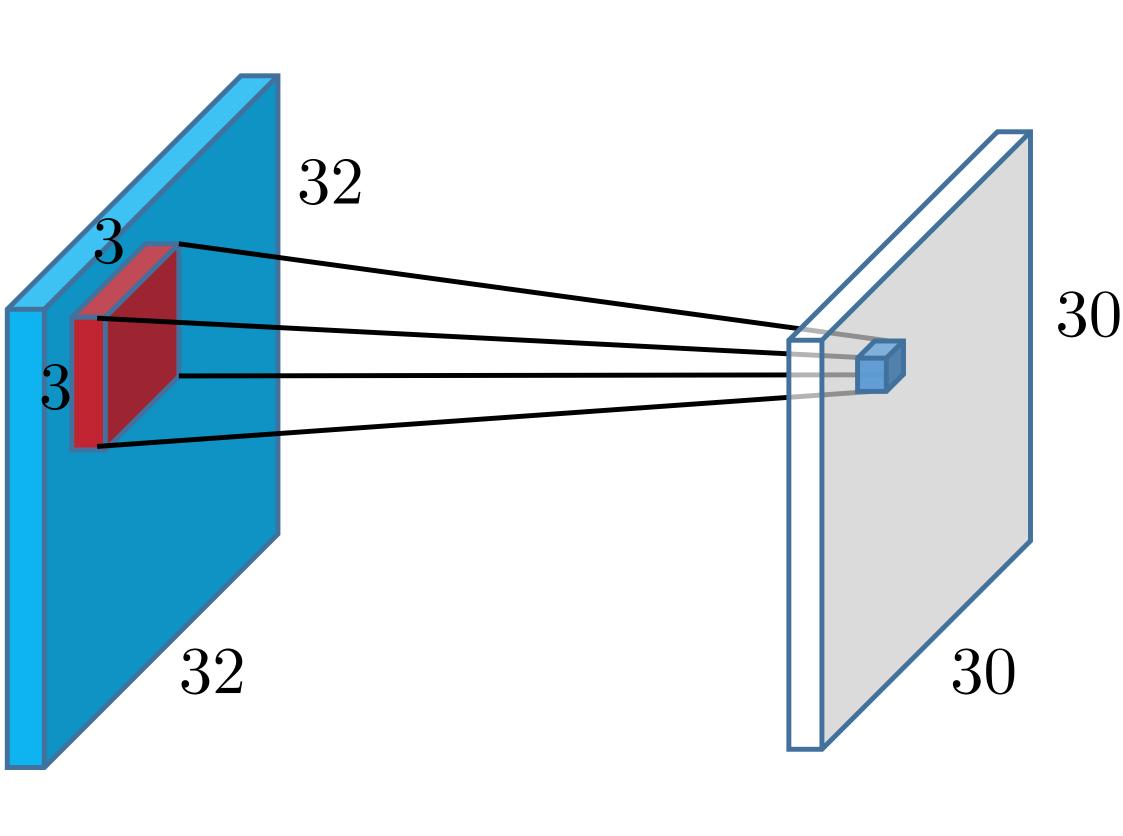
- Use the encoder part of a stacked autoencoder for weight initialization of a different network
- Semi-supervised setup

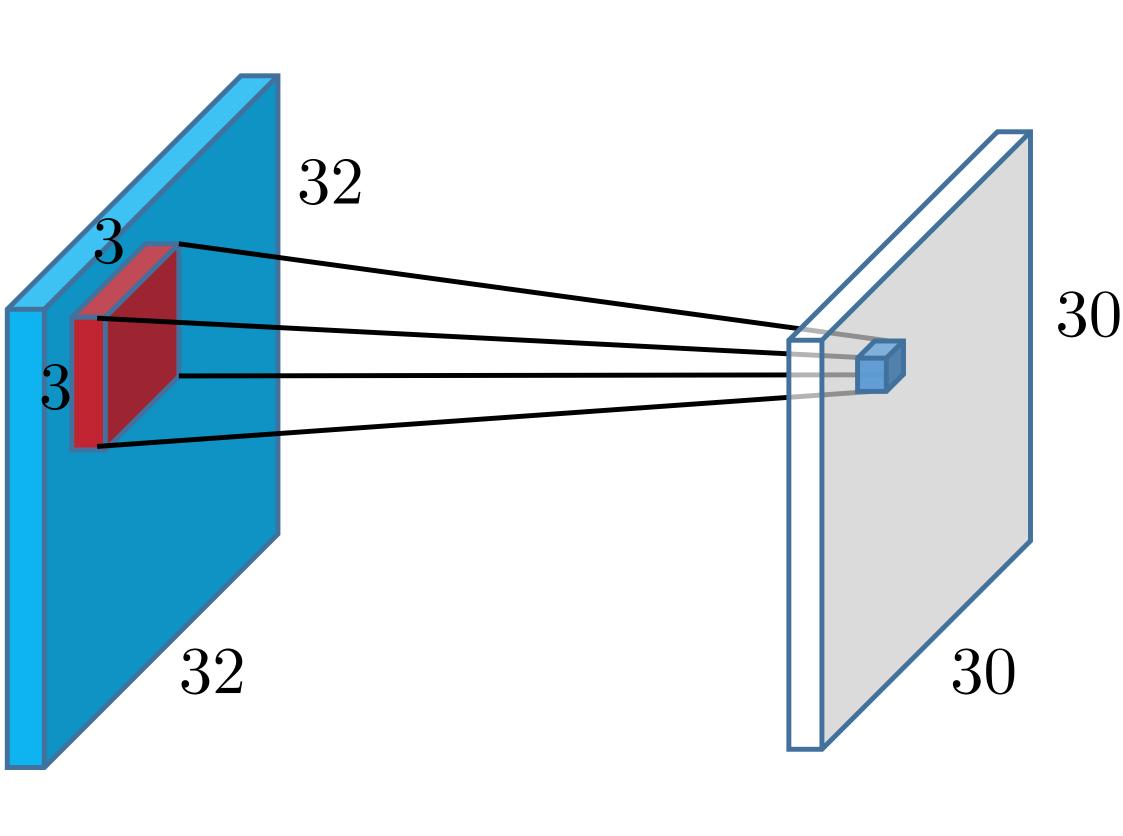


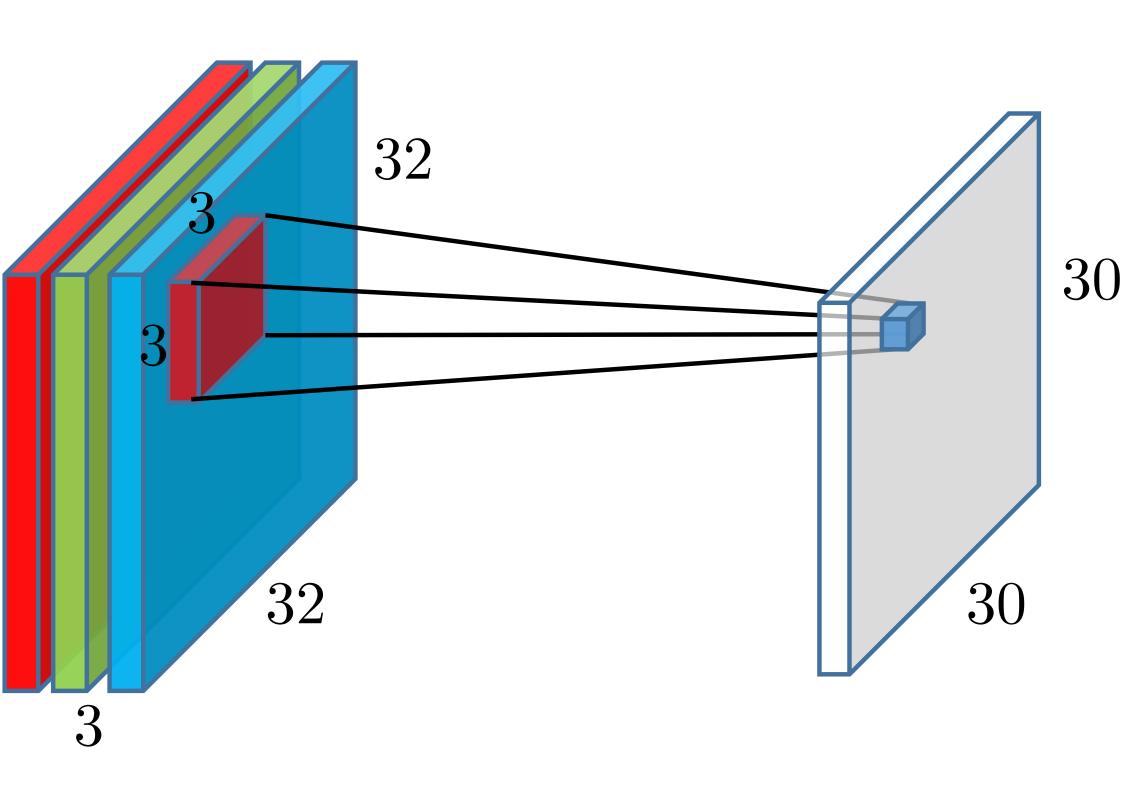


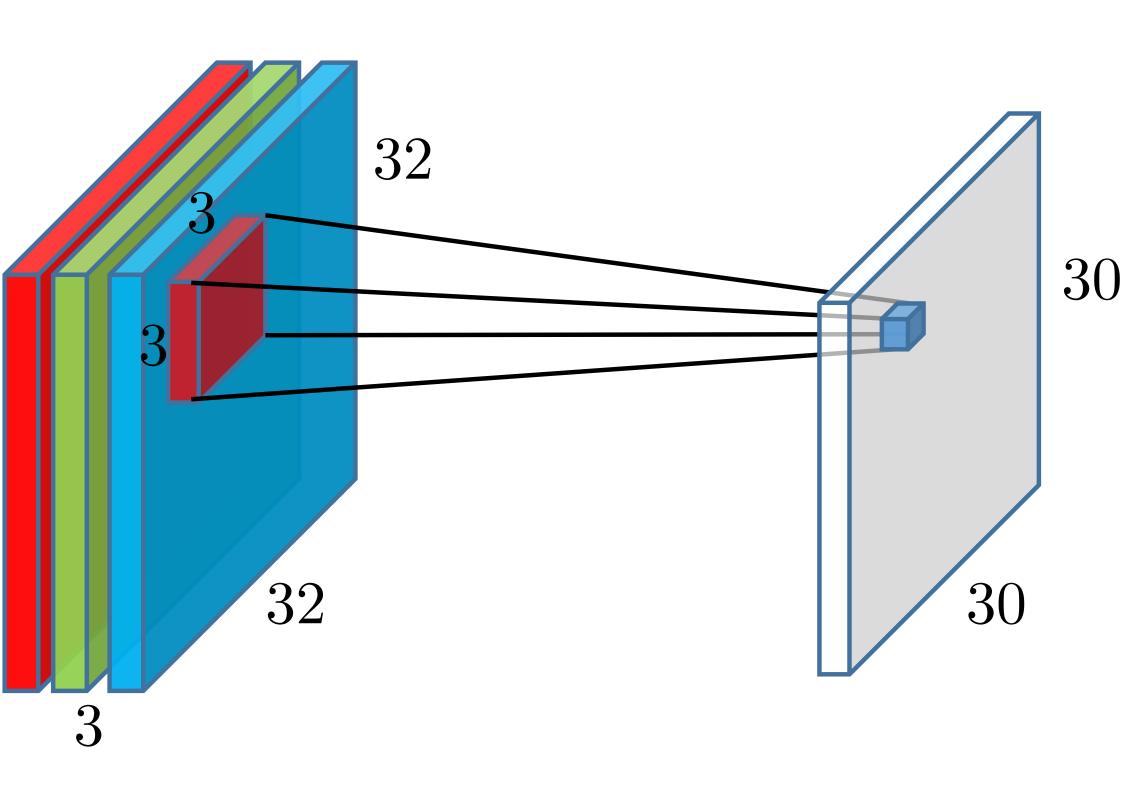


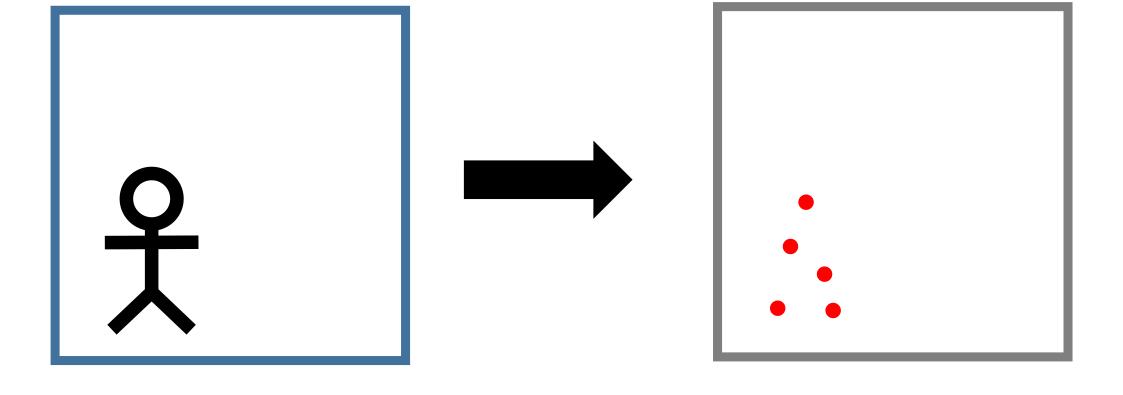


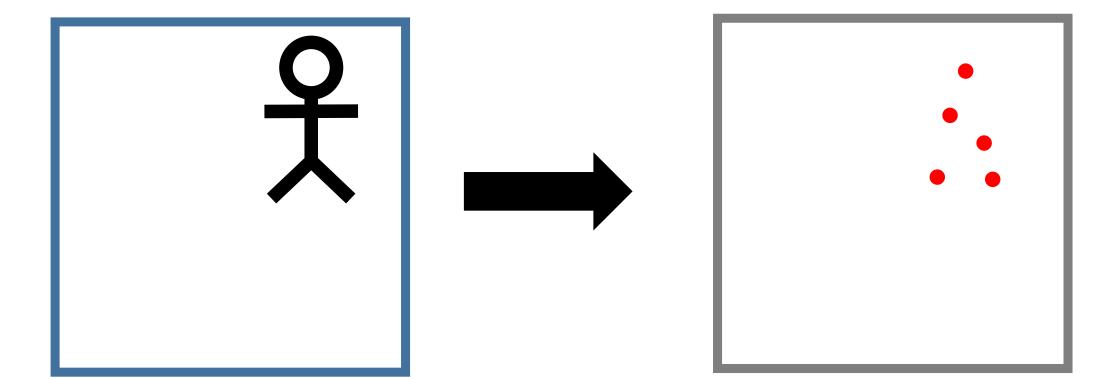


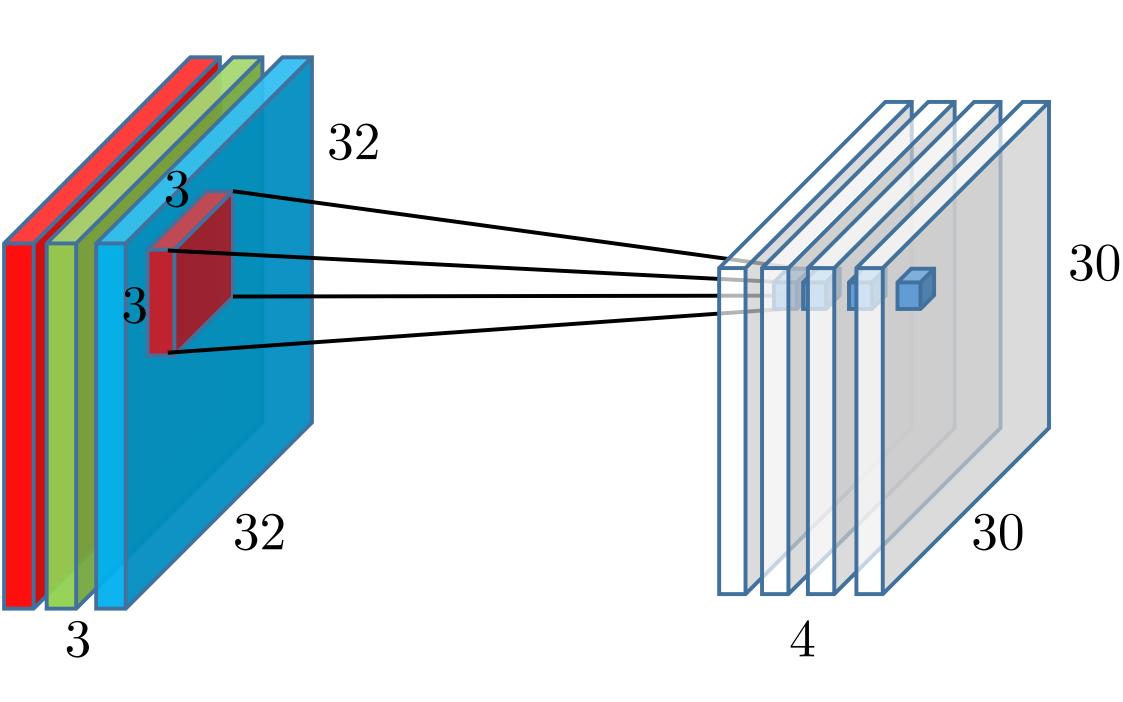


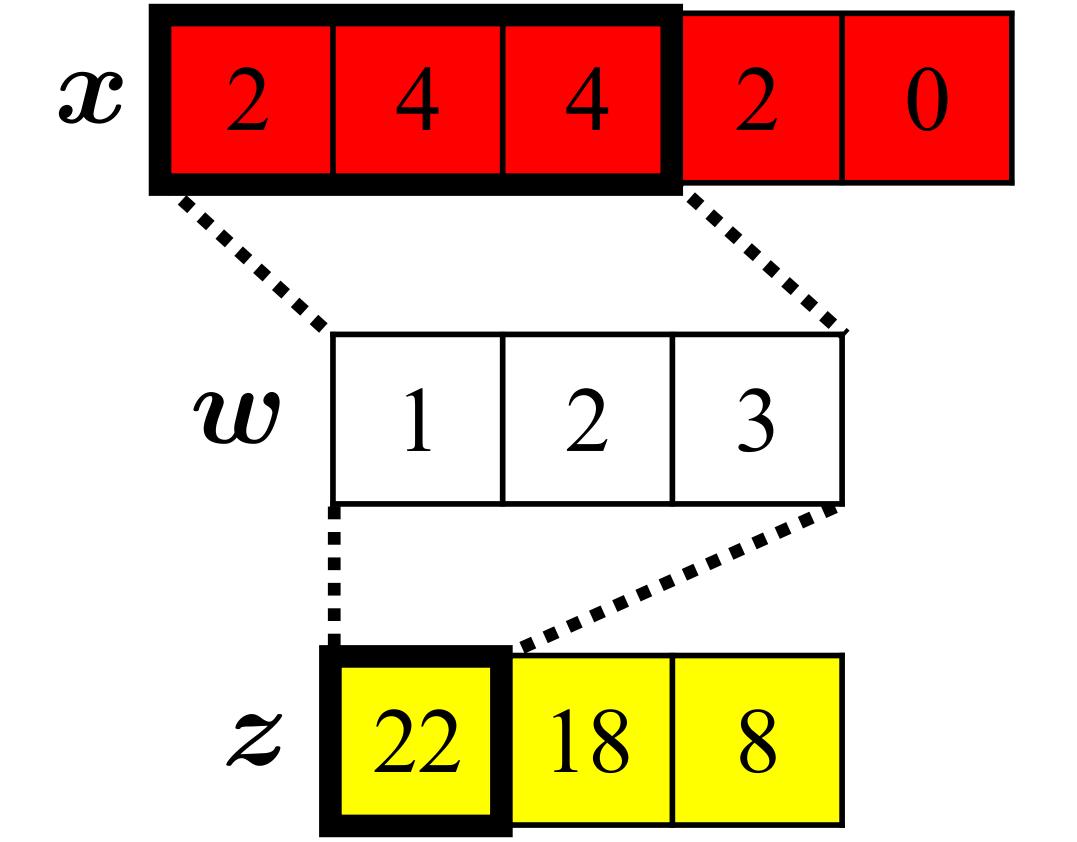


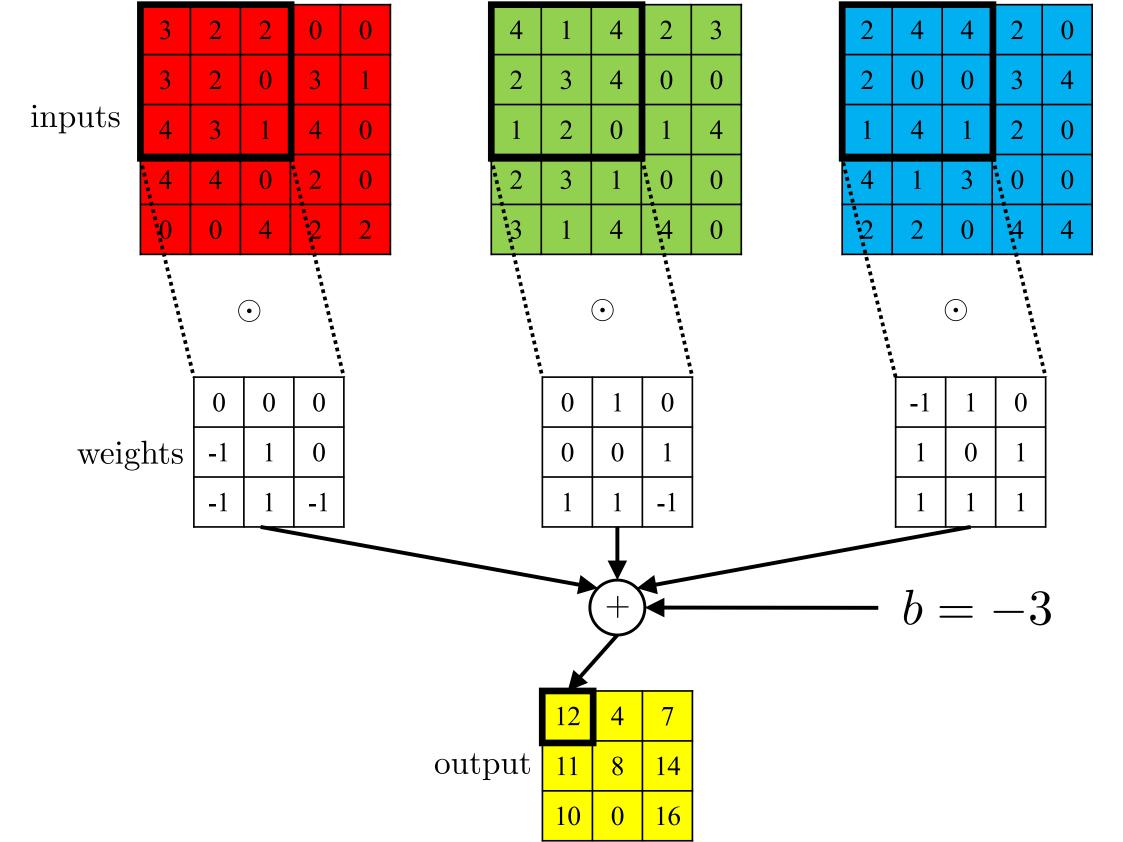


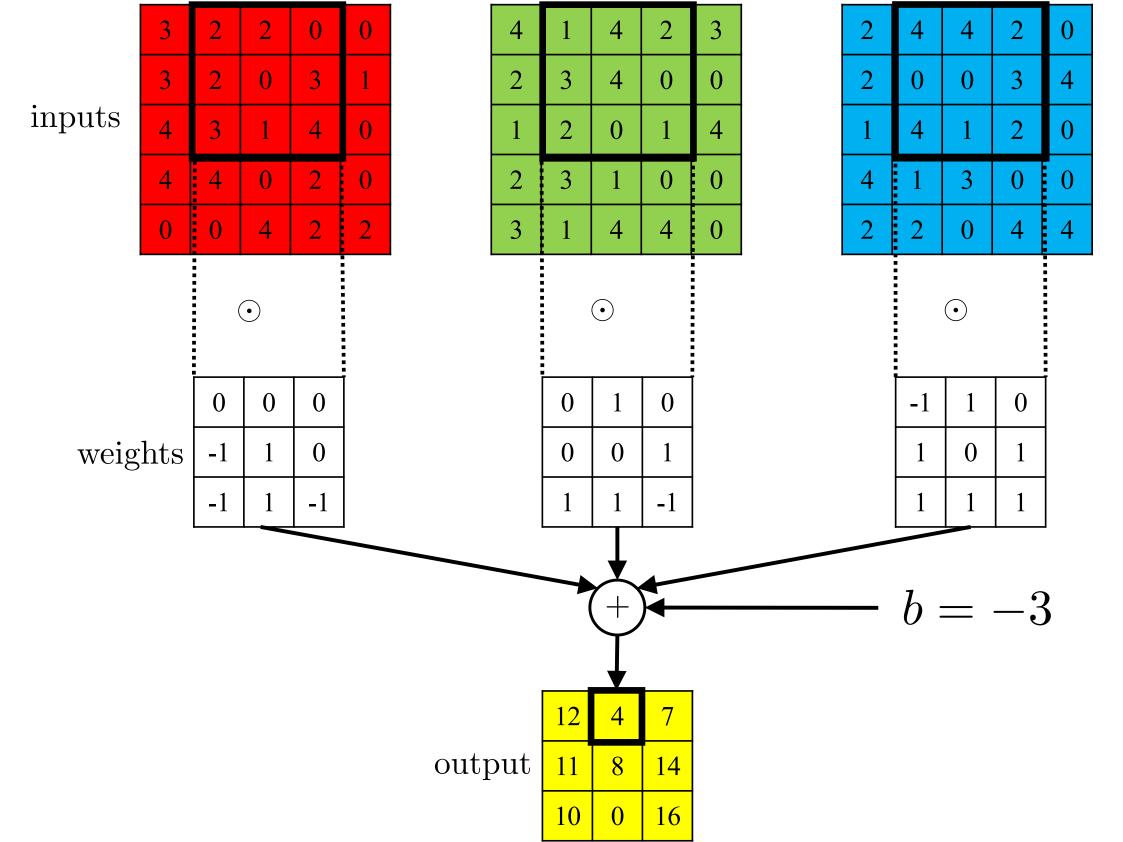


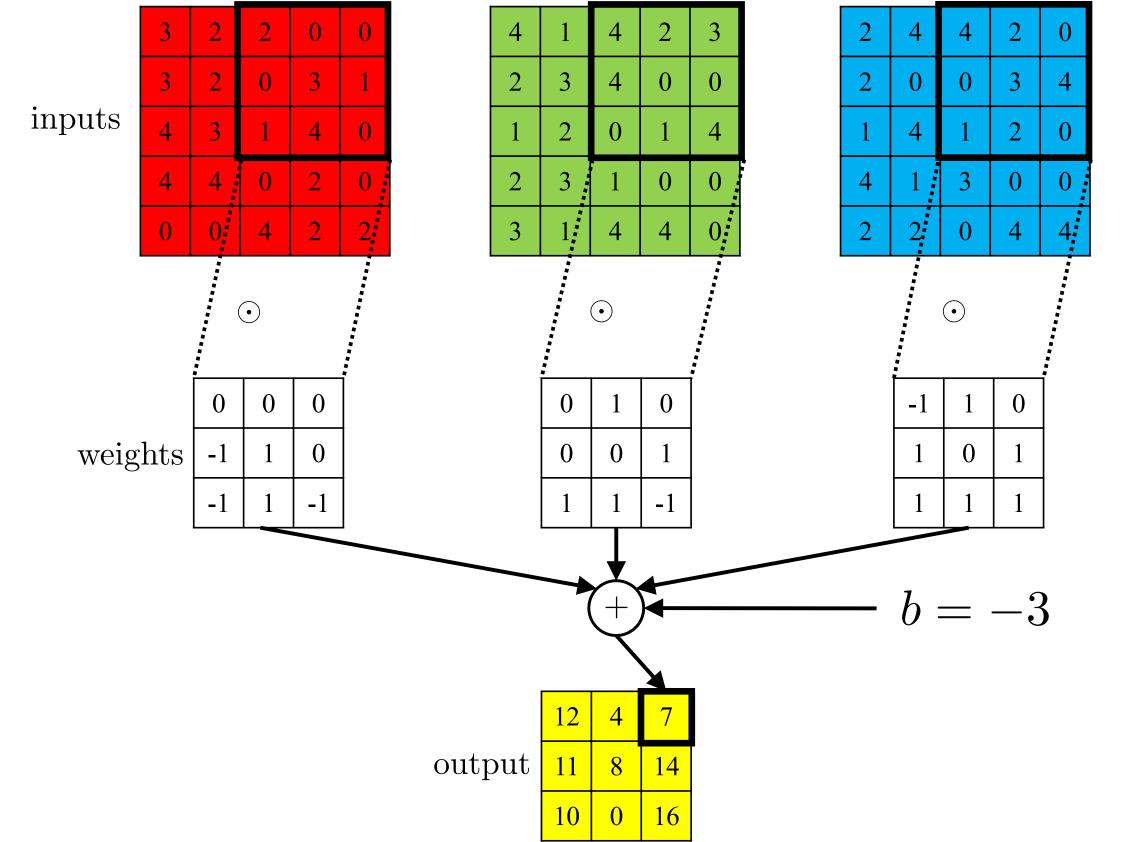


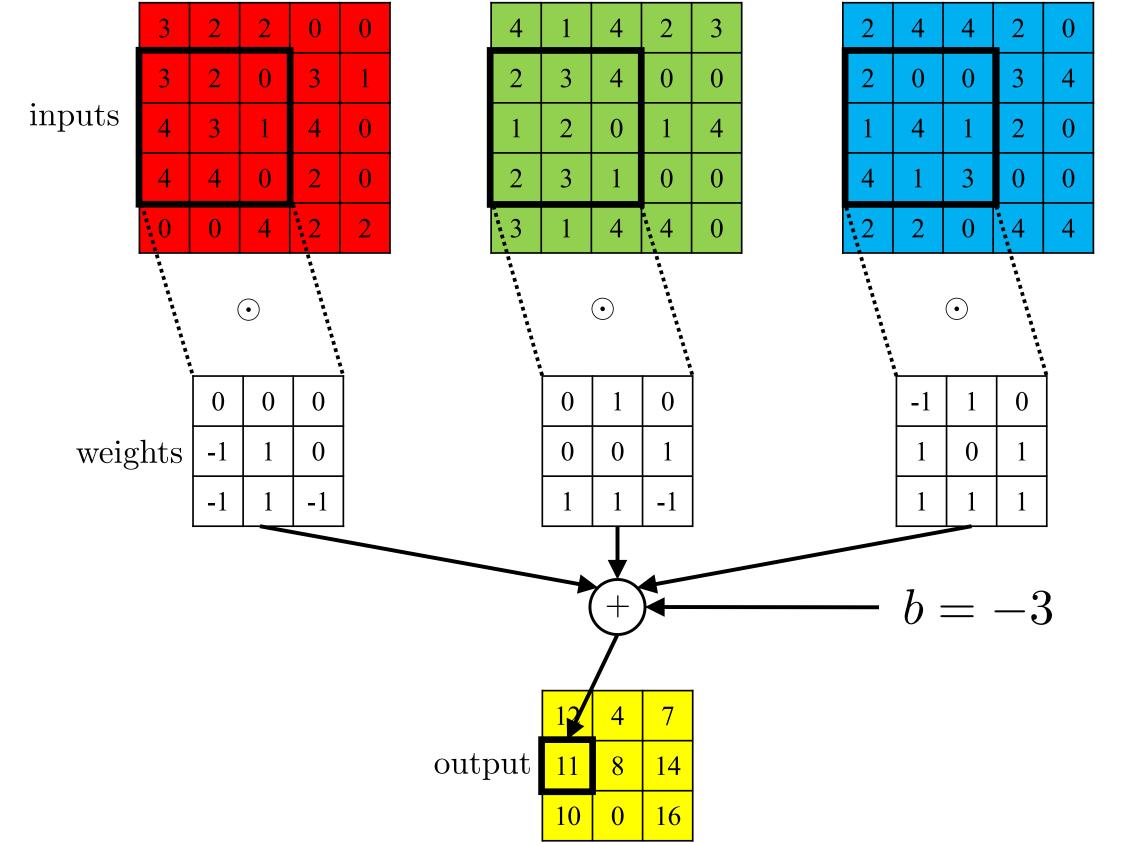


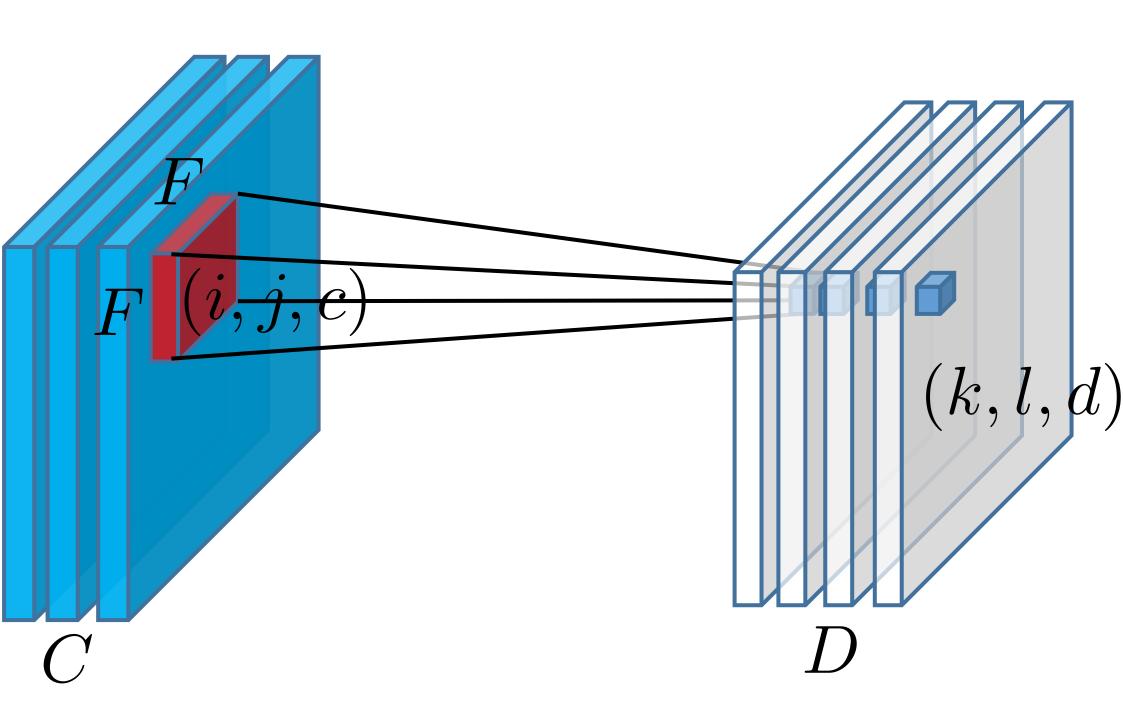


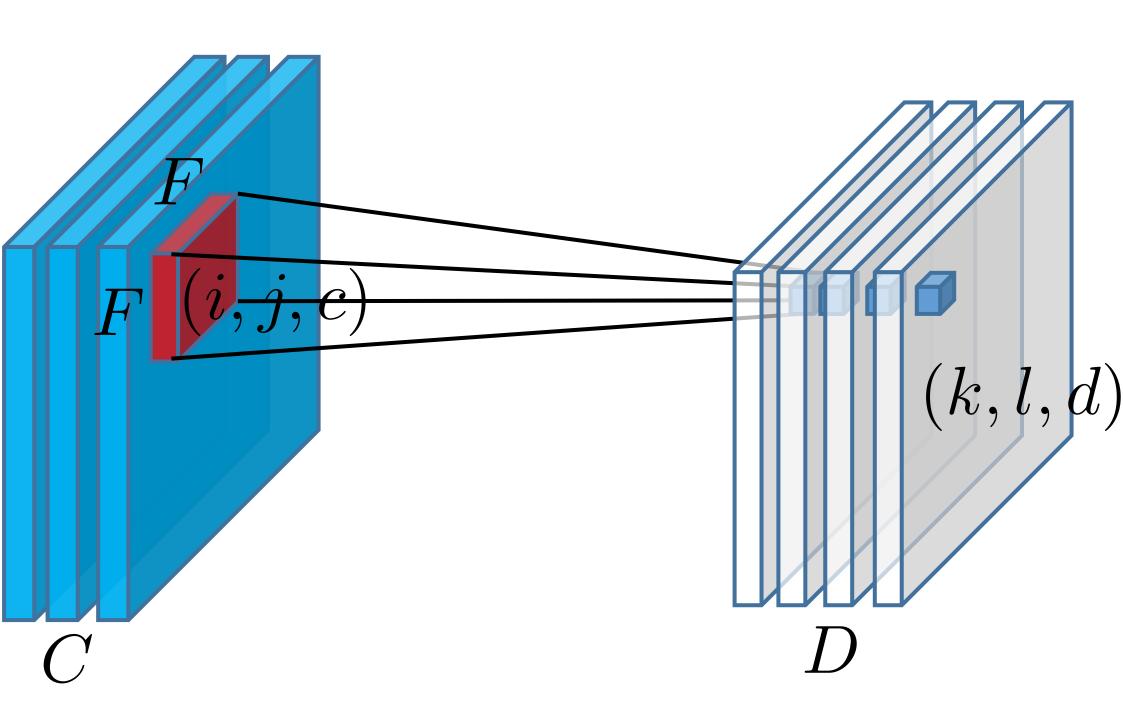


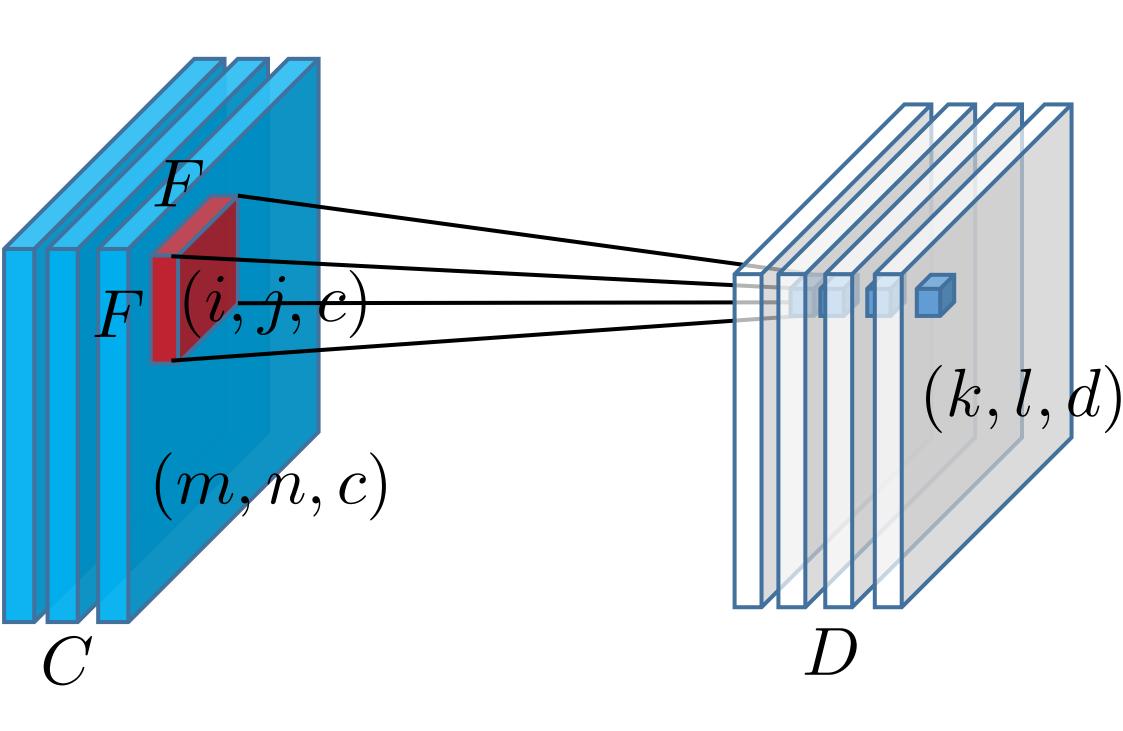












$$S = 1$$

$$S = 2$$

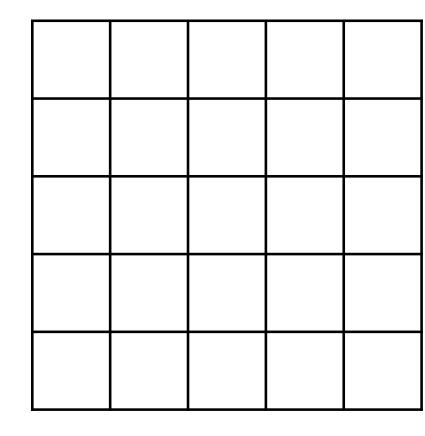
$$S=1$$

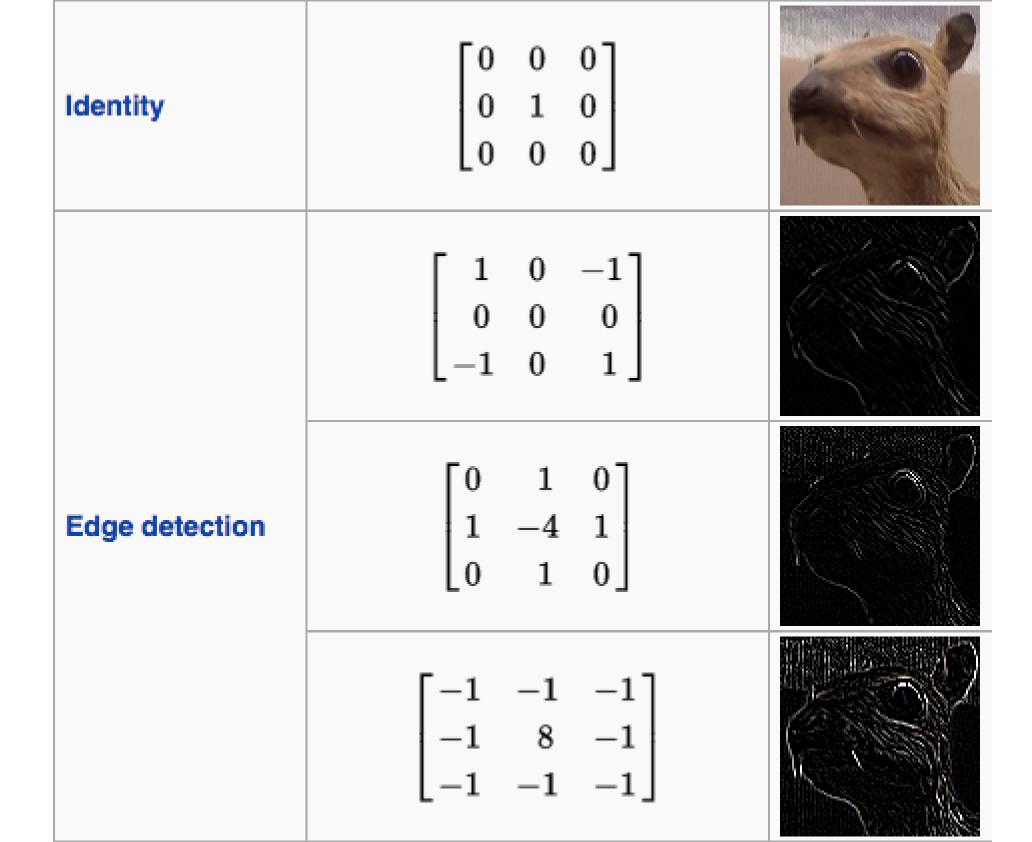
$$S=2$$

$$S=2$$

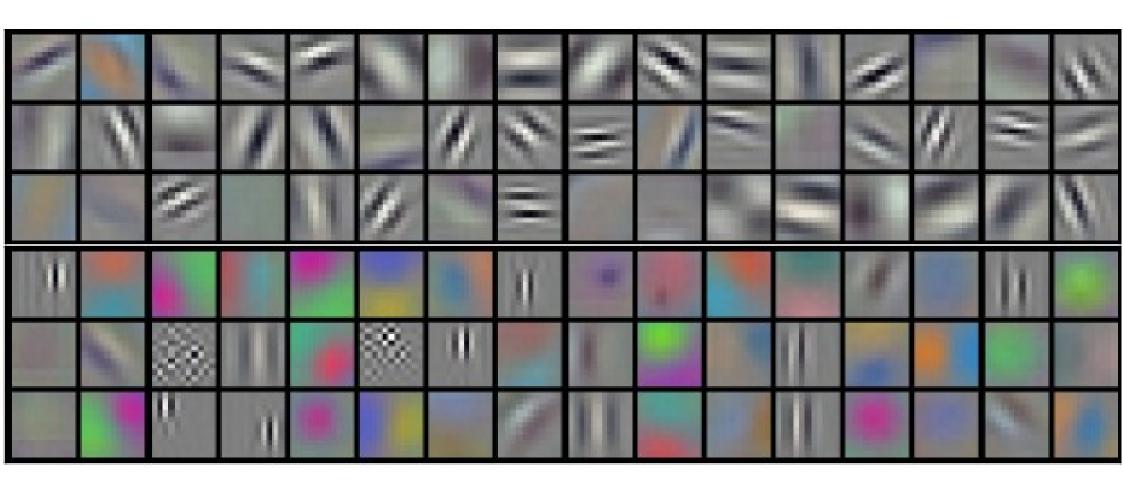
P	=	1,	S	=	1
		•			

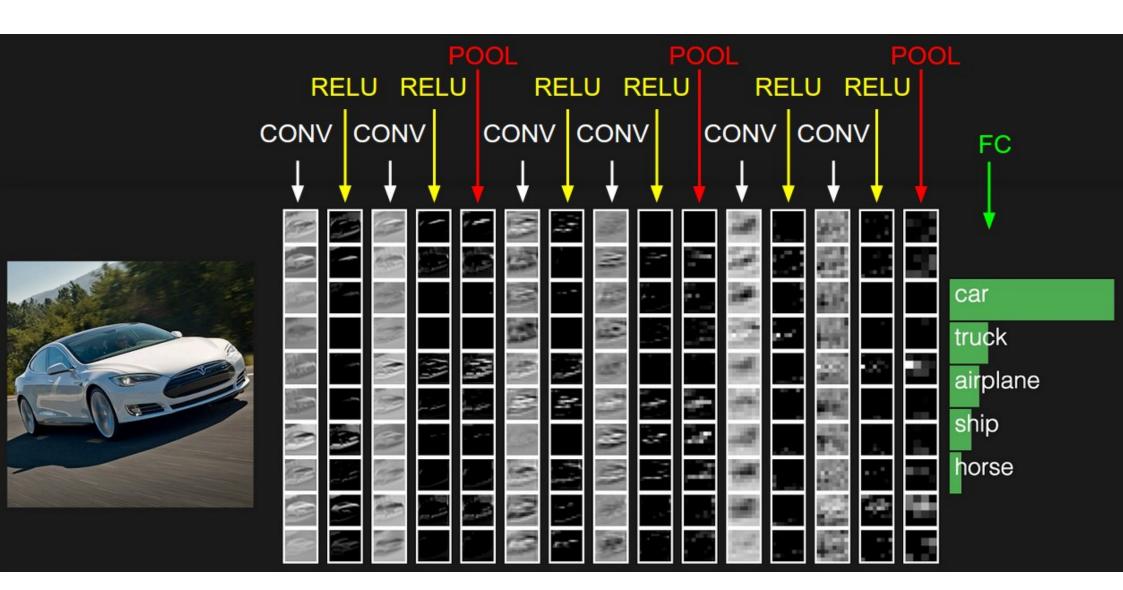
0	0	0	0	0	0
0					0
0					0
0					0
0					0
0	0	0	0	0	0





Sharpen	$\begin{bmatrix} 0 & -1 & 0 \\ -1 & 5 & -1 \\ 0 & -1 & 0 \end{bmatrix}$	
Box blur (normalized)	$\frac{1}{9} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$	
Gaussian blur (approximation)	$\frac{1}{16} \begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix}$	





Input feature map

Output feature map

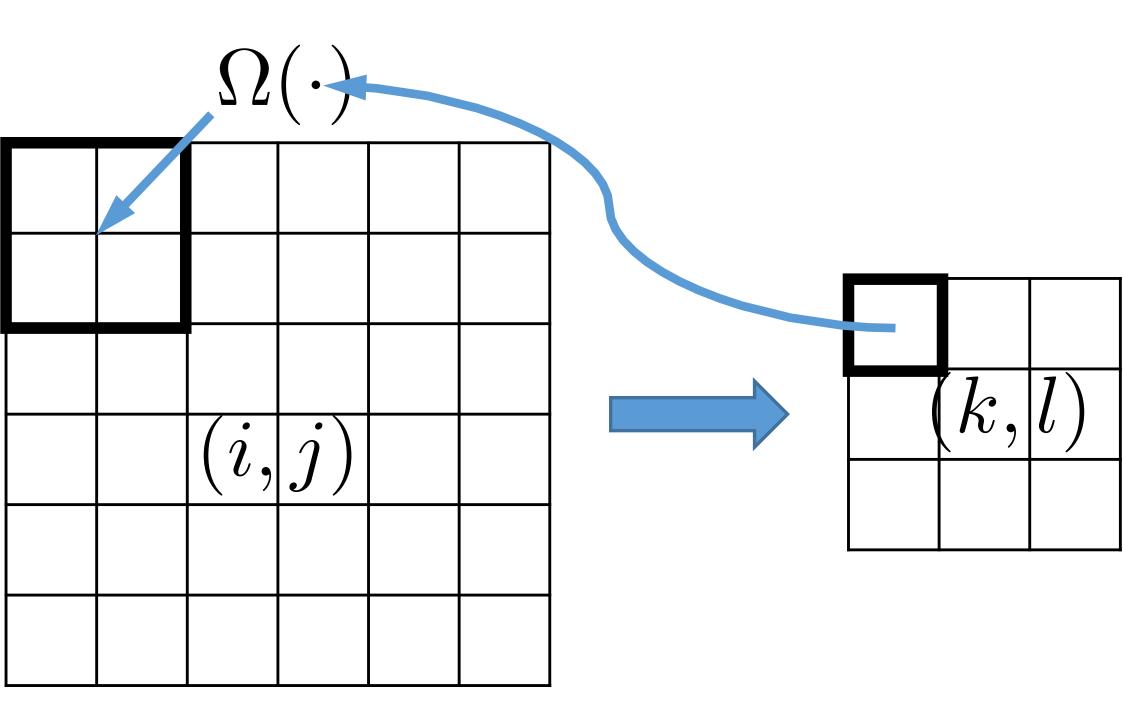
Black = negative; white = positive values

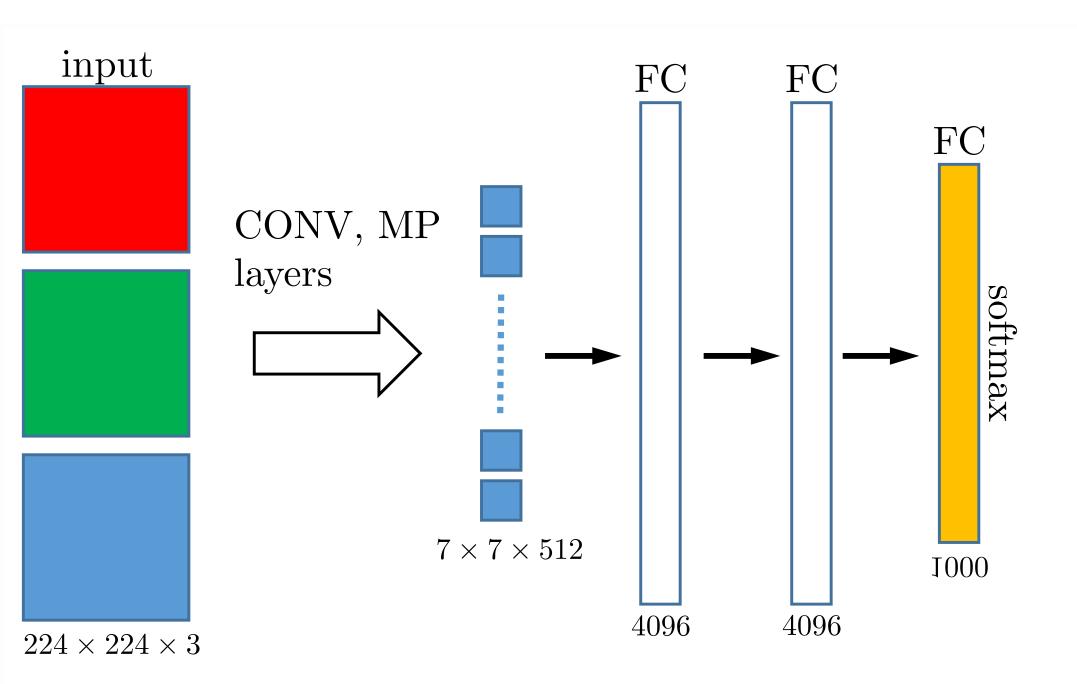
Only non-negative values

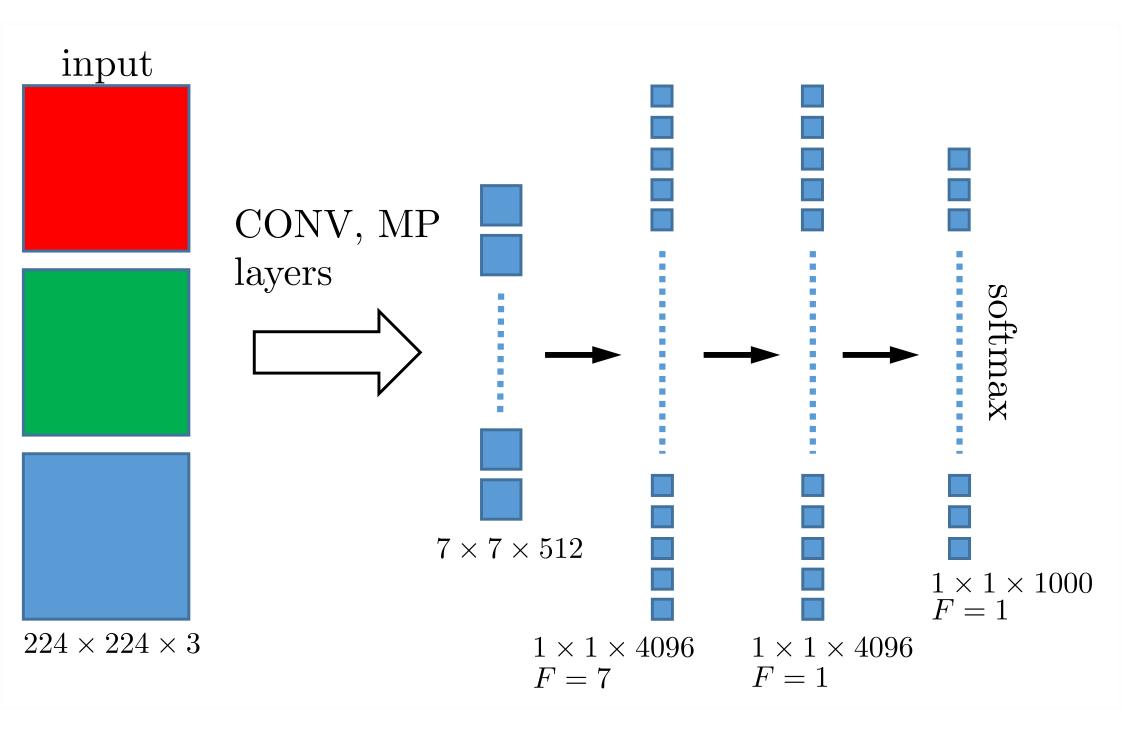
F = 2, S = 2

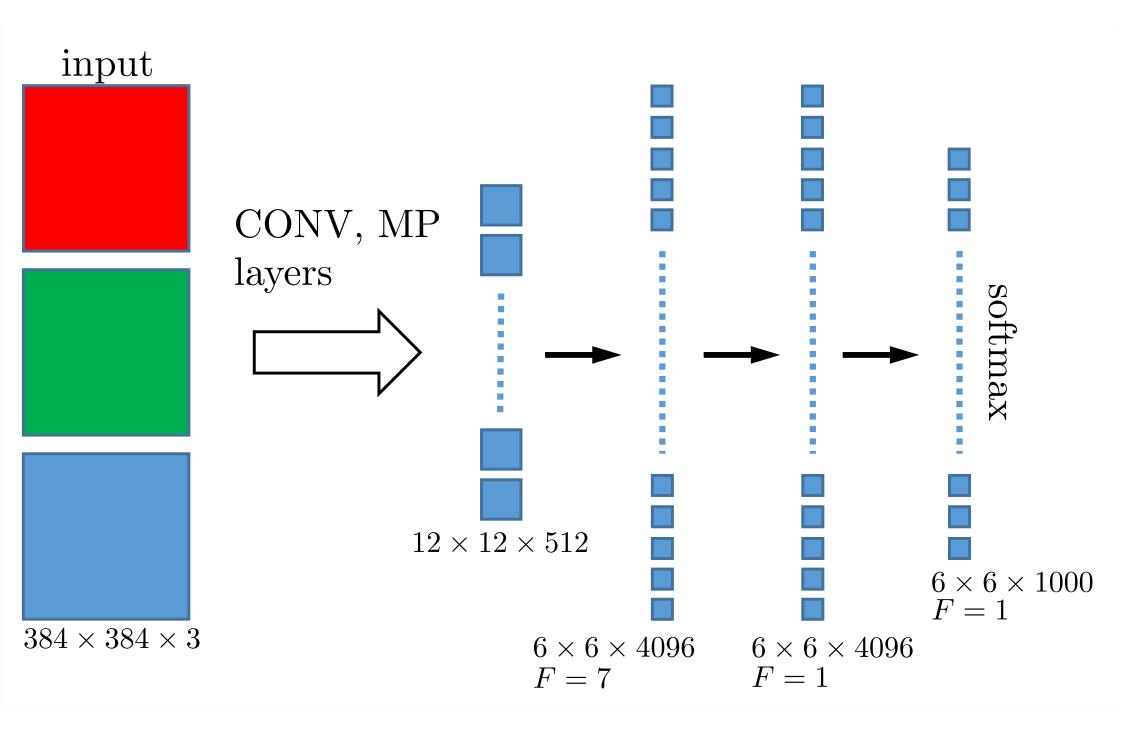
2	2	0	4	3	4
0	0	5	0	4	1
4	5	2	5	1	4
5	2	1	0	2	1
2	3	3	3	5	3
0	3	0	4	0	1

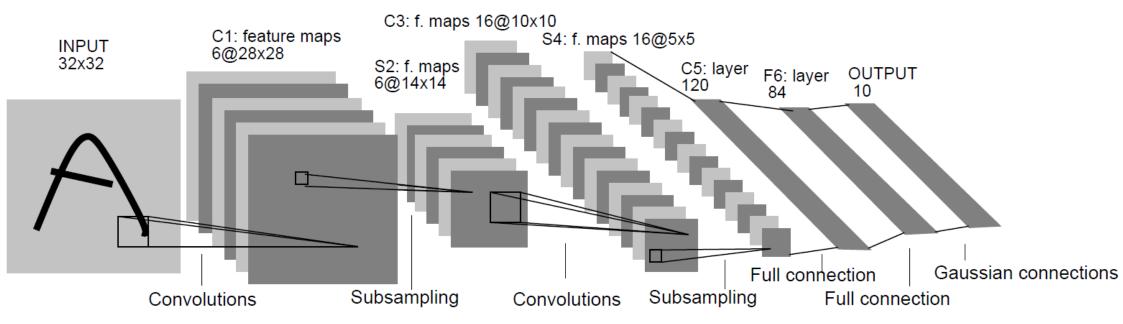
2	5	4
5	5	4
3	4	5

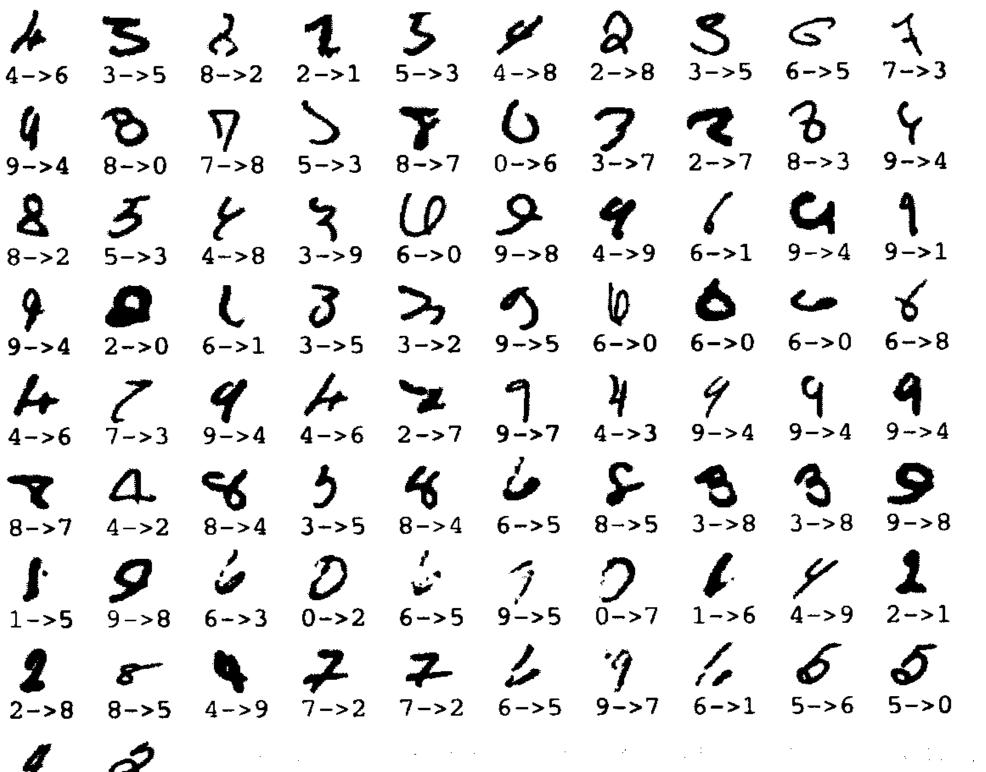




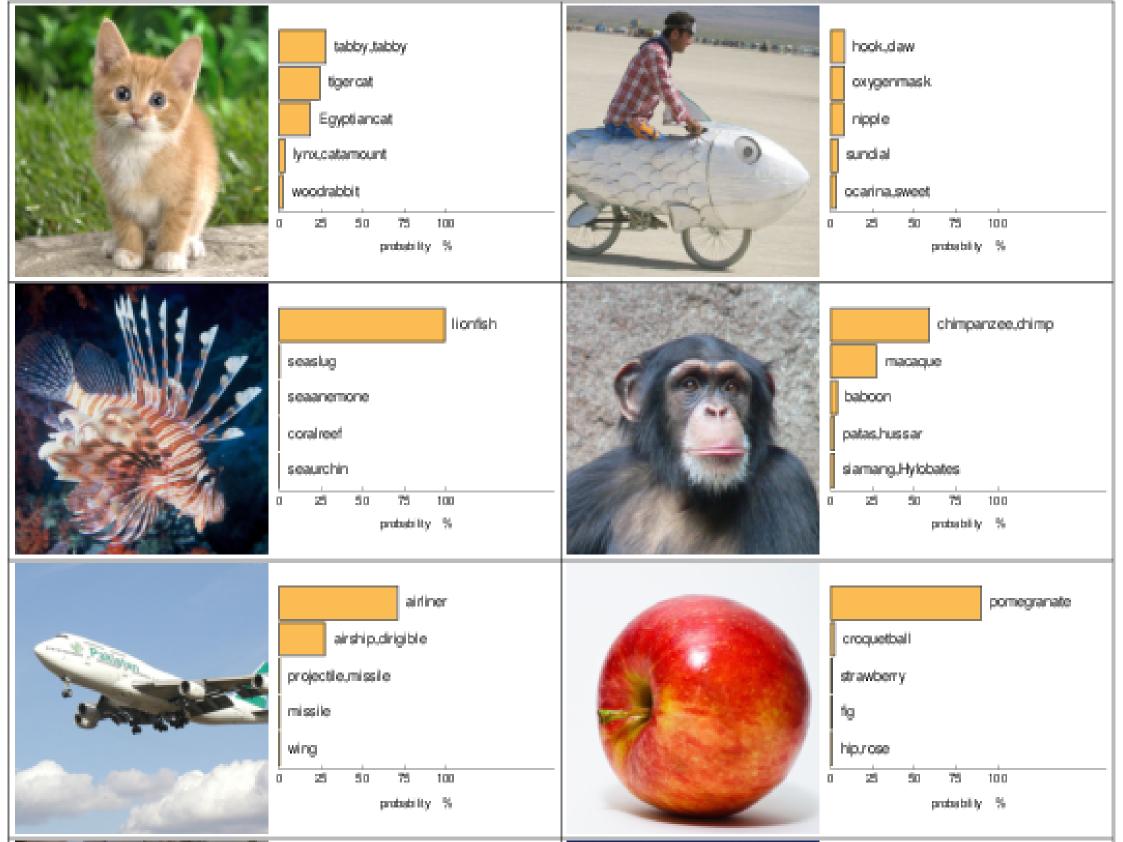








2 4->9 2->8

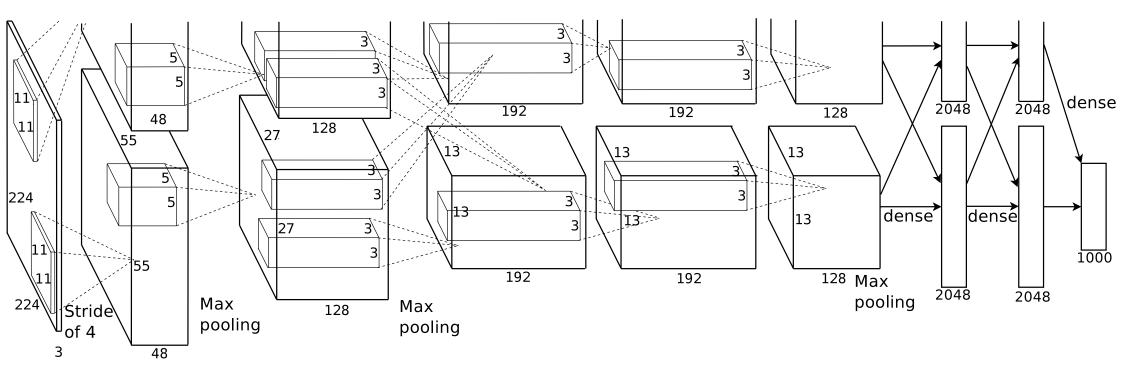


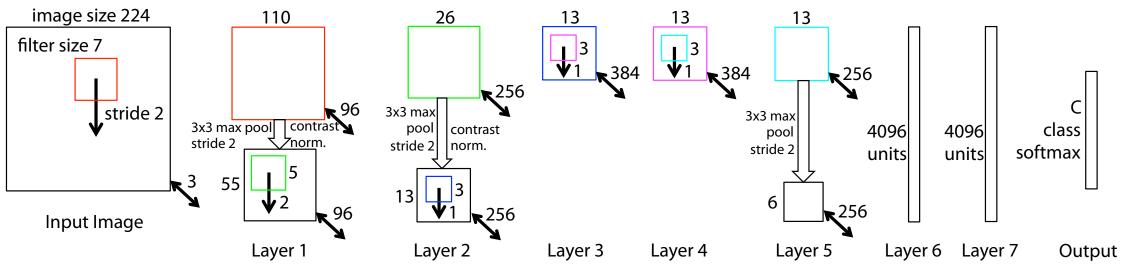


(a) Siberian husky

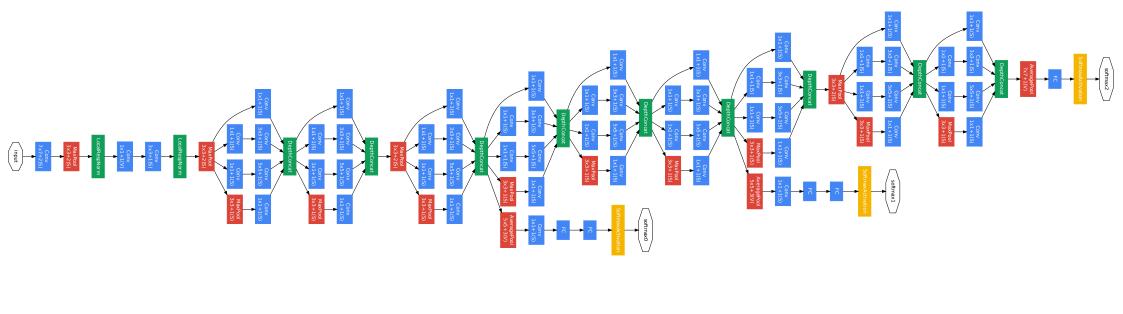


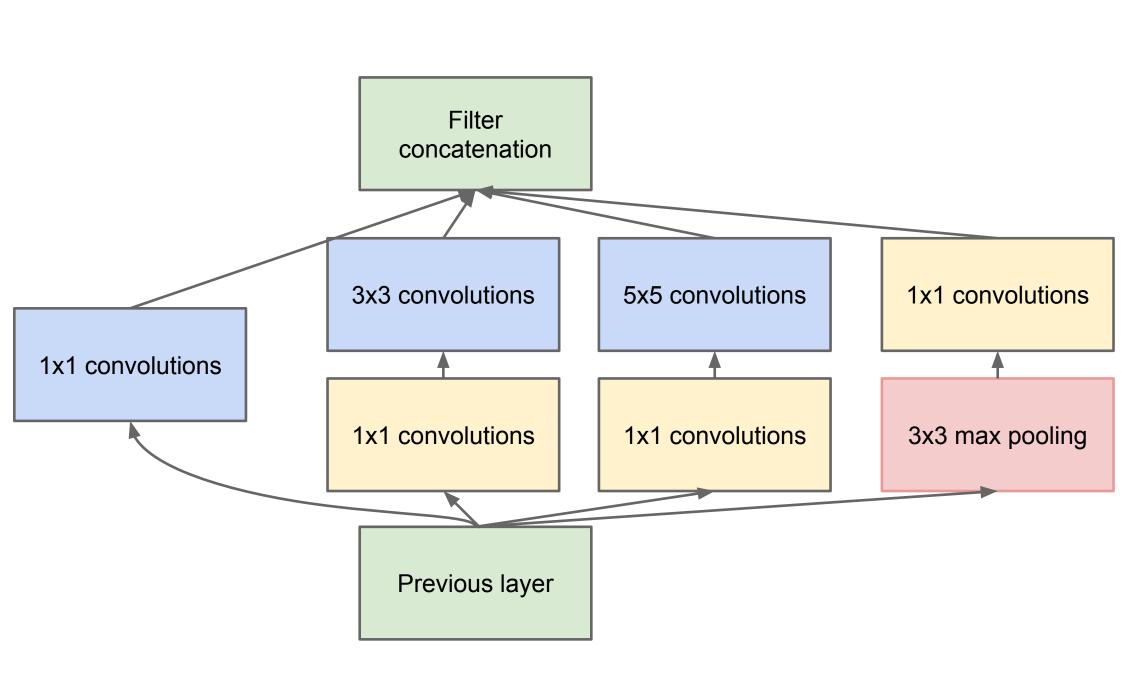
(b) Eskimo dog

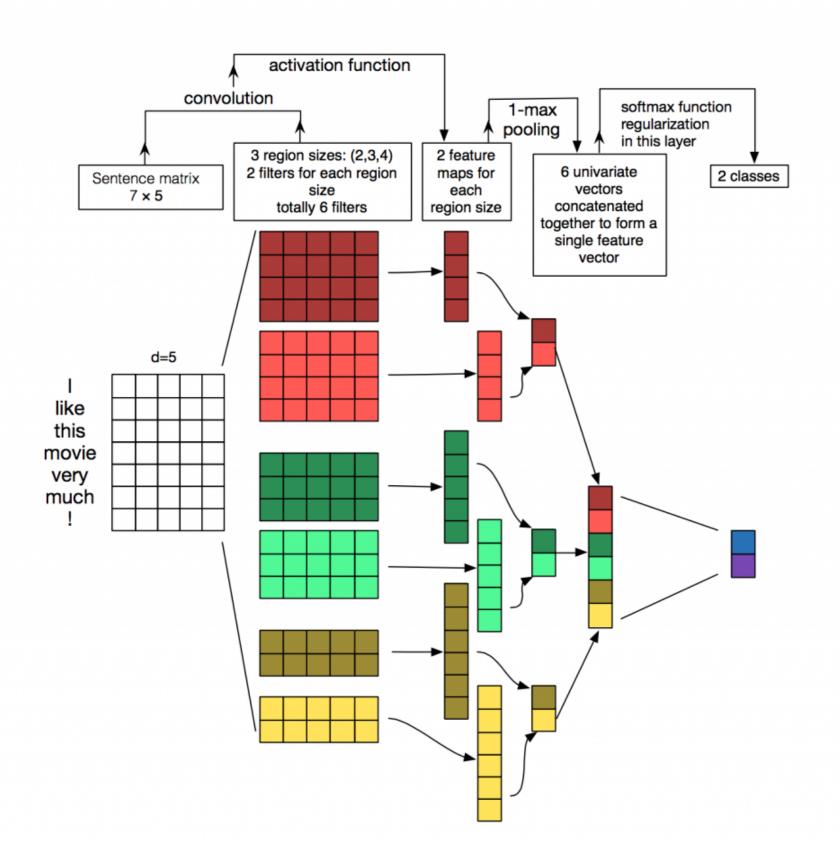


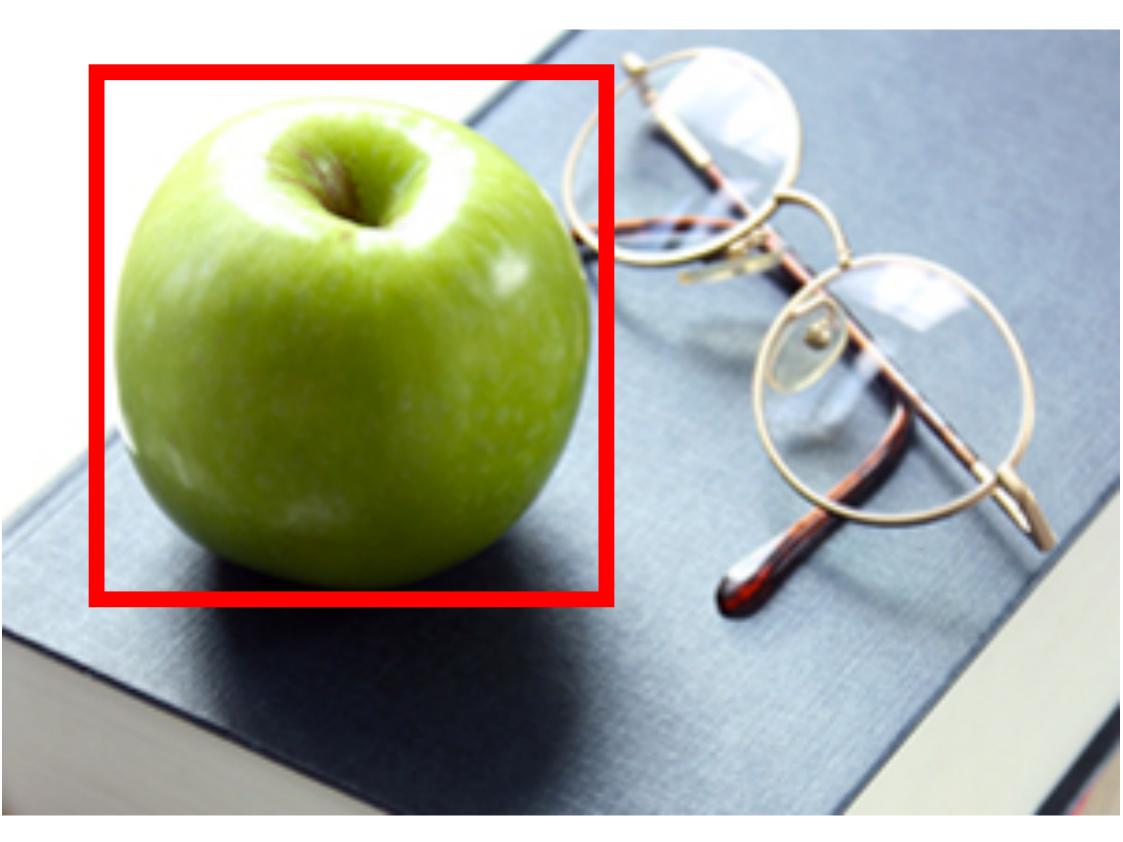


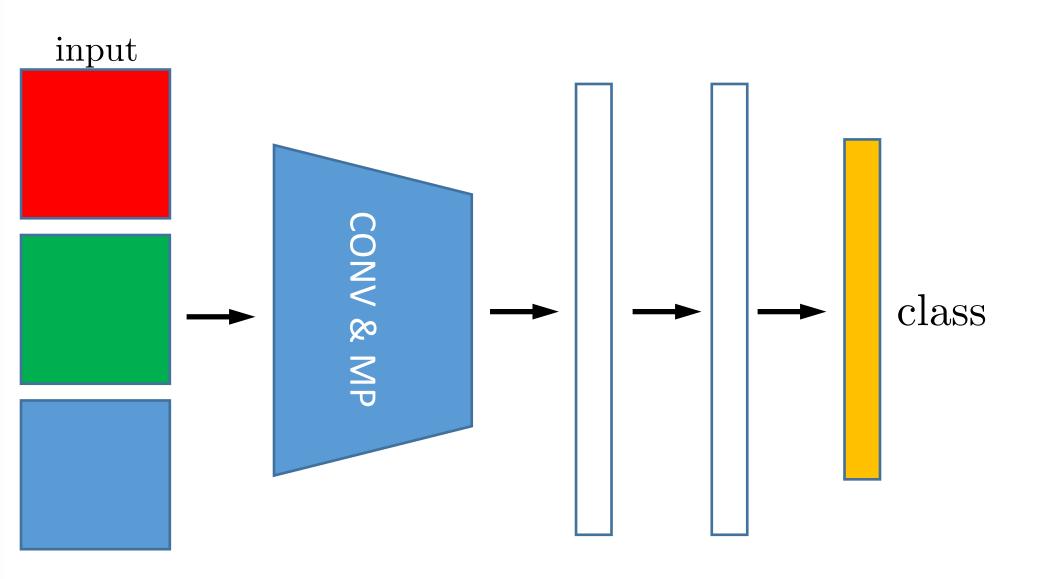
	input	conv3-64	conv3-64	MP	conv3-128	conv3-128	MP	conv3-256	conv3-256	conv3-256	MP	conv3-512	conv3-512	conv3-512	MP	conv3-512	conv3-512	conv3-512	MP	FC - 4096	FC - 4096	FC - 1000	softmax
parameters		1.7k	37k		74k	147k		295k	590k	590k		1.2M	2.4M	2.4M		2.4M	2.4M	2.4M		103M	16.7M	4M	
activations 1	150k	3.2M	3.2M	800k	1.6M	1.6M	400k	800k	800k	800k	200k	400k	400k	400k	100k	100k	100k	100k	25k	4096	4096	1000	1000
	224 × 224 × 3	224 x 224 x 64		112 x 112 x 64	112×112×128		56 x 56 x 128	56 x 56 x 256			28 x 28 x 256	28 × 28 × 512			14×14 512	14 x 14 x 512			7×7×512	1××1×4096	1 × 1 × 4096	1×1×1000	

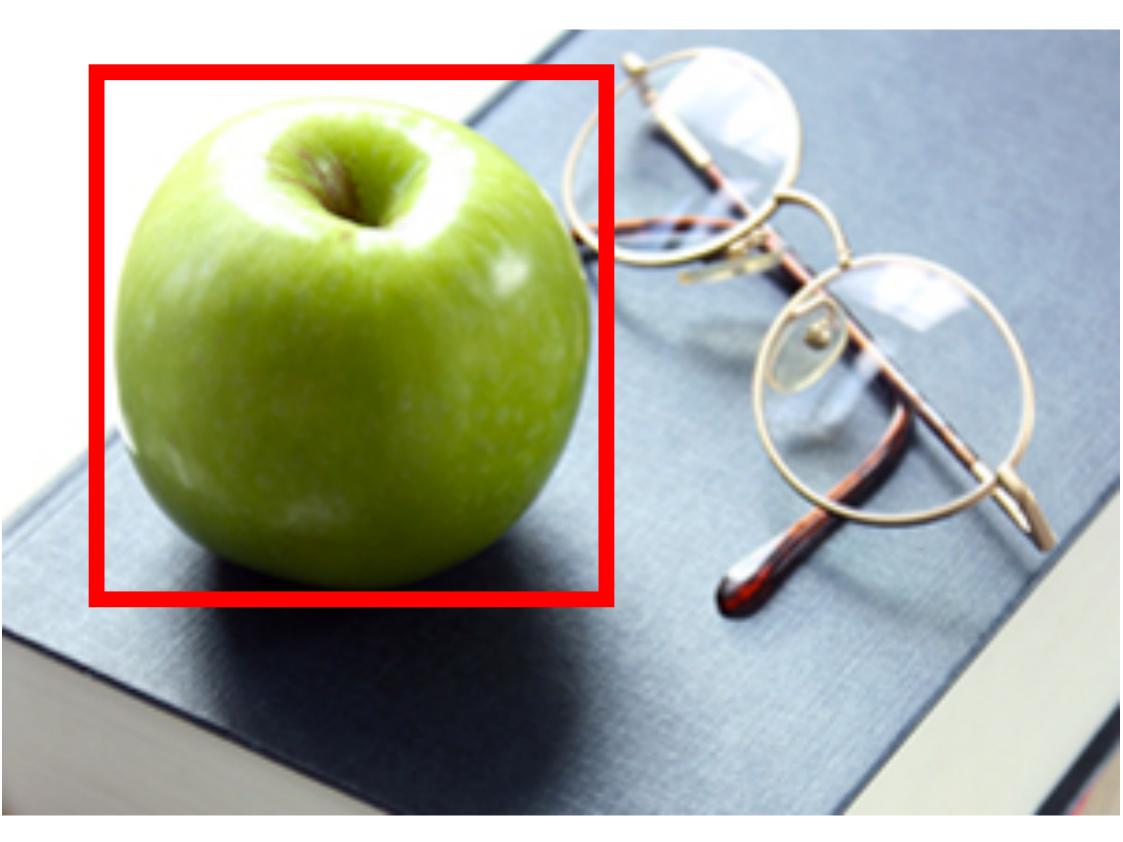


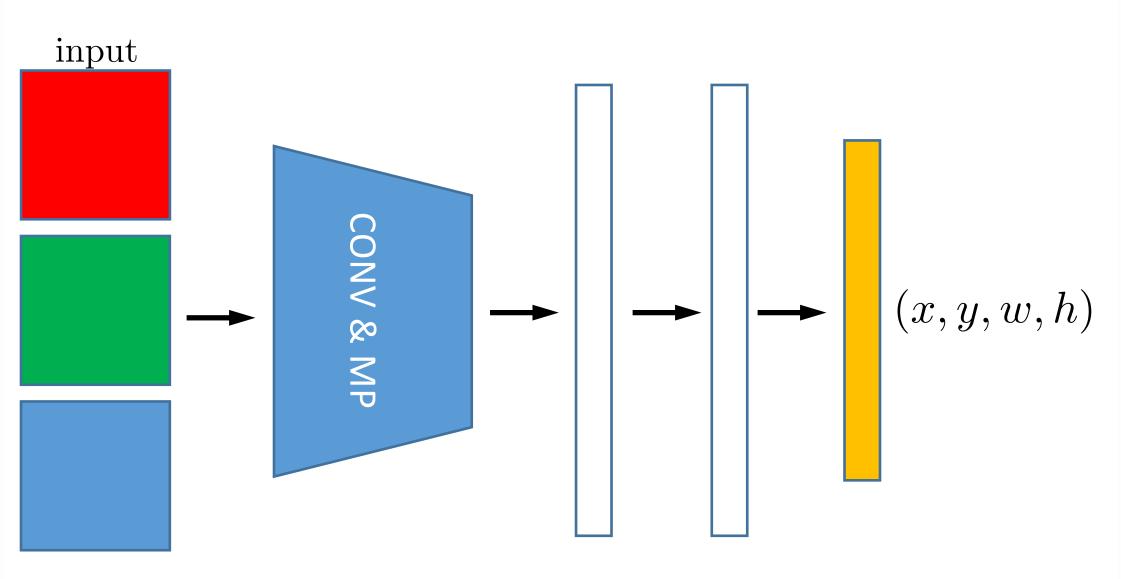


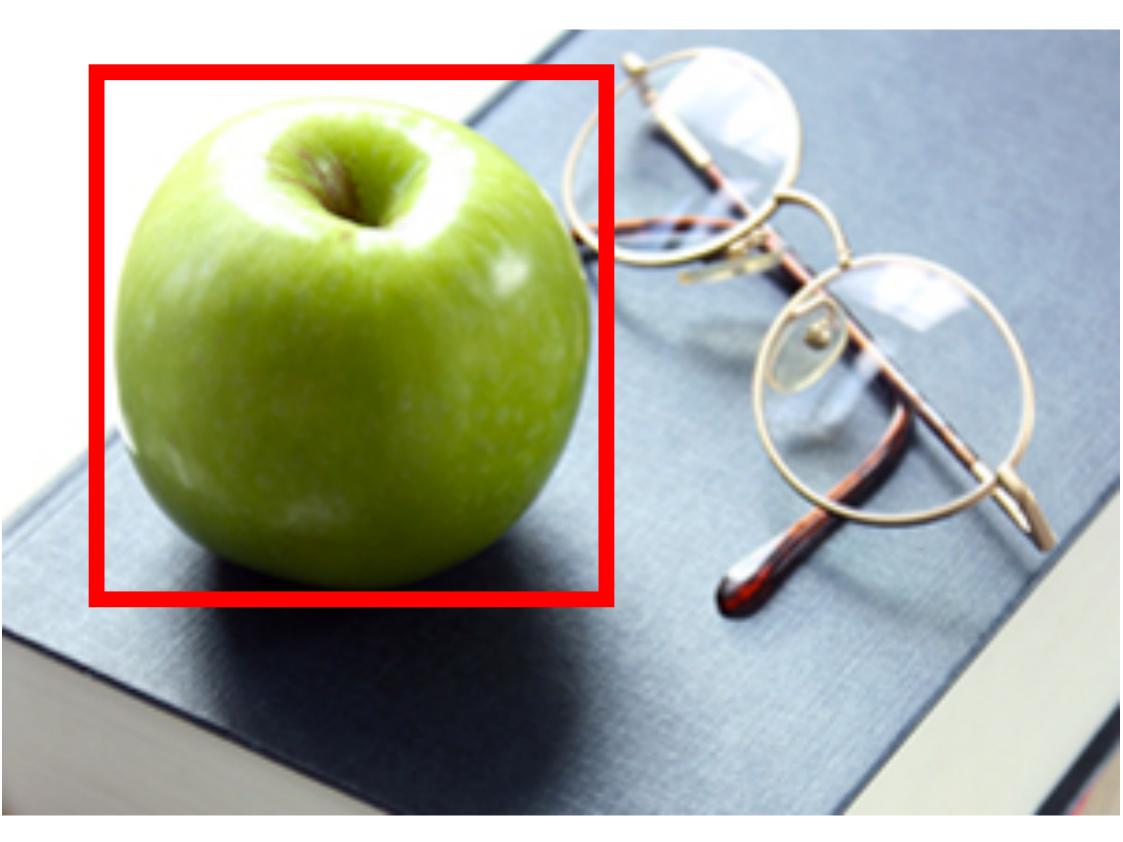


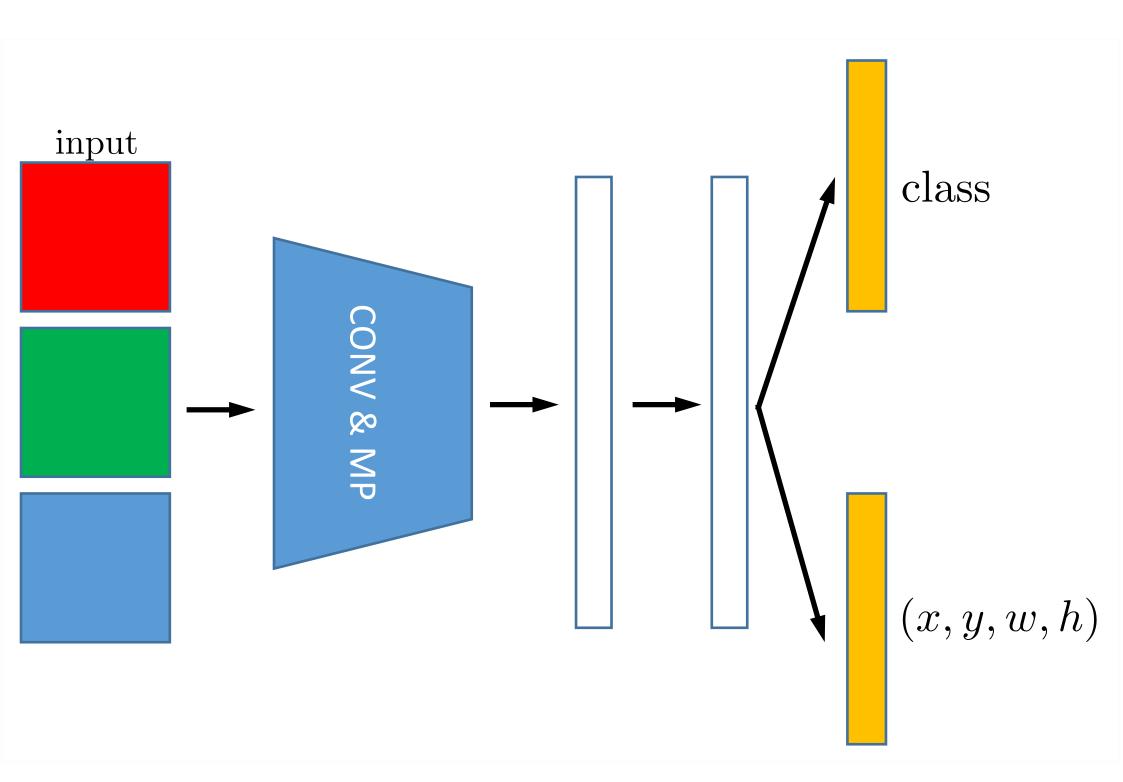


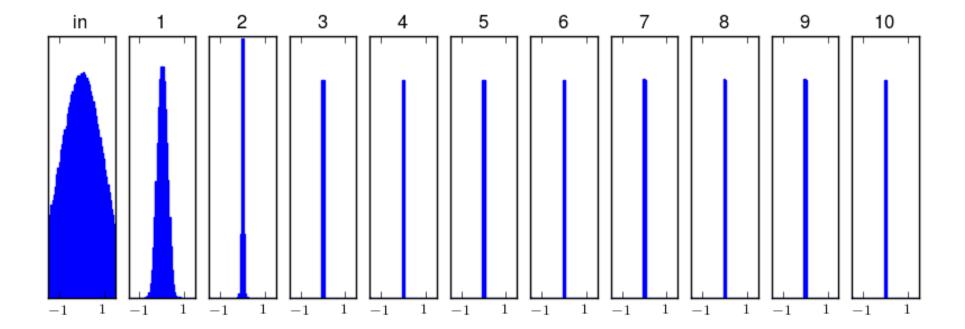


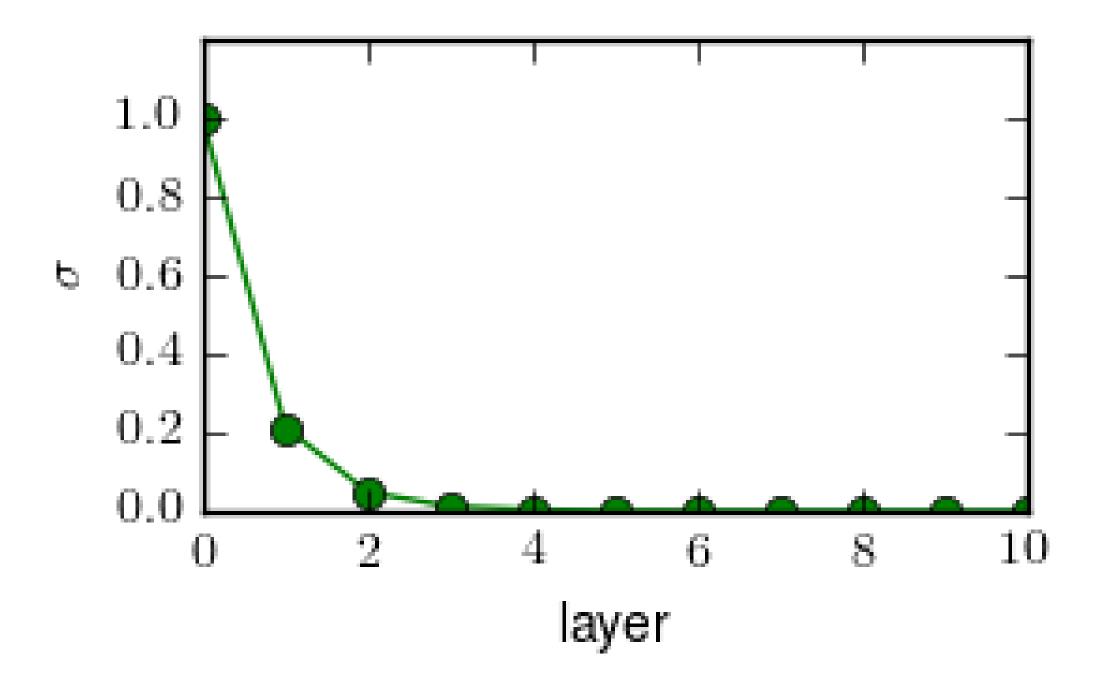


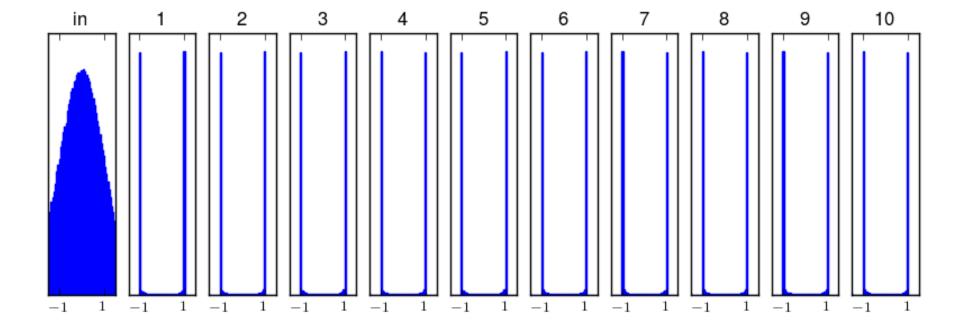


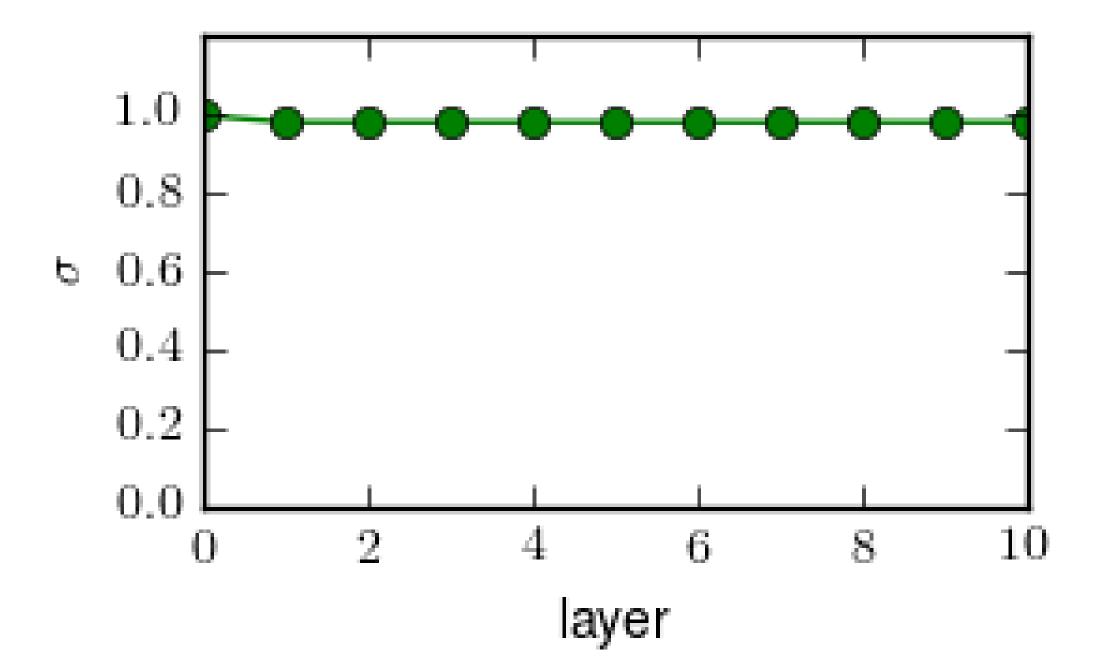


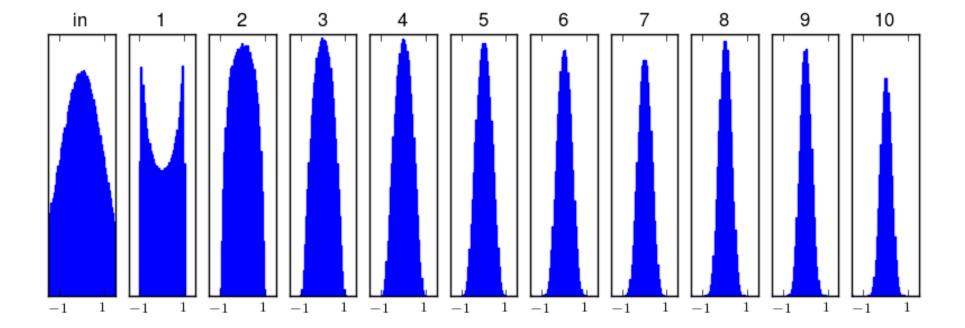


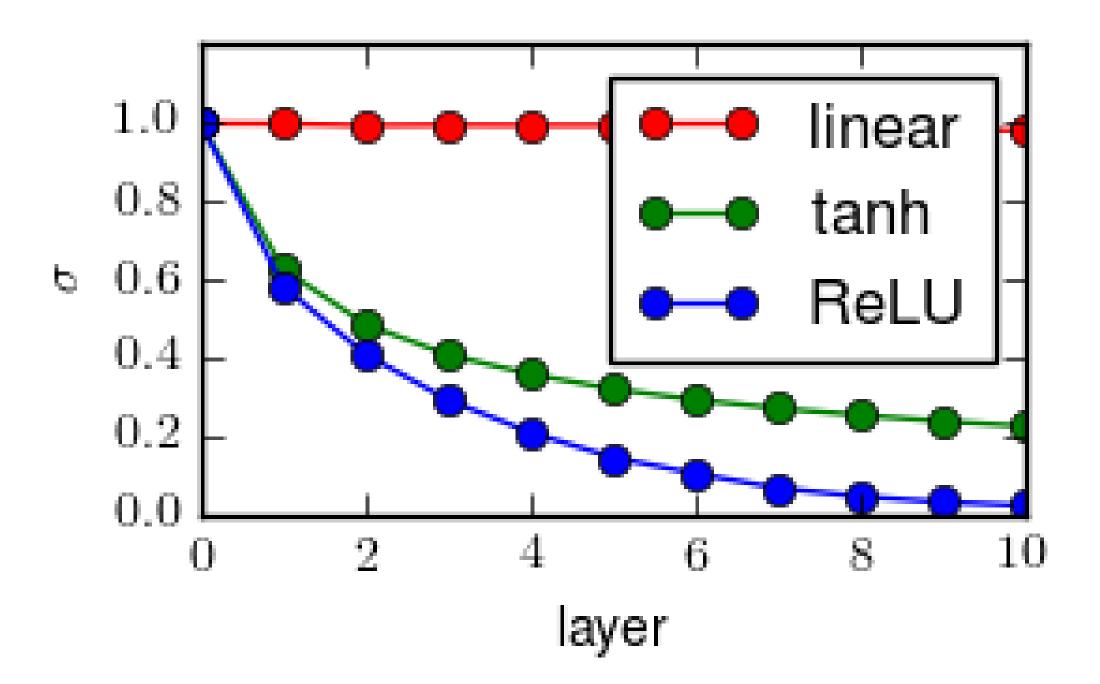


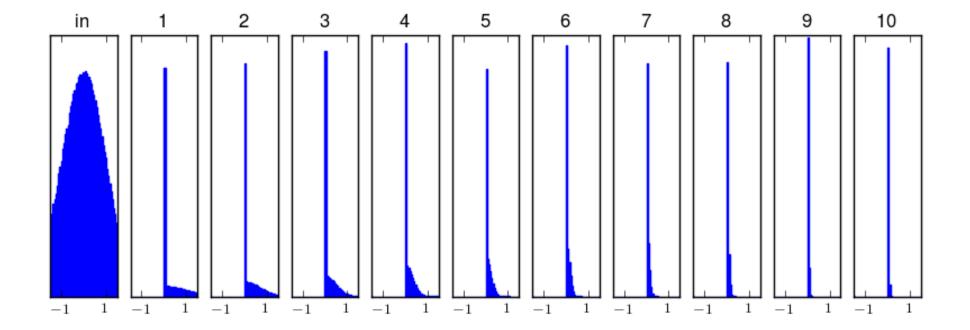


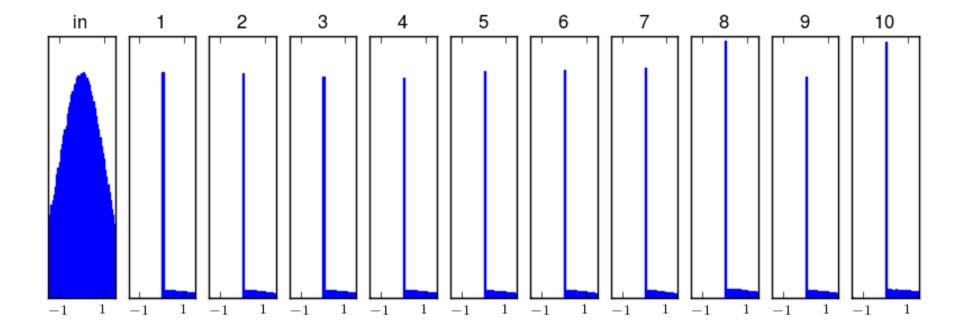


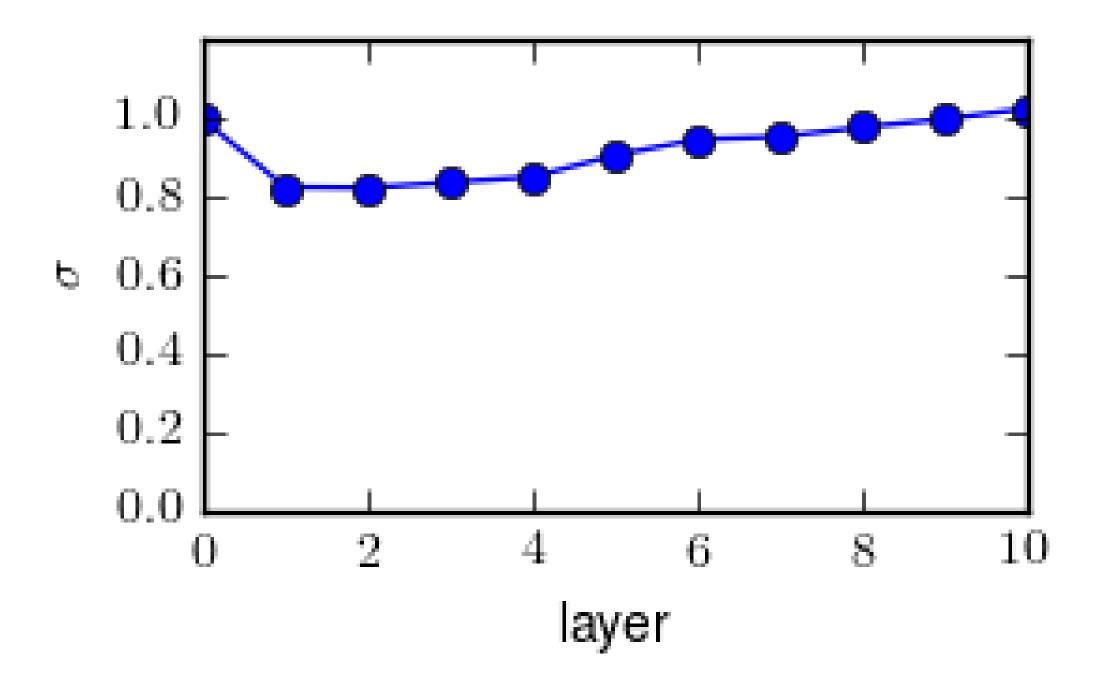




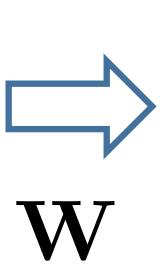








input



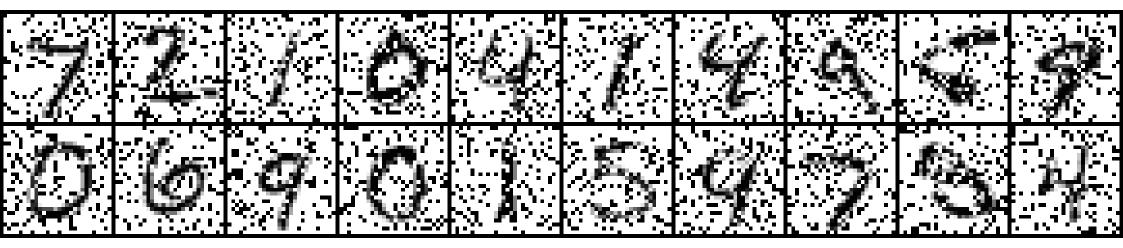
hidden



output

7	2	/	0	4	/	Ч	٥	1,8	9
O	0	9	0	j	U	9	J	\mathcal{O}	4

	2								
0	0	9	0	1	())	9	7	Ø	4

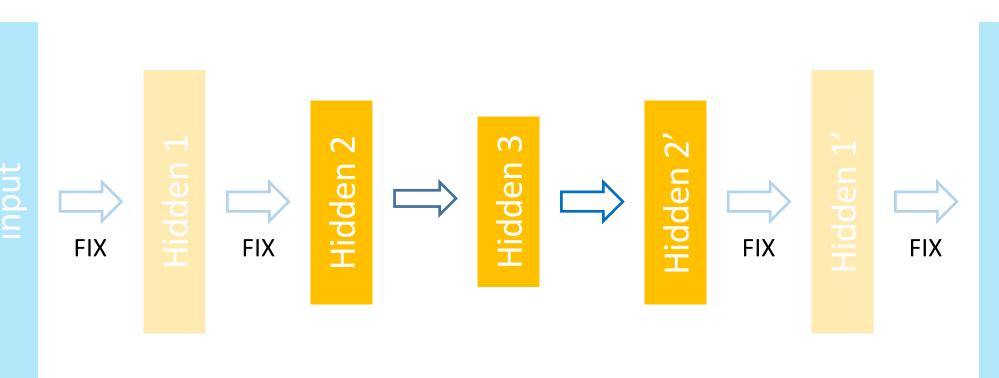


7	2	F	0	14	1	4	4	5	9
3	6	9	0	-	3	4	4	(3)	1



Hidden 1









Hidden 1



Hidden 2



Hidden 3



Hidden 2'



Hidden 1'





Hidden 1



Hidden 2



Hidden 3



Classifier