Introduction to Neural Networks

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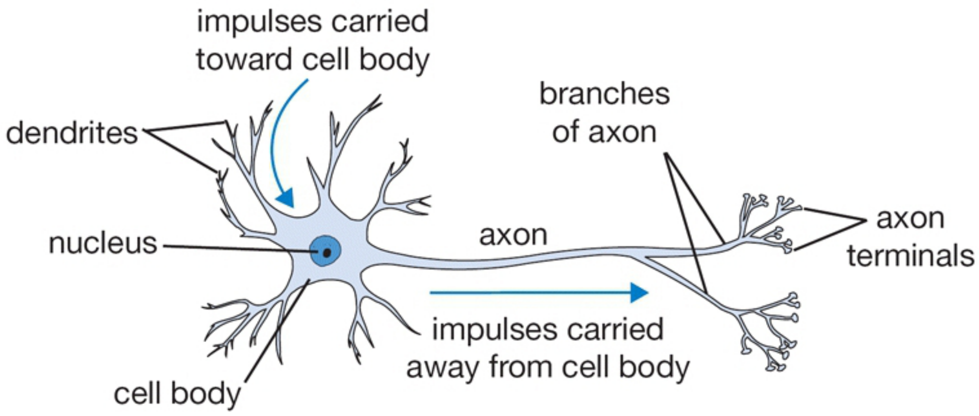
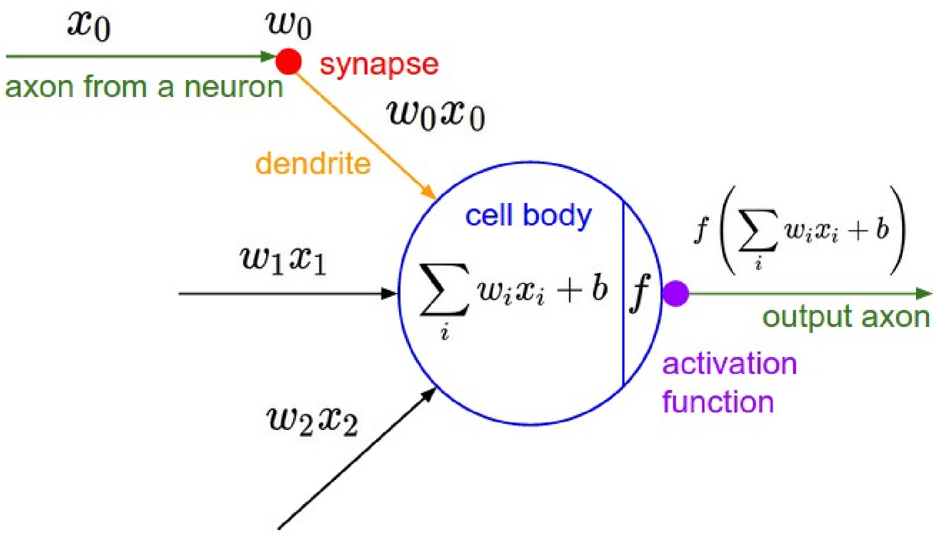
Biological motivation

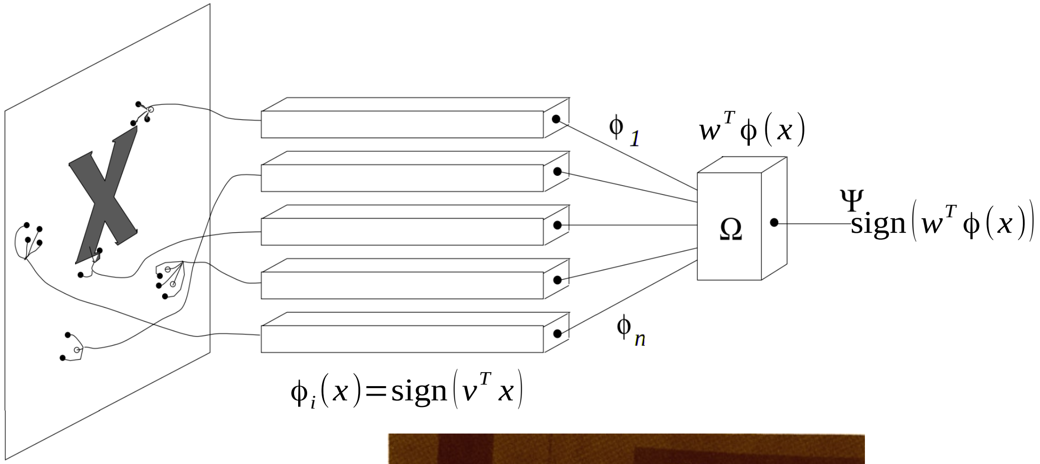
- Neuron is basic computational unit of the brain
  - about 10^11 neurons in human brain
- Simplified neuron model as linear threshold unit (McCulloch & Pitts, 1943)
  - Firing rate of electrical spikes modeled as continuous output quantity
  - Connection strength modeled by multiplicative weight
  - Cell activation given by sum of inputs
  - Output is non linear function of activation
- Basic component in neural circuits for complex tasks



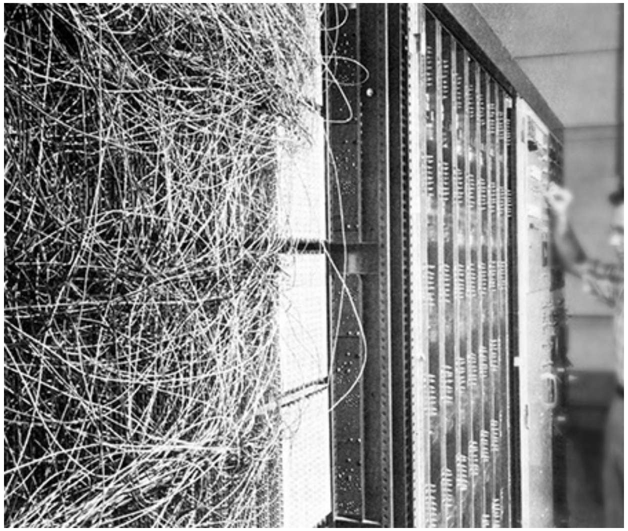


1957: Rosenblatt's Perceptron

- Binary classification based on sign of generalized linear function
  - Weight vector w learned using special purpose machines
  - Fixed associative units in first layer, sign activation prevents learning



20x20 pixel sensor



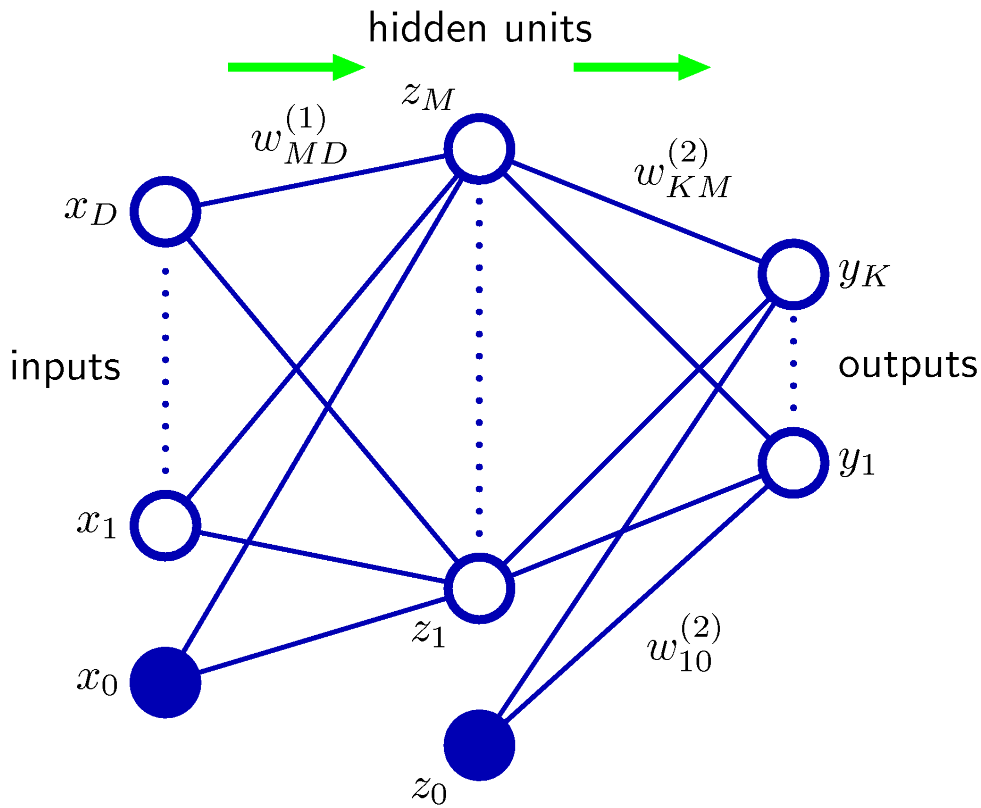
Random wiring of associative units

Multi-Layer Perceptron (MLP)

- Instead of using a generalized linear function, learn the features as well
- Each unit in MLP computes
  - Linear function of features in previous layer
  - Followed by scalar non-linearity
- Do **not** use the “step” non-linear activation function of original perceptron

$$z_j = h\left(\sum_i x_i w_{ij}^{(1)}\right)$$
$$z = h\left(W^{(1)} x\right)$$

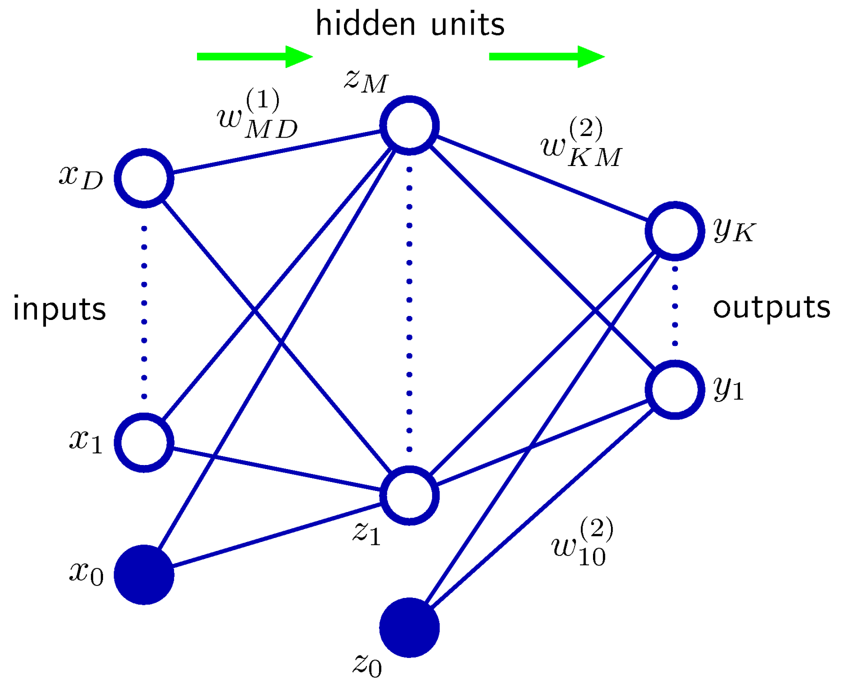
$$y_k = \sigma\left(\sum_j z_j w_{jk}^{(2)}\right)$$
$$y = \sigma\left(W^{(2)} z\right)$$



Multi-Layer Perceptron (MLP)

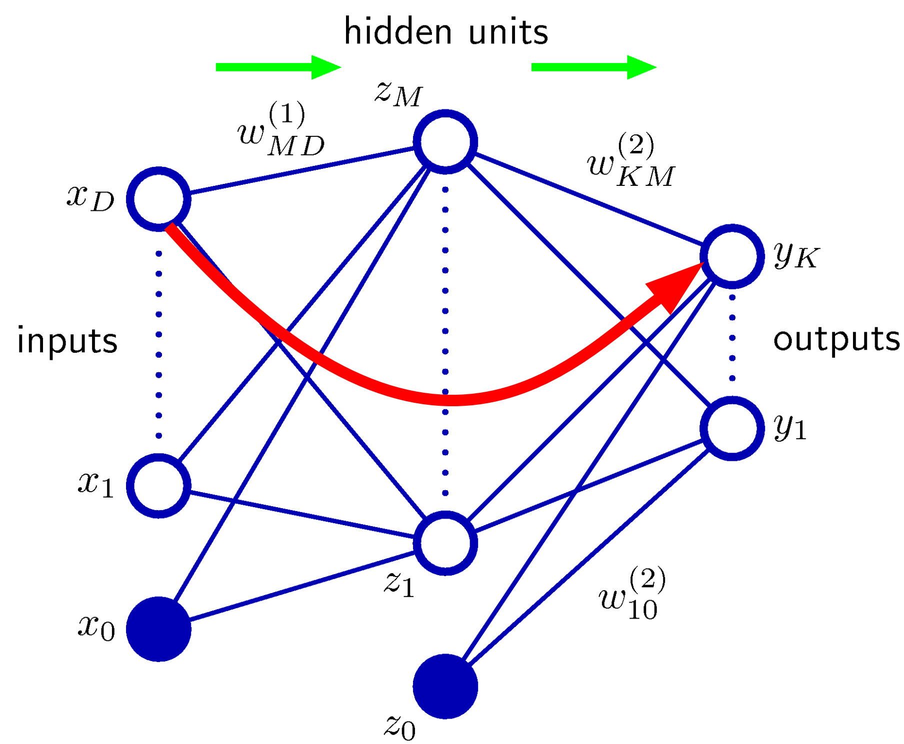
- Linear activation function leads to composition of linear functions
  - Remains a linear model, layers just induce a certain factorization

- Two-layer MLP can uniformly approximate any continuous function on a compact input domain to arbitrary accuracy provided the network has a sufficiently large number of hidden units
  - Holds for many non-linearities, but not for polynomials



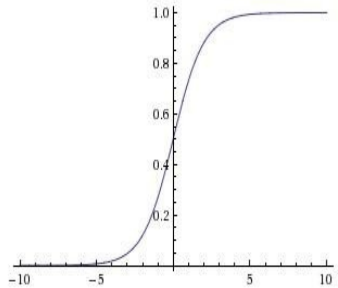
Feed-forward neural networks

- MLP Architecture can be generalized
  - More than two layers of computation
  - Skip-connections from previous layers
- Feed-forward nets are restricted to directed acyclic graphs of connections
  - Ensures that output can be computed from the input in a single feed-forward pass from the input to the output
- Important issues in practice
  - Designing network architecture
    - Nr nodes, layers, non-linearities, etc
  - Learning the network parameters
    - Non-convex optimization
  - Sufficient training data
    - Data augmentation, synthesis

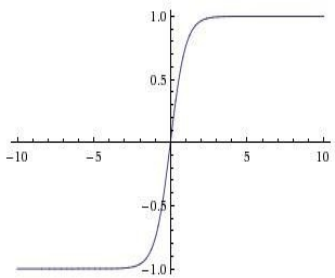


Activation functions

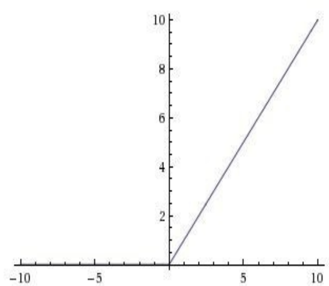
Sigmoid $1/(1+e^{-x})$



tanh

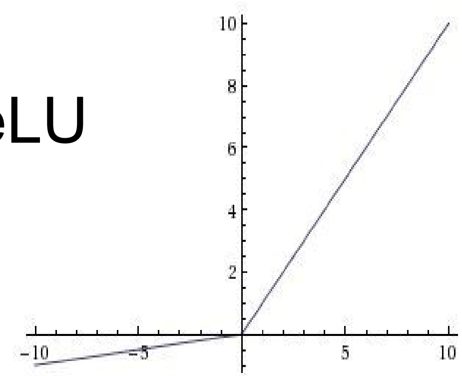


ReLU $\max(0, x)$

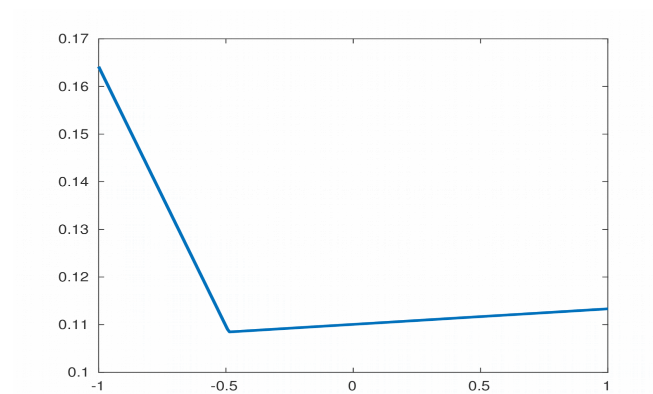


Leaky ReLU

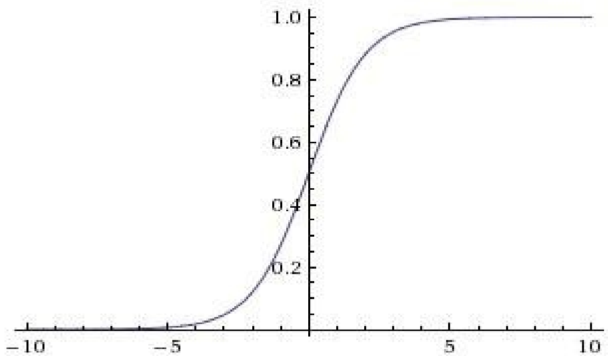
$\max(\alpha x, x)$



Maxout $\max(w_1^T x, w_2^T x)$

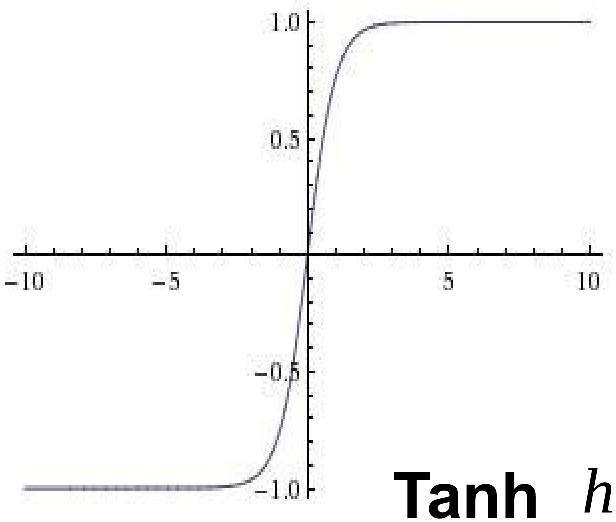


Activation Functions



- Squashes reals to range [0,1]
- Tanh outputs centered at zero: [-1, 1]
- Smooth step function
- Historically popular since they have nice interpretation as a saturating "firing rate" of a neuron

Sigmoid $\sigma(x) = 1/(1+e^{-x})$



1. Saturated neurons "kill" the gradients, need activations to be exactly in right regime to obtain non-constant output
2. exp() is a bit compute expensive

Tanh $h(x) = 2\sigma(x) - 1$

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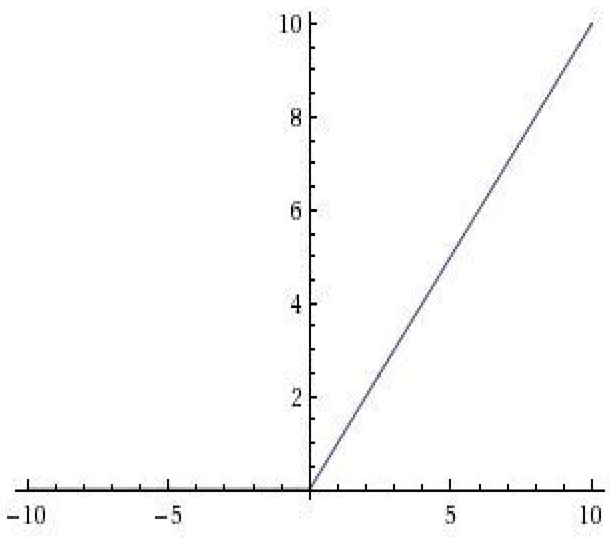
Activation Functions



ReLU
(Rectified Linear Unit)

Computes **f(x) = max(0,x)**

- Does not saturate (in +region)
- Very computationally efficient
- Converges much faster than sigmoid/tanh in practice (e.g. 6x)
- Most commonly used today

[Nair & Hinton, 2010]

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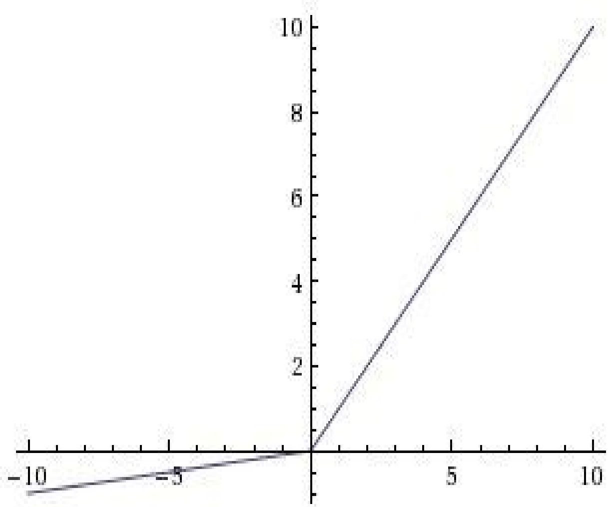
Activation Functions



Leaky ReLU

- Does not saturate: will not "die"
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)

$$f(x) = \max(0.01x, x)$$

[Mass et al., 2013] [He et al., 2015]

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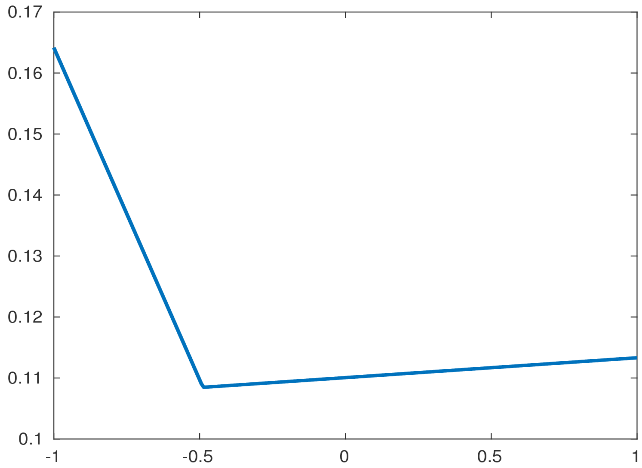
Activation Functions



Maxout

$$\max\left(w_1^T x, w_2^T x\right)$$

- Does not saturate: will not "die"
- Computationally efficient

- Maxout networks can implement ReLU networks and vice-versa
- More parameters per node

[Goodfellow et al., 2013]

Training feed-forward neural network

- Non-convex optimization problem in general
  - Typically number of weights is very large (millions in vision applications)
  - Seems that many different local minima exist with similar quality

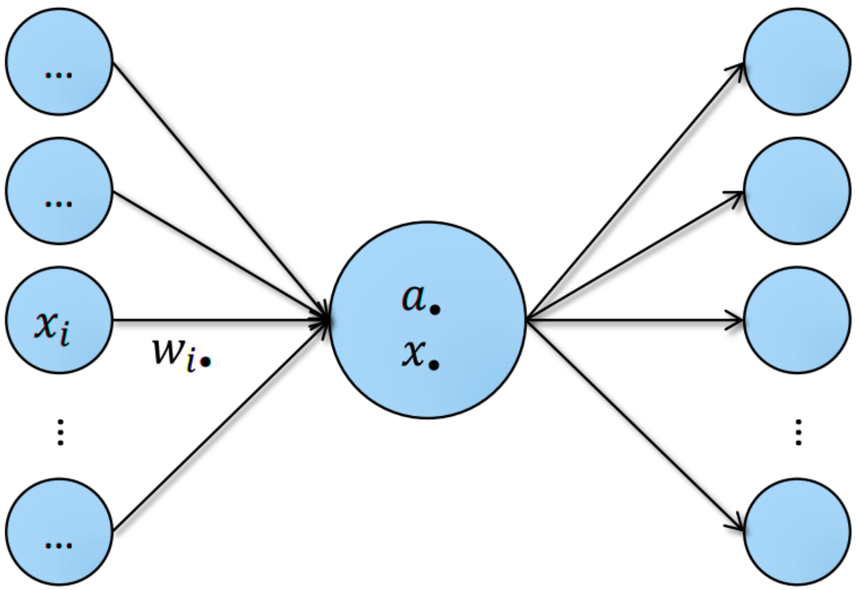
$$\frac{1}{N}\sum_{i=1}^{N} L\left(f\left(x_i\right), y_i; W\right) + \lambda\,\Omega\left(W\right)$$

- Regularization
  - L2 regularization: sum of squares of weights
  - “Drop-out”: deactivate random subset of weights in each iteration
    - Similar to using many networks with less weights (shared among them)

- Training using simple gradient descend techniques
  - Stochastic gradient descend for large datasets (large N)
  - Estimate gradient of loss terms by averaging over a relatively small number of samples

Training the network: forward propagation

- Forward propagation from input nodes to output nodes
  - Accumulate inputs via weighted sum into activation
  - Apply non-linear activation function f to compute output
- Use Pre(j) to denote all nodes feeding into j



$$a_j = \sum_{i \in Pre(j)} w_{ij} x_i$$

$$x_j = f(a_j)$$

Training the network: backward propagation

- Node activation and output

$$a_j = \sum_{i \in Pre(j)} w_{ij} x_i$$

$$x_j = f(a_j)$$

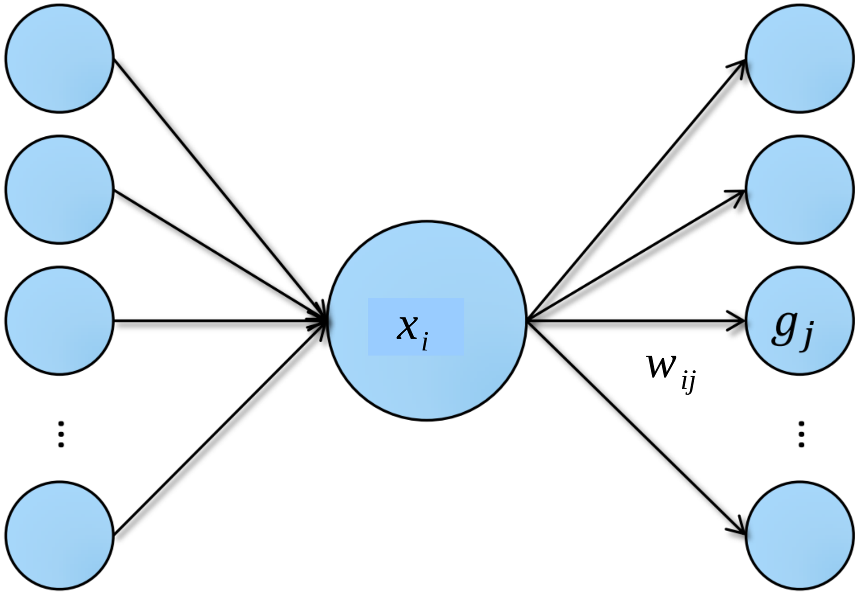
- Partial derivative of loss w.r.t. activation

$$g_j = \frac{\partial L}{\partial a_j}$$

- Partial derivative w.r.t. learnable weights

$$\frac{\partial L}{\partial w_{ij}} = \frac{\partial L}{\partial a_j} \frac{\partial a_j}{\partial w_{ij}} = g_j x_i$$

- Gradient of weight matrix between two layers given by outer-product of x and g



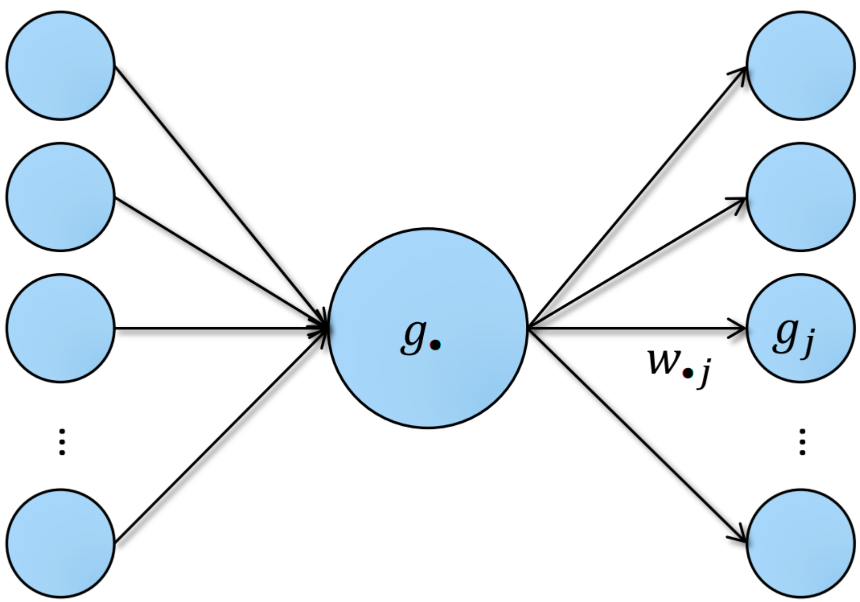
Training the network: backward propagation

- Back-propagation layer-by-layer of gradient from loss to internal nodes
  - Application of chain-rule of derivatives
- Accumulate gradients from downstream nodes
  - Post(i) denotes all nodes that i feeds into
  - Weights propagate gradient back
- Multiply with derivative of local activation function

$$a_j = \sum_{i \in Pre(j)} w_{ij} x_i$$

$$x_j = f(a_j)$$

$$g_i = \frac{\partial L}{\partial a_i}$$



$$\frac{\partial L}{\partial x_i} = \sum_{j \in Post(i)} \frac{\partial L}{\partial a_j} \frac{\partial a_j}{\partial x_i} = \sum_{j \in Post(i)} g_j w_{ij}$$

$$g_i = \frac{\partial x_i}{\partial a_i} \frac{\partial L}{\partial x_i} = f'(a_i) \sum_{j \in Post(i)} w_{ij} g_j$$

Training the network: forward and backward propagation

- Special case for Rectified Linear Unit (ReLU) activations

$$f(a) = max(0, a)$$

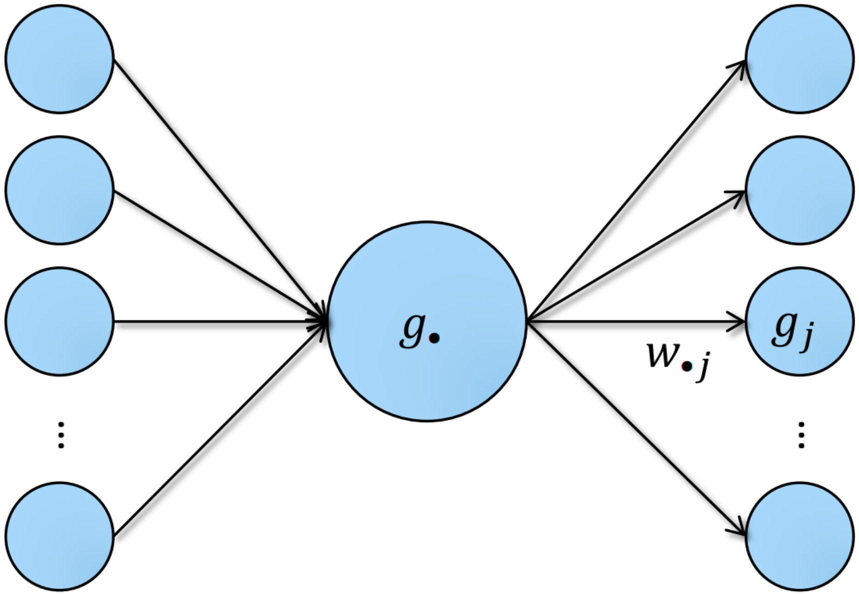
- Sub-gradient is step function

$$f'(a) = \begin{cases} 0 & \text{if } a \leq 0 \\ 1 & \text{otherwise} \end{cases}$$

- Sum gradients from downstream nodes

$$g_i = \begin{cases} 0 & \text{if } a_i \leq 0 \\ \sum_{j \in Post(i)} w_{ij} g_j & \text{otherwise} \end{cases}$$

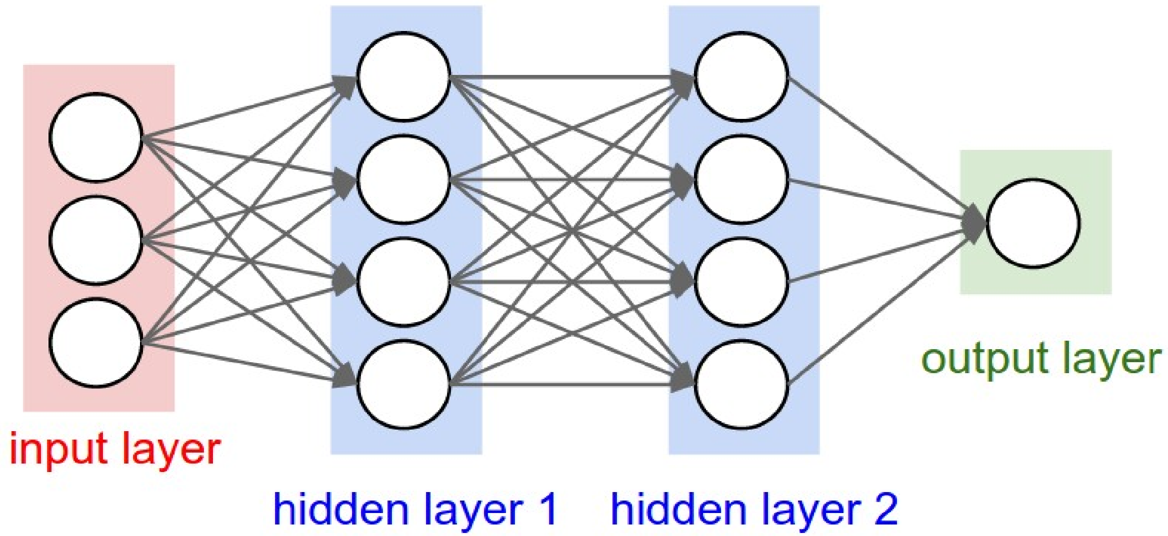
  - Set to zero if in ReLU zero-regime
  - Compute sum only for active units



- Gradient on incoming weights is “killed” by inactive units
  - Generates tendency for those units to remain inactive

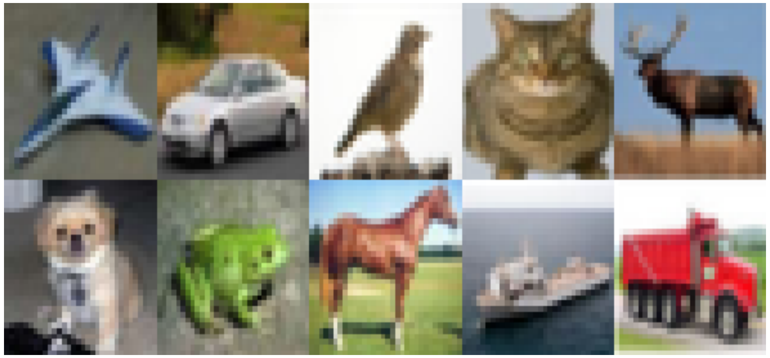
$$\frac{\partial L}{\partial w_{ij}} = \frac{\partial L}{\partial a_j} \frac{\partial a_j}{\partial w_{ij}} = g_j x_i$$

Convolutional Neural Networks



How to represent the image at the network input?

Input example : an image

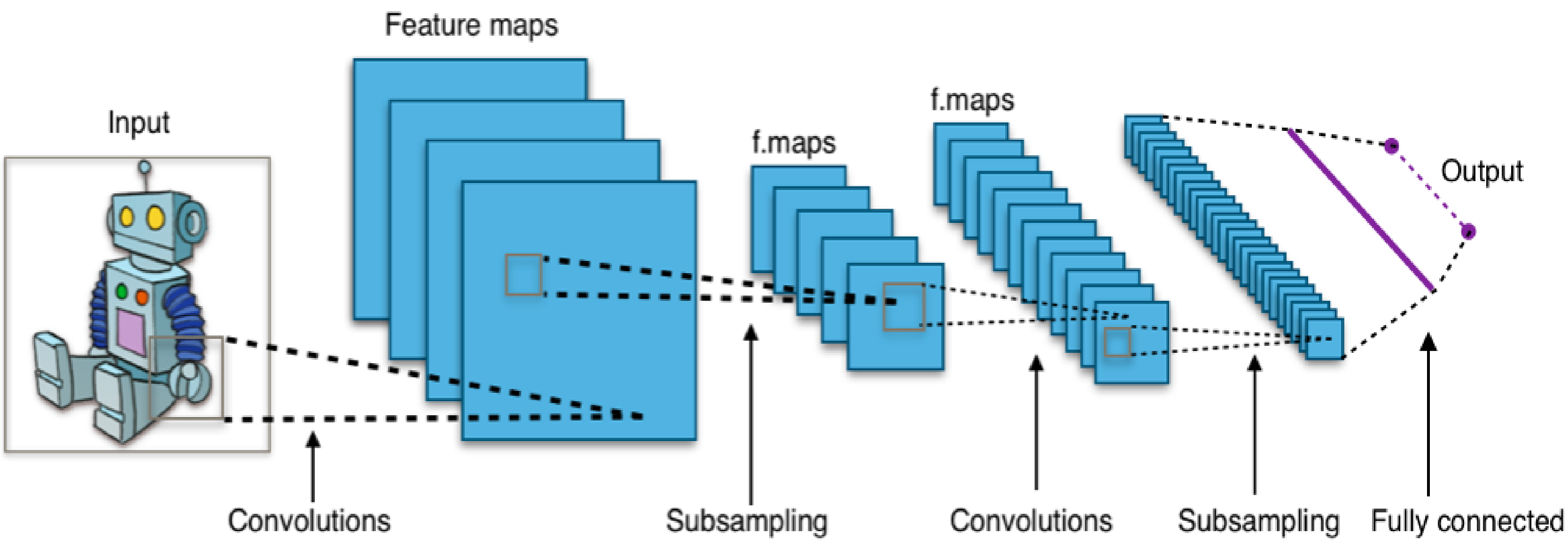


Output example: class label

airplane	dog
automobile	frog
bird	horse
cat	ship
deer	truck

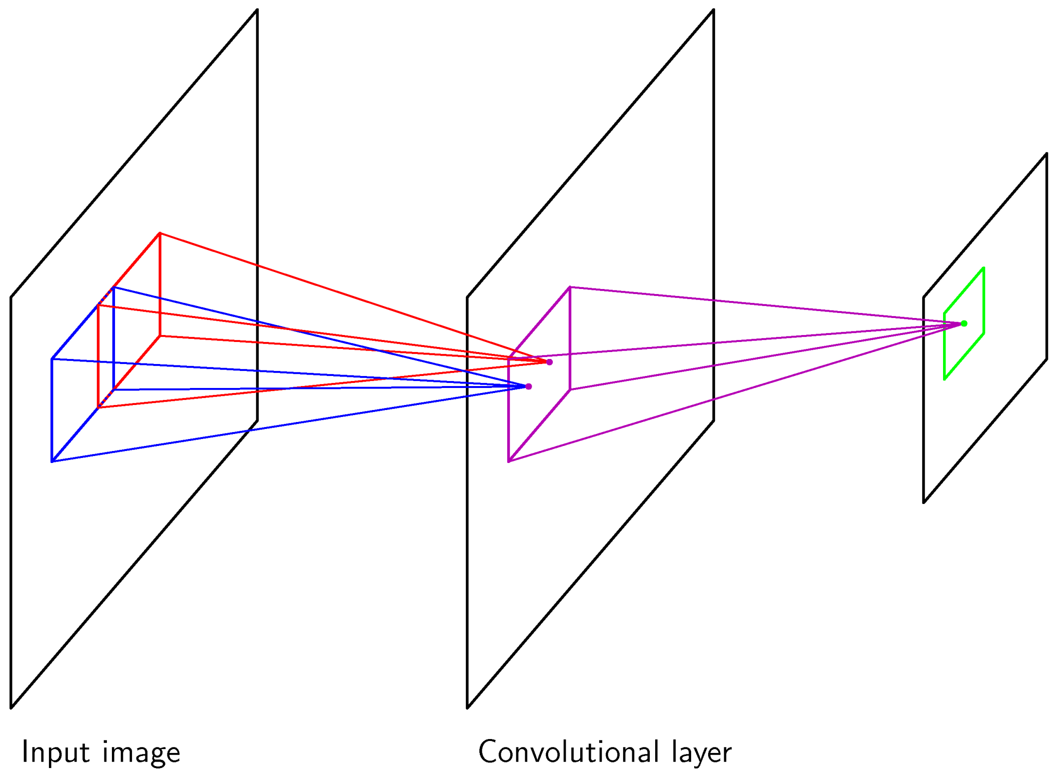
Convolutional neural networks

- A convolutional neural network is a feedforward network where
  - Hidden units are organizes into images or “response maps”
  - Linear mapping from layer to layer is replaced by convolution

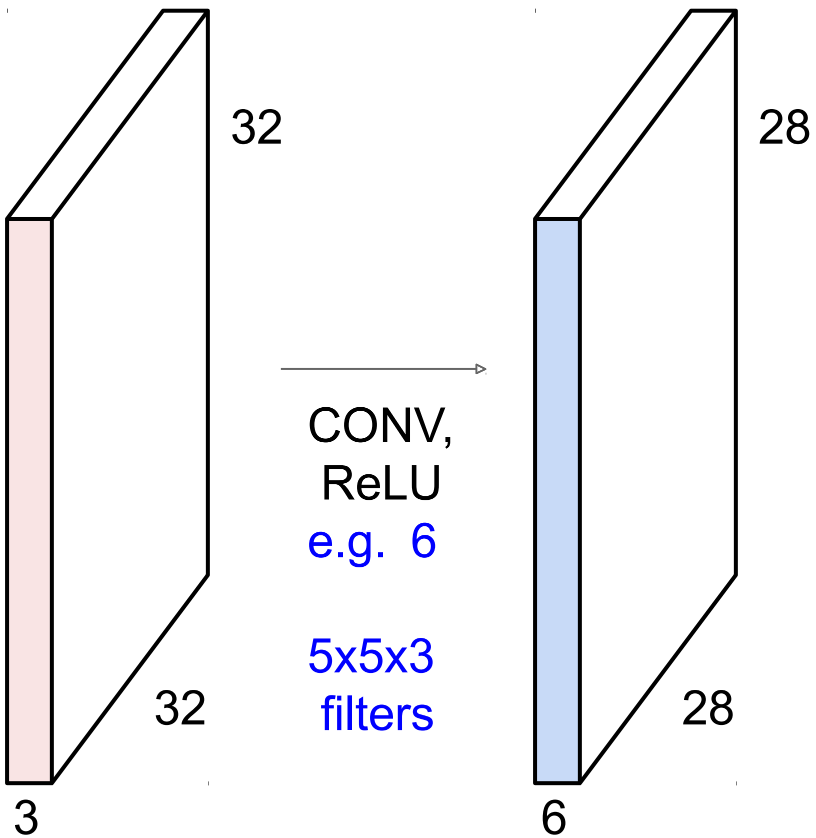


Convolutional neural networks

- Local connections: motivation from findings in early vision
  - Simple cells detect local features
  - Complex cells pool simple cells in retinotopic region
- Convolutions: motivated by translation invariance
  - Same processing should be useful in different image regions



Preview: ConvNet is a sequence of Convolution Layers, interspersed with activation functions



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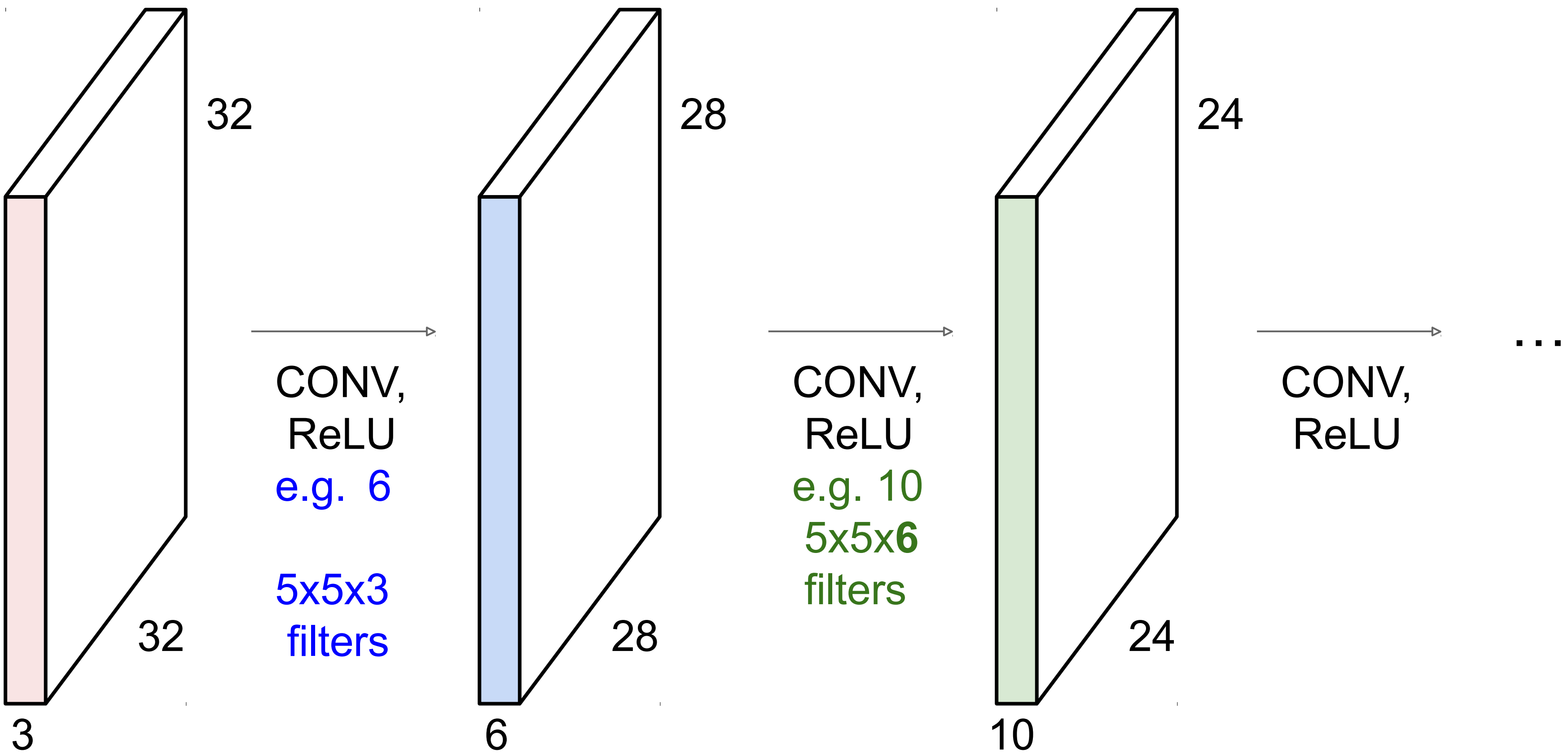
Preview: ConvNet is a sequence of Convolutional Layers, interspersed with activation functions



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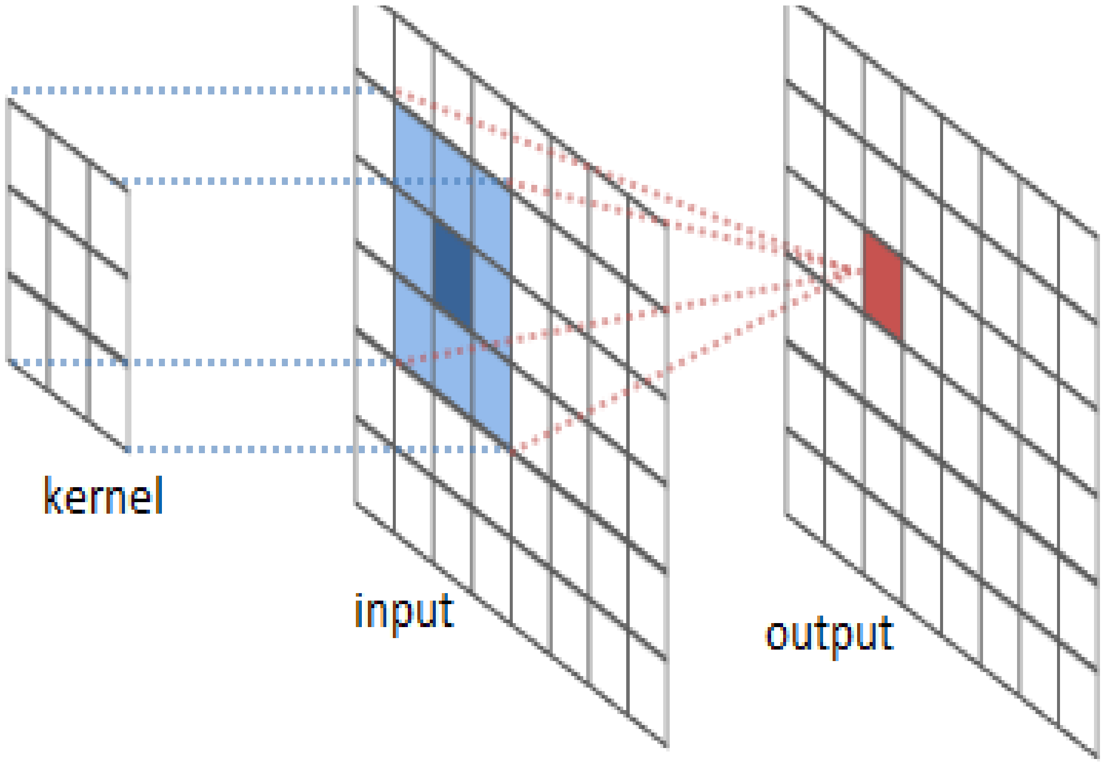
The convolution operation



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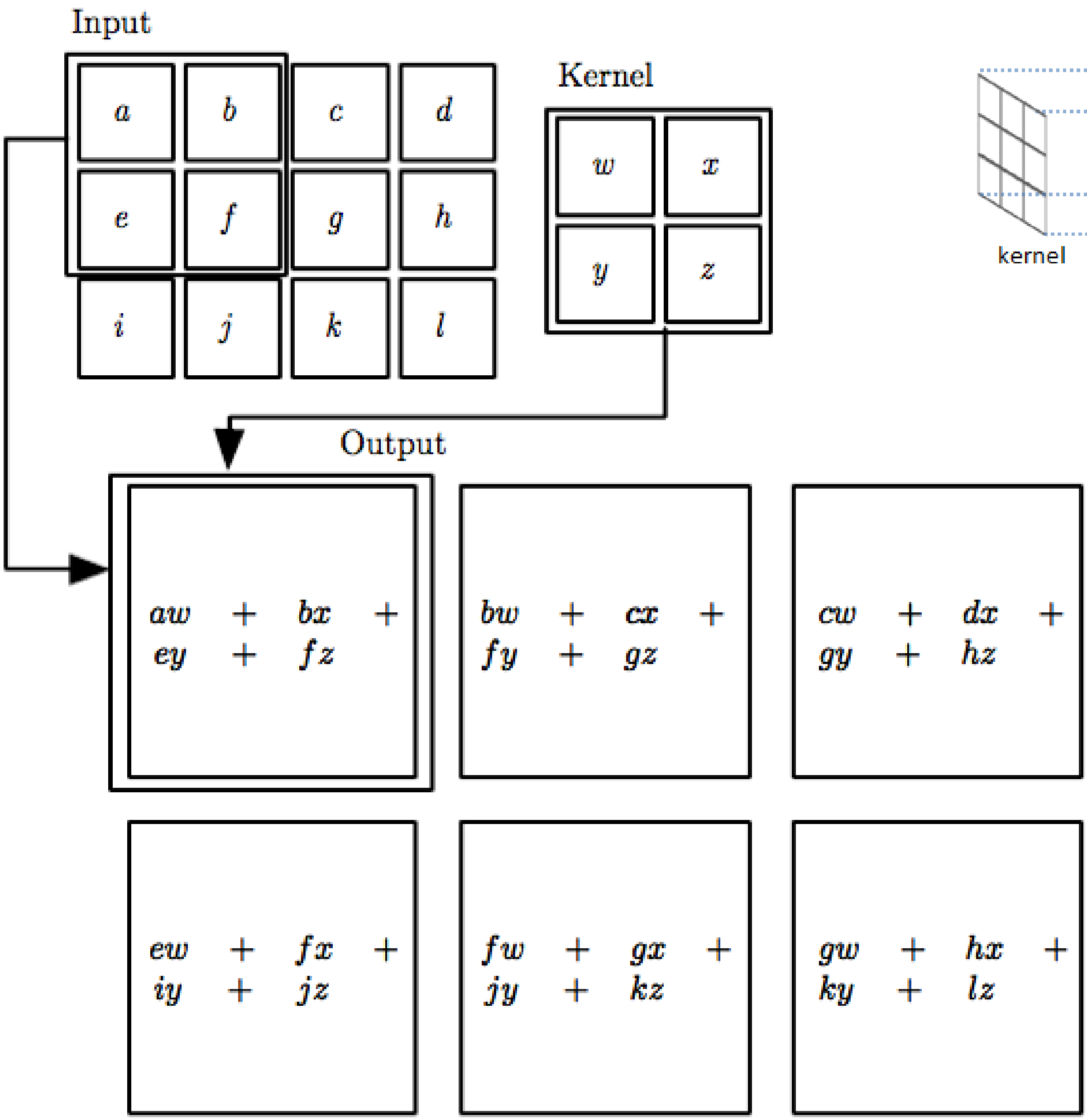
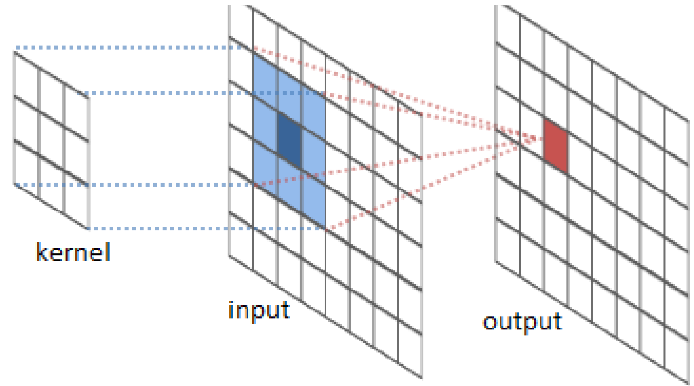
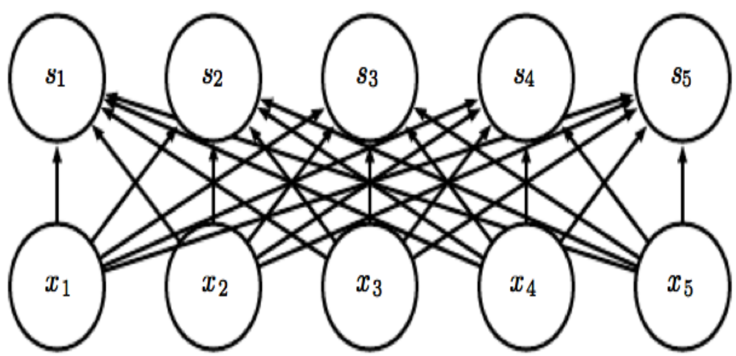




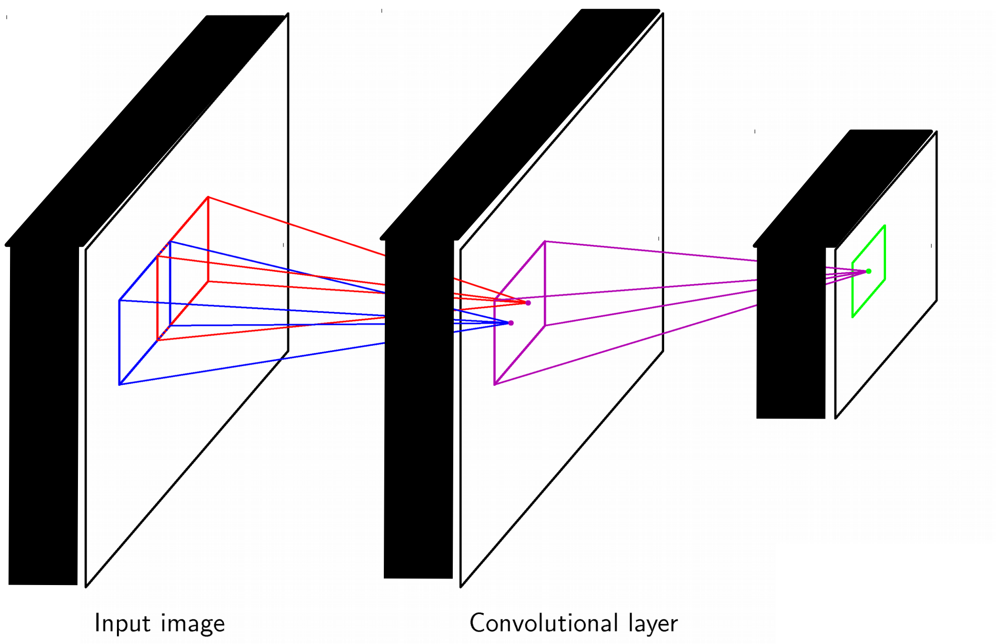
Local connectivity

Fully connected layer
as used in MLP



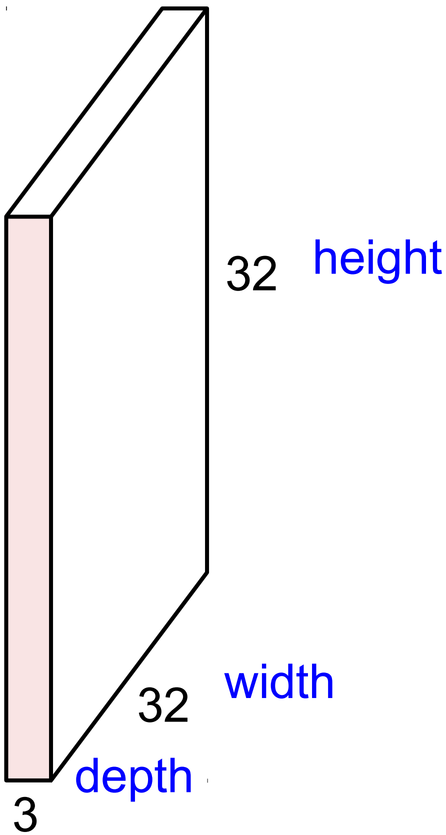
Convolutional neural networks

- Hidden units form another “image” or “response map”
  - Followed by point-wise non-linearity as in MLP
- Both input and output of the convolution can have multiple channels
  - E.g. three channels for an RGB input image
- Sharing of weights across spatial positions decouples the number of parameters from input and representation size
  - Enables training of models for large input images



Convolution Layer

32x32x3 image



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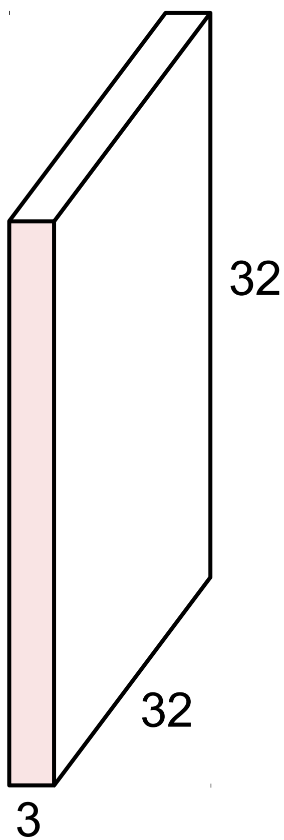
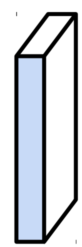
Convolution Layer

32x32x3 image



5x5x3 filter



Convolve the filter with the image
i.e. “slide over the image spatially,
computing dot products”

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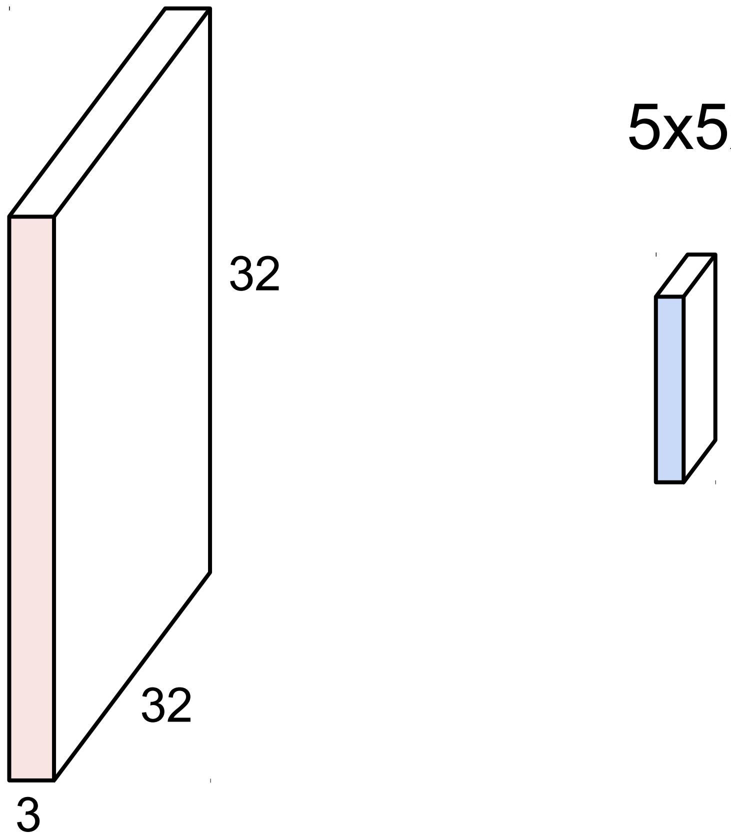
Convolution Layer

32x32x3 image

Filters always extend the full depth of the input volume

5x5x3 filter



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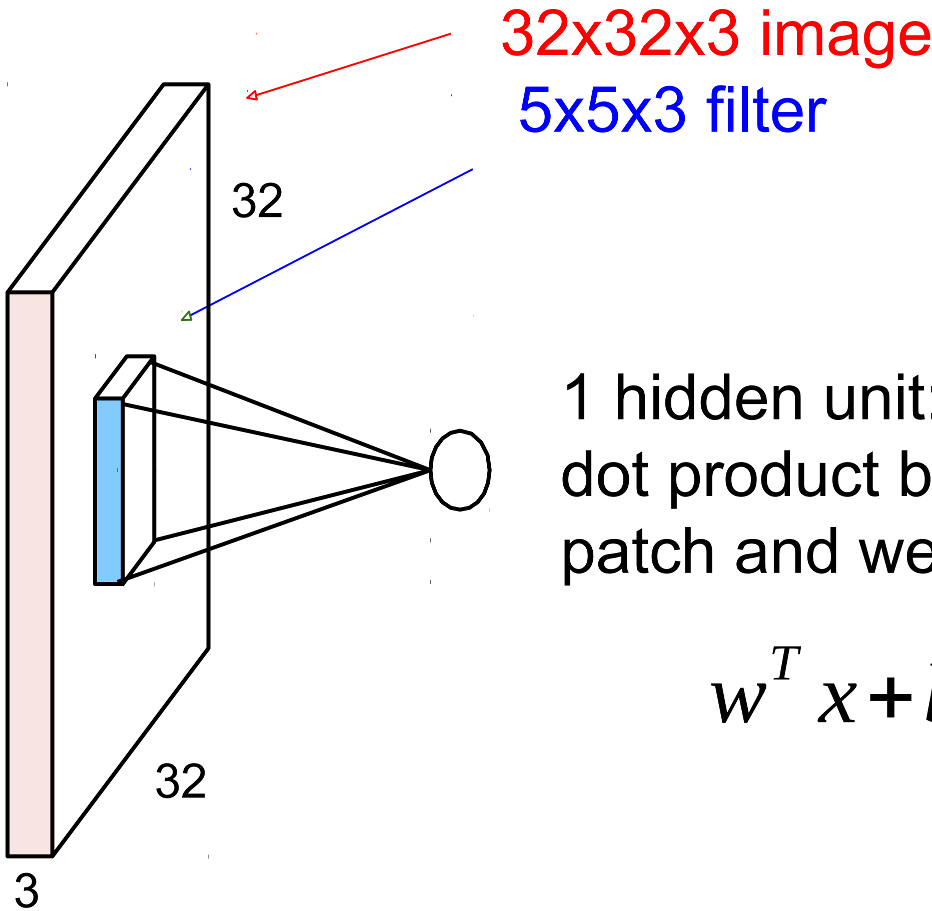
Convolution Layer



1 hidden unit:
dot product between 5x5x3=75 input patch and weight vector + bias

$$w^T x + b$$

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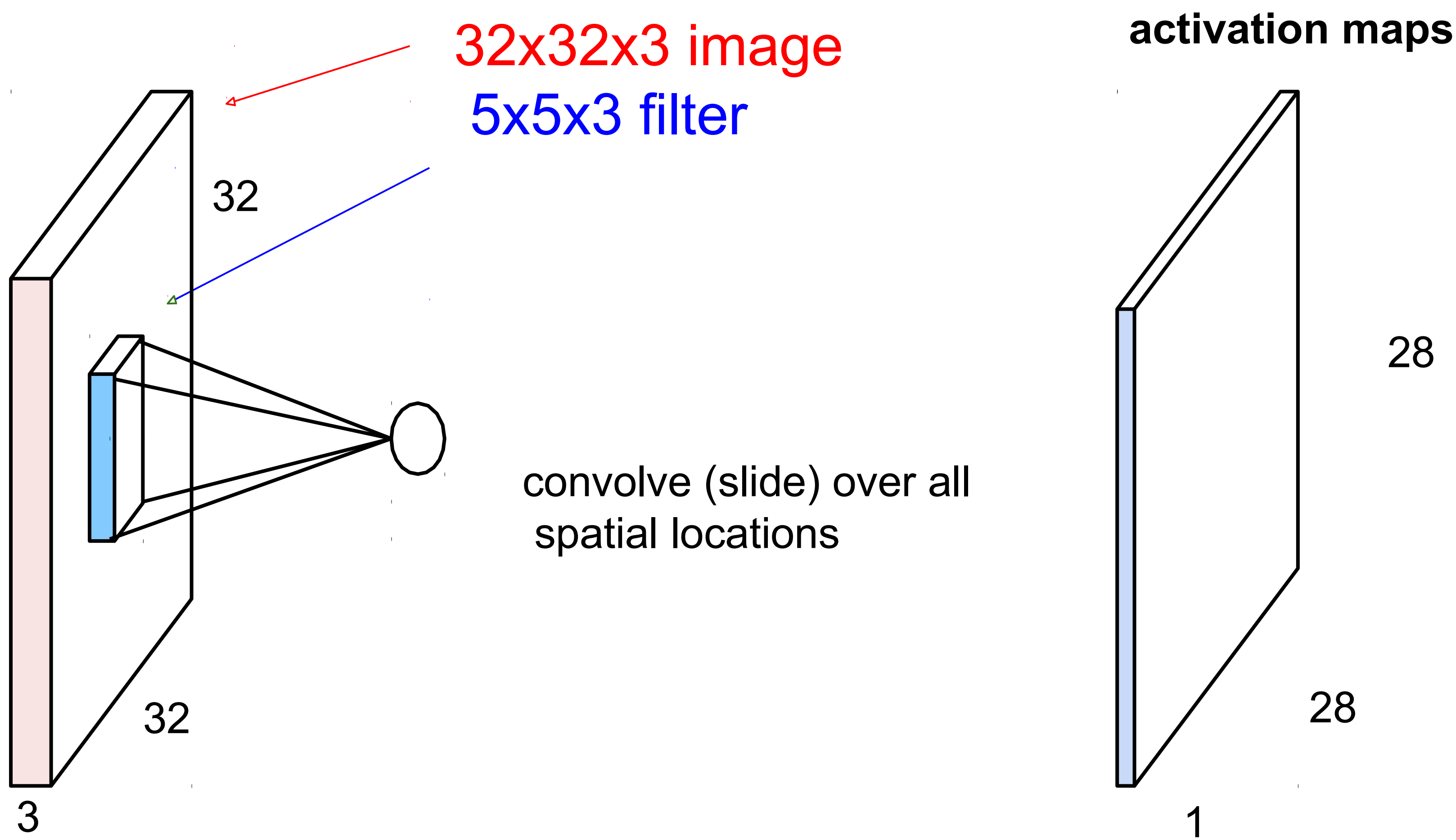
Convolution Layer



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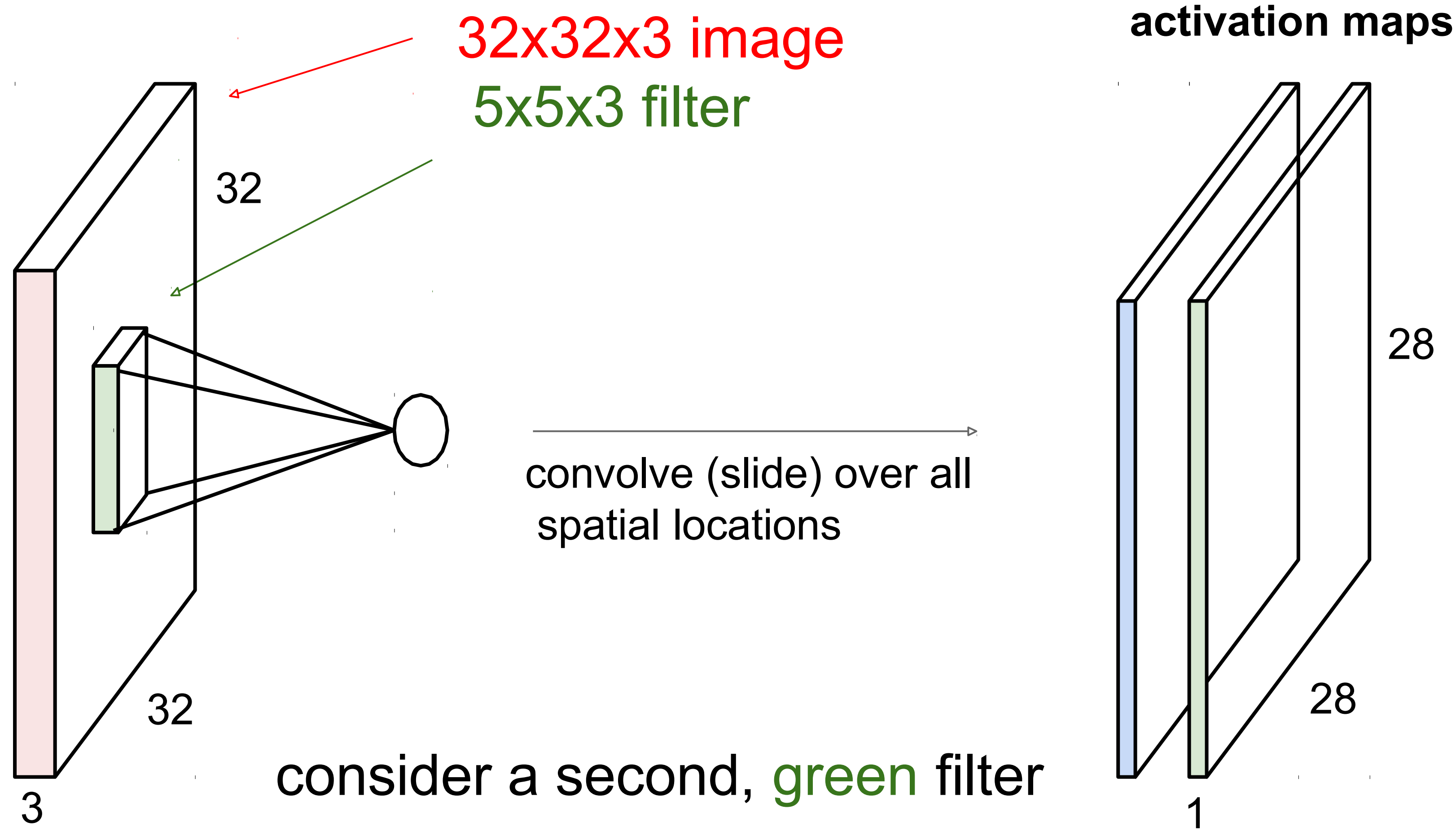
Convolution Layer



consider a second, green filter

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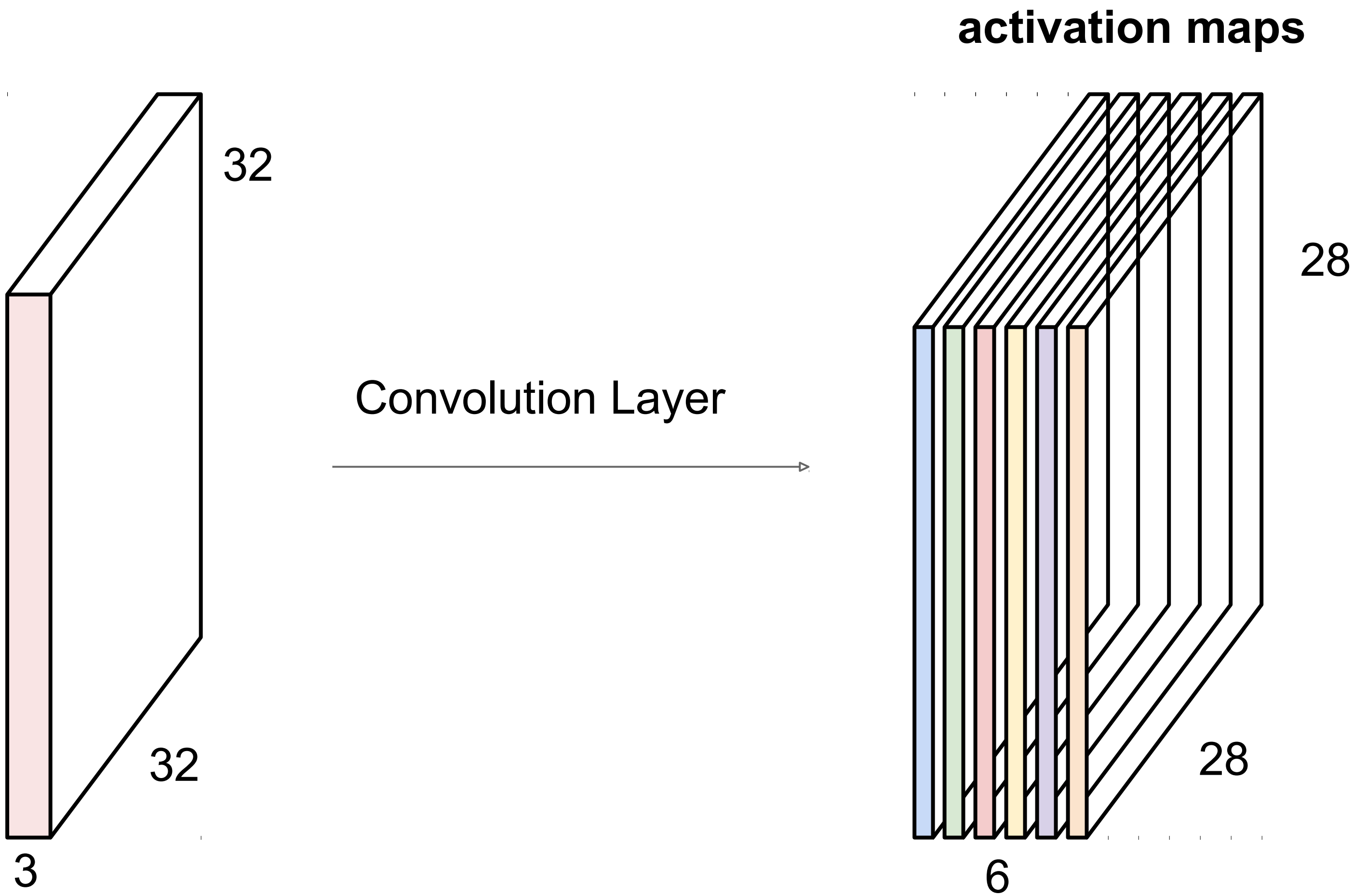
For example, if we had 6 5x5 filters, we'll get 6 separate activation maps:



We stack these up to get a "new image" of size 28x28x6!

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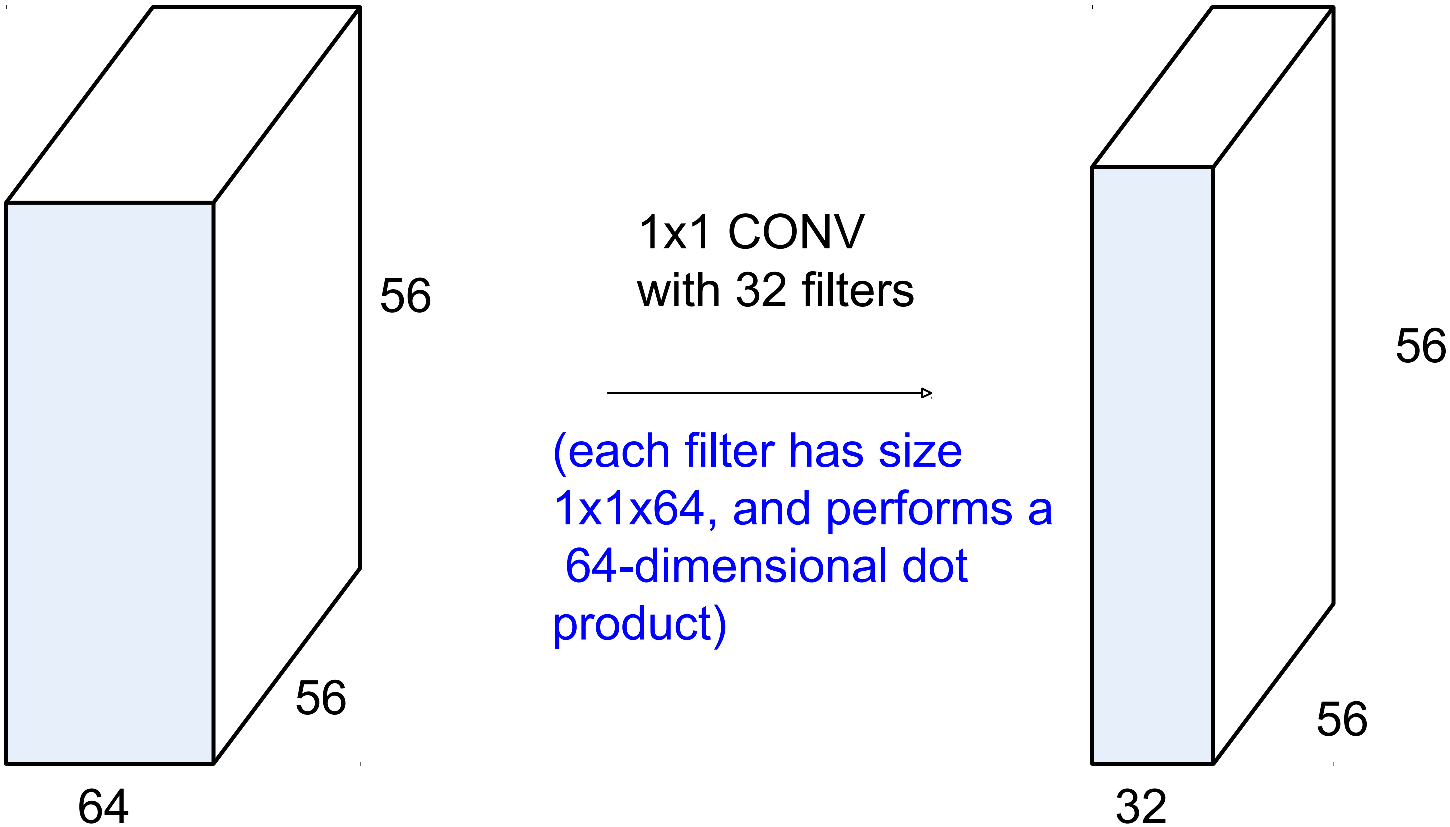
Convolution with 1x1 filters makes perfect sense



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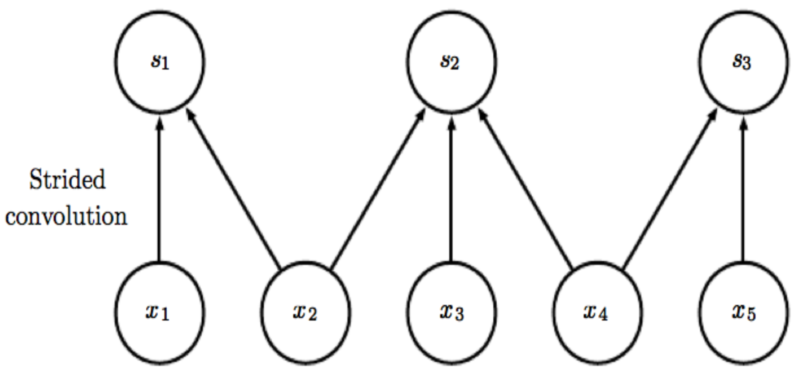
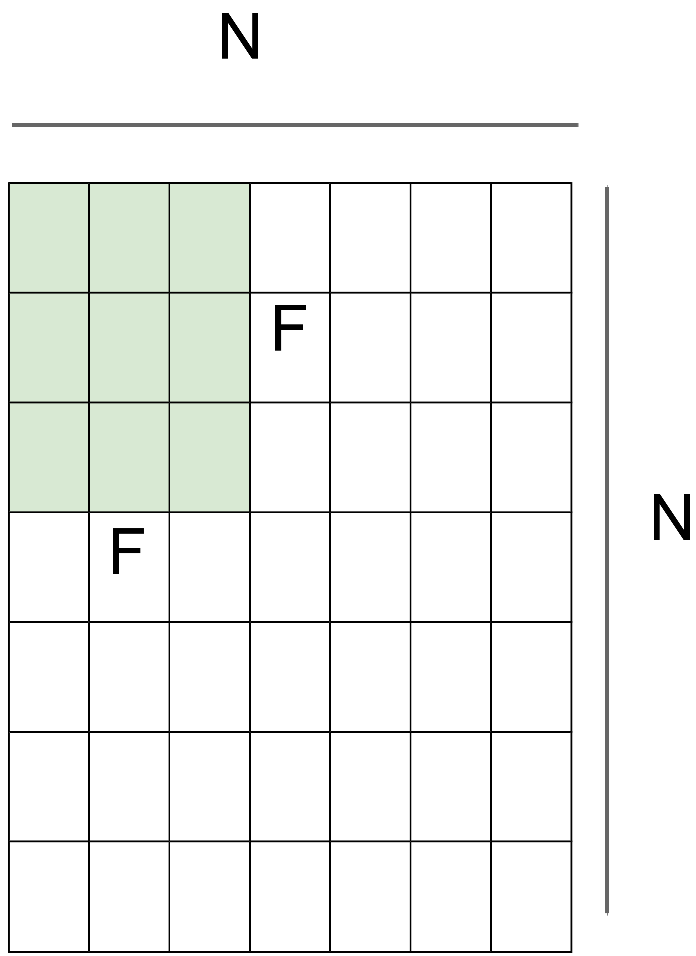
Stride





Output size:
(N - F) / stride + 1

e.g. N = 7, F = 3:
stride 1 => (7 - 3)/1 + 1 = 5
stride 2 => (7 - 3)/2 + 1 = 3
stride 3 => (7 - 3)/3 + 1 = 2.33 :\

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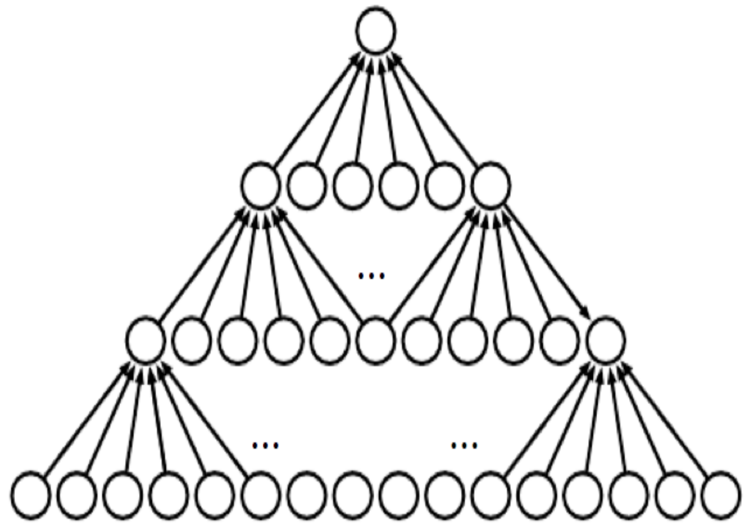
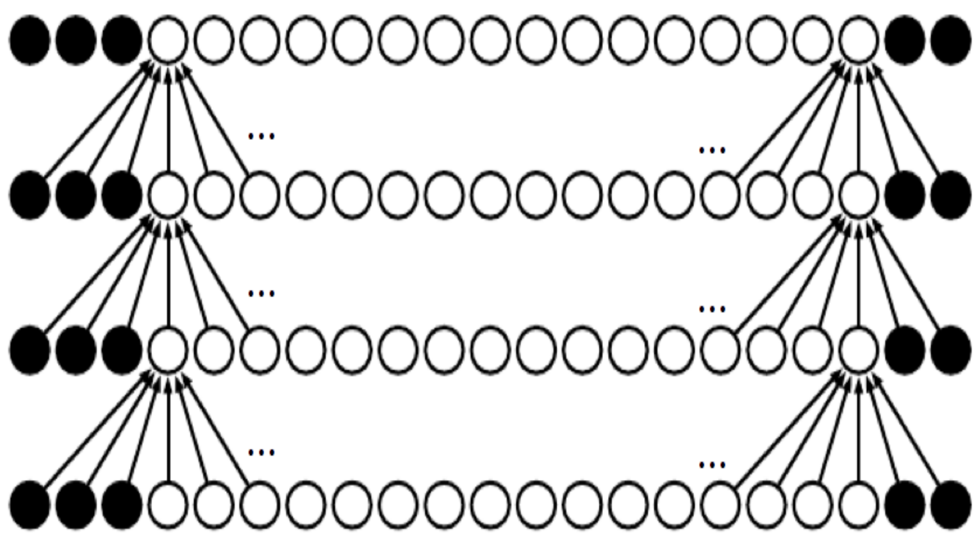
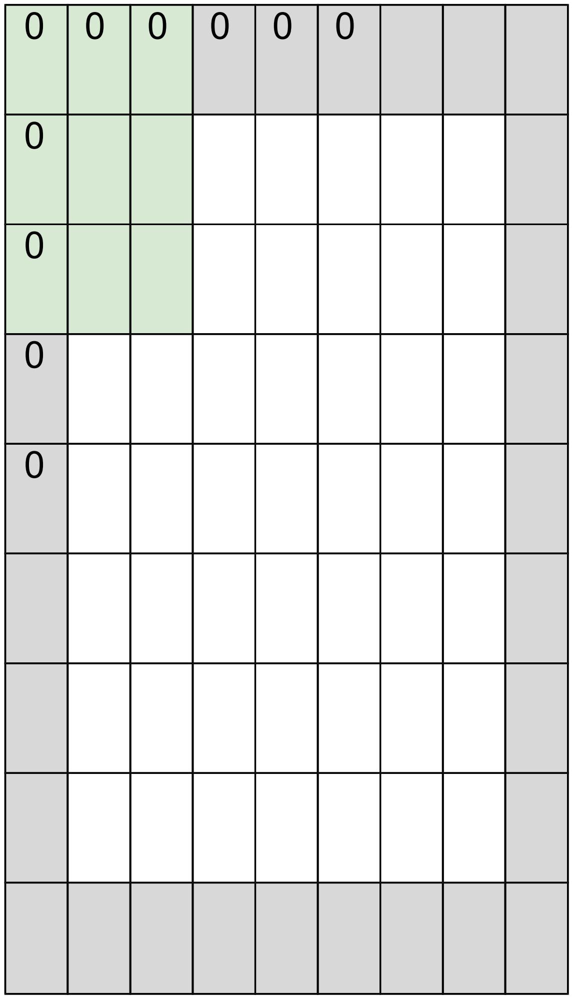
(Zero)-Padding





Zero-Padding: common to the border



e.g. input 7x7
3x3 filter, applied with **stride 1**
pad with 1 pixel border => what is the output?

7x7 output!

In general, common to see CONV layers with stride 1, filters of size FxF, and zero-padding with (F-1)/2. (will preserve size spatially)

e.g. F = 3 => zero pad with 1
F = 5 => zero pad with 2
F = 7 => zero pad with 3

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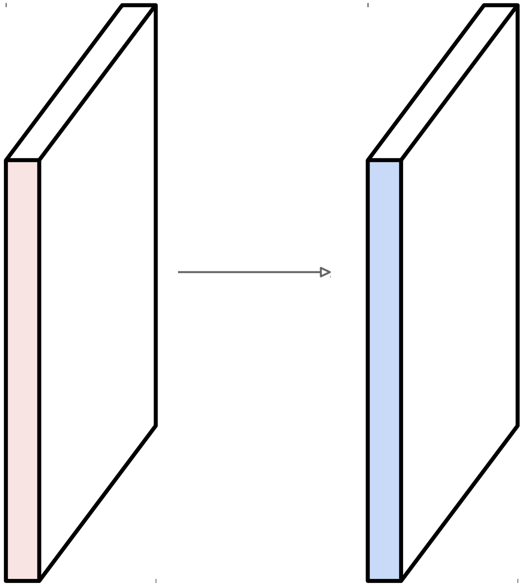
Example:



Input volume: **32x32x3**
10 5x5 filters with stride 1, pad 2

Output volume size: ?

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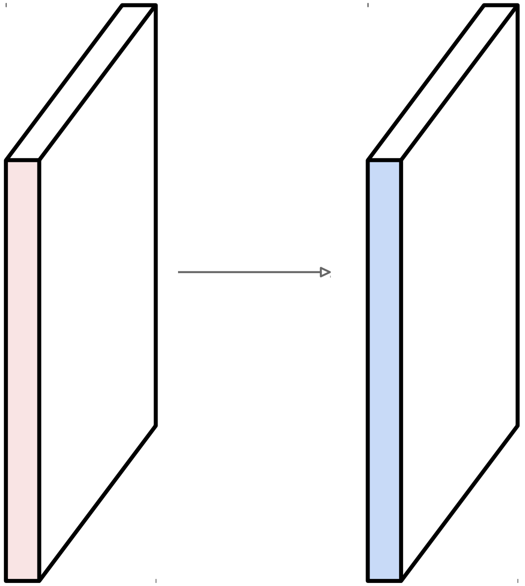
Example:

Input volume: **32x32x3**

10 5x5 filters with stride 1, pad 2



Output volume size:

(32+2*2-5)/1+1 = 32 spatially, so

32x32x10

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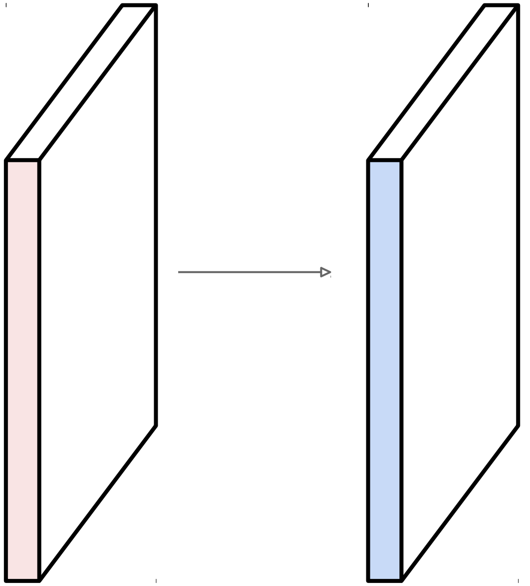
Example:

Input volume: **32x32x3**
10 5x5 filters with stride 1, pad 2



Number of parameters in this layer?

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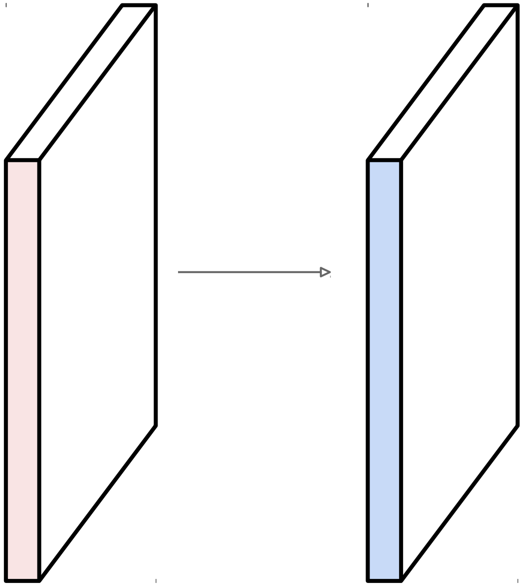
Example:



Input volume: **32x32x3**

10 5x5 filters with stride 1, pad 2

Number of parameters in this layer?

each filter has 5*5*3 + 1 = 76 params

(+1 for bias)

=> 76*10 = **760**

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Common settings:

K = (powers of 2, e.g. 32, 64, 128, 512)

- F = 3, S = 1, P = 1
- F = 5, S = 1, P = 2
- F = 5, S = 2, P = ? (whatever fits)
- F = 1, S = 1, P = 0

Summary. To summarize, the Conv Layer:

- Accepts a volume of size $W_1 \times H_1 \times D_1$
- Requires four hyperparameters:
  - Number of filters K,
  - their spatial extent F,
  - the stride S,
  - the amount of zero padding P.
- Produces a volume of size $W_2 \times H_2 \times D_2$ where:
  - $W_2 = (W_1 - F + 2P)/S + 1$
  - $H_2 = (H_1 - F + 2P)/S + 1$ (i.e. width and height are computed equally by symmetry)
  - $D_2 = K$
- With parameter sharing, it introduces $F \cdot F \cdot D_1$ weights per filter, for a total of $(F \cdot F \cdot D_1) \cdot K$ weights and K biases.
- In the output volume, the d-th depth slice (of size $W_2 \times H_2$) is the result of performing a valid convolution of the d-th filter over the input volume with a stride of S, and then offset by d-th bias.

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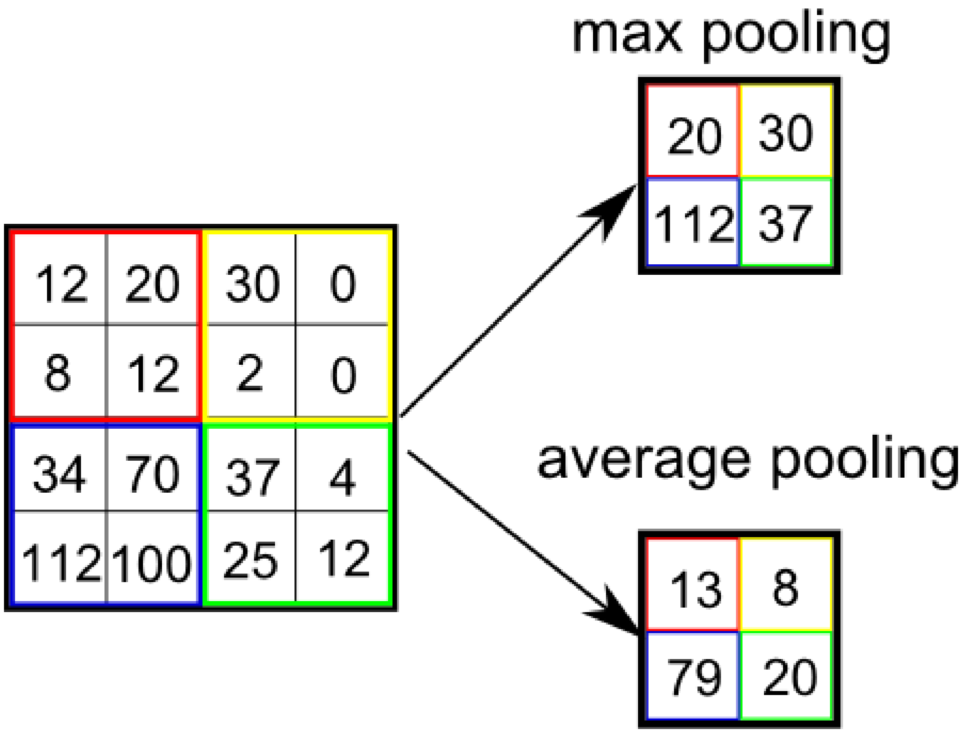
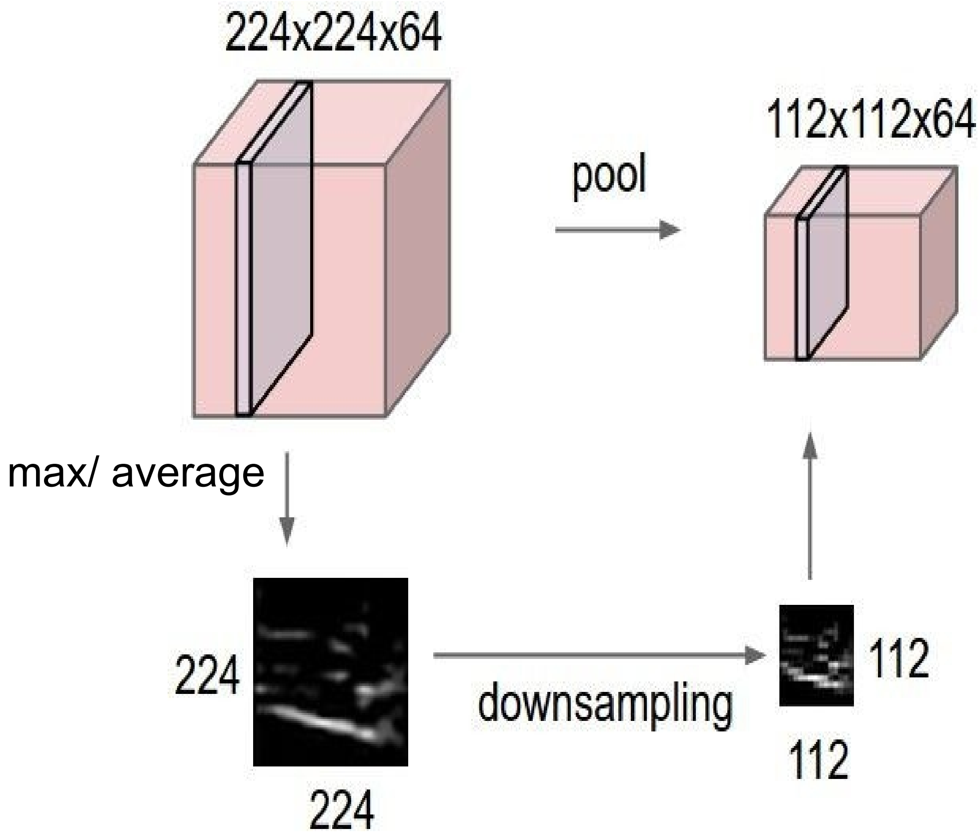
Pooling



Effect = invariance to small translations of the input

Pooling

- Makes representation smaller and computationally less expensive
- Operates over each activation map independently



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Summary

Common settings:

F = 2, S = 2
F = 3, S = 2

- Accepts a volume of size $W_1 \times H_1 \times D_1$
- Requires three hyperparameters:
  - their spatial extent F,
  - the stride S,
- Produces a volume of size $W_2 \times H_2 \times D_2$ where:
  - $W_2 = (W_1 - F)/S + 1$
  - $H_2 = (H_1 - F)/S + 1$
  - $D_2 = D_1$
- Introduces zero parameters since it computes a fixed function of the input
- Note that it is not common to use zero-padding for Pooling layers

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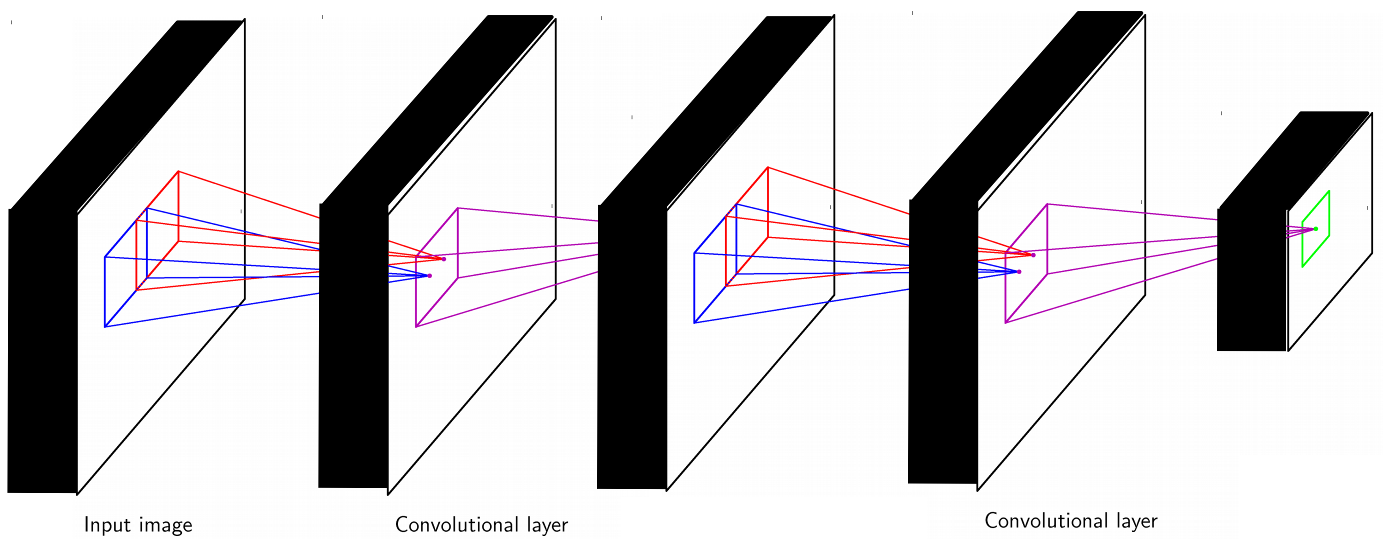
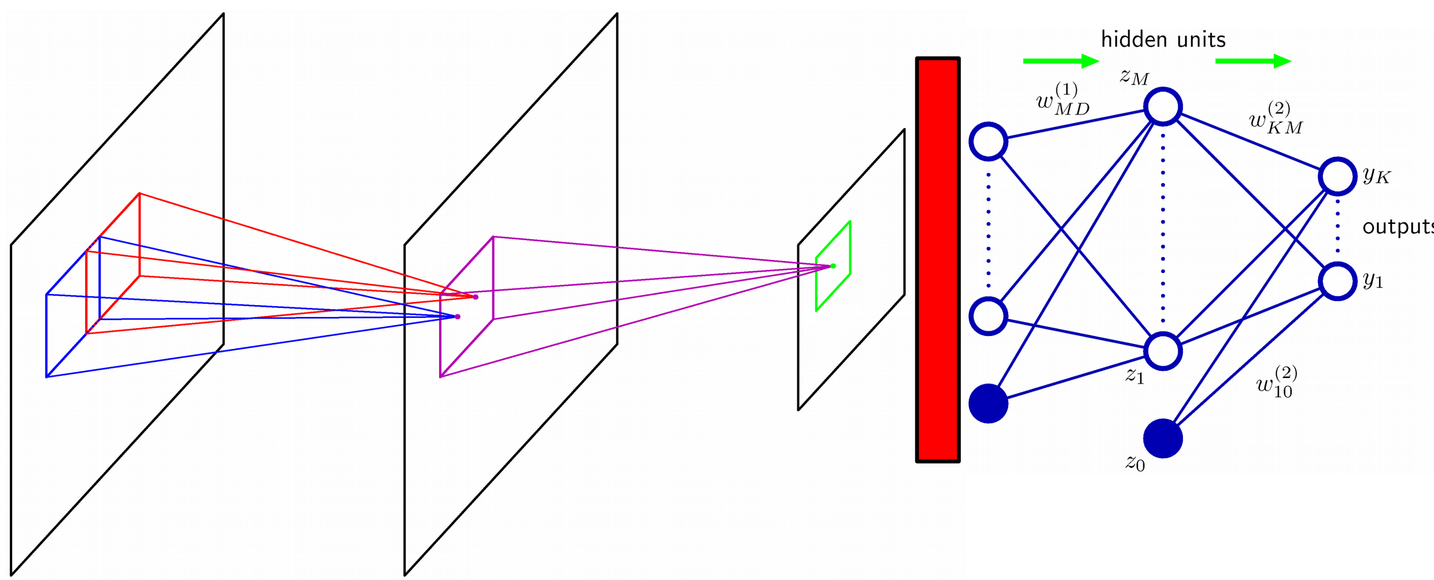
Receptive fields

- "Receptive field" is area in original image impacting a certain unit
  - Later layers can capture more complex patterns over larger areas
- Receptive field size grows linearly over convolutional layers
  - If we use a convolutional filter of size w x w, then each layer the receptive field increases by (w-1)
- Receptive field size increases exponentially over layers with striding
  - Regardless whether they do pooling or convolution



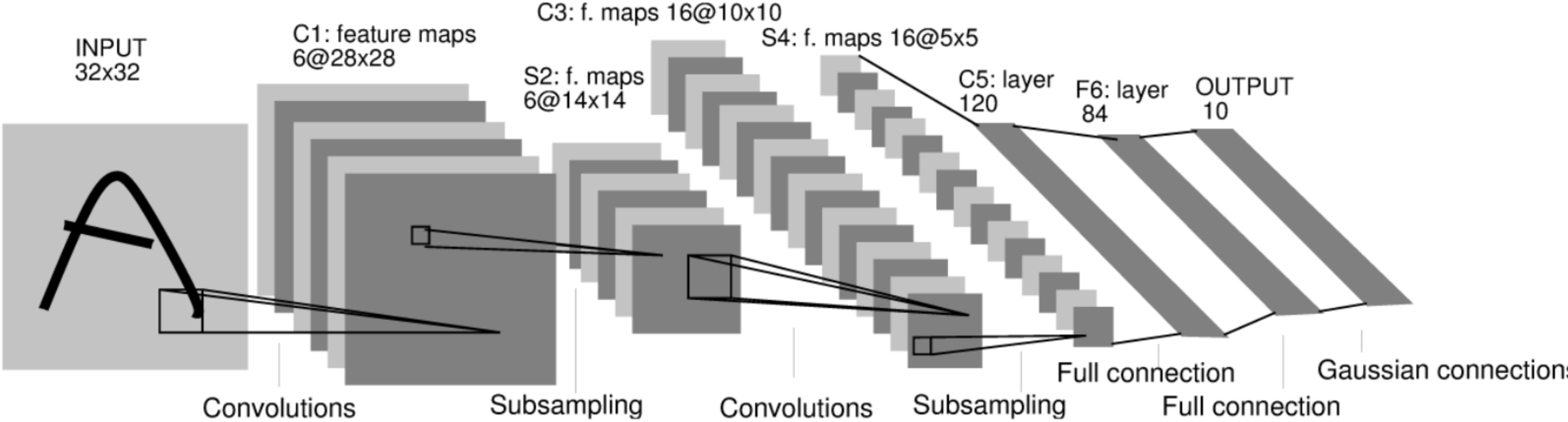
Fully connected layers

- Convolutional and pooling layers typically followed by several “fully connected” (FC) layers, i.e. a standard MLP
  - FC layer connects all units in previous layer to all units in next layer
  - Assembles all local information into global vectorial representation
- FC layers followed by softmax for classification
- First FC layer that connects response map to vector has many parameters
  - Conv layer of size 16x16x256 with following FC layer with 4096 units leads to a connection with 256 million parameters !
  - Large 16x16 filter without padding gives 1x1 sized output map



Convolutional neural network architectures

- LeNet by LeCun et al 1998
- Surprisingly little difference between todays architectures and those of late eighties and nineties
  - Convolutional layers, same
  - Nonlinearities: ReLU dominant now, tanh before
  - Subsampling: more strided convolution now than max/average pooling



Handwritten digit recognition network. LeCun, Bottou, Bengio, Haffner, Proceedings IEEE, 1998

Convolutional neural network architectures

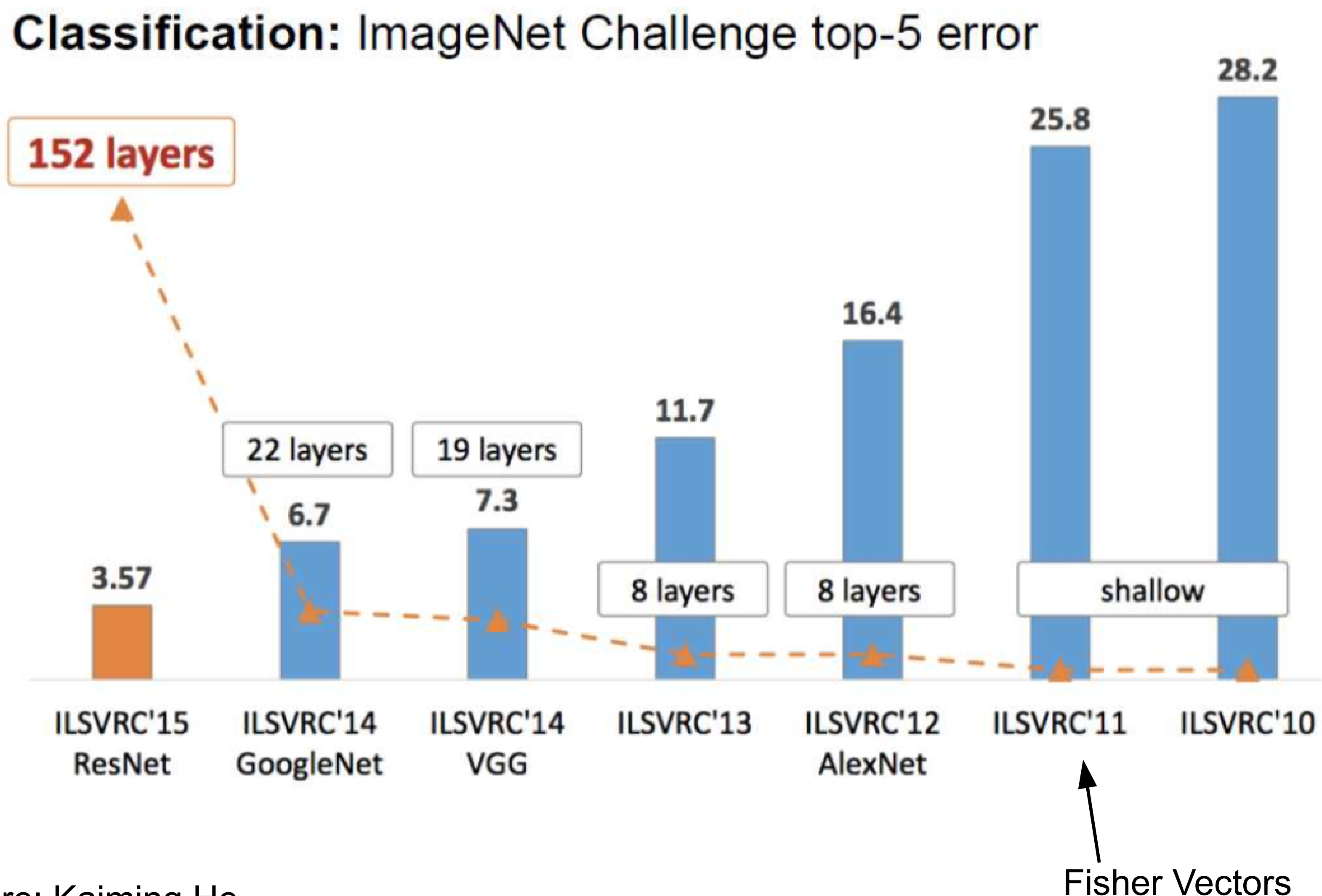
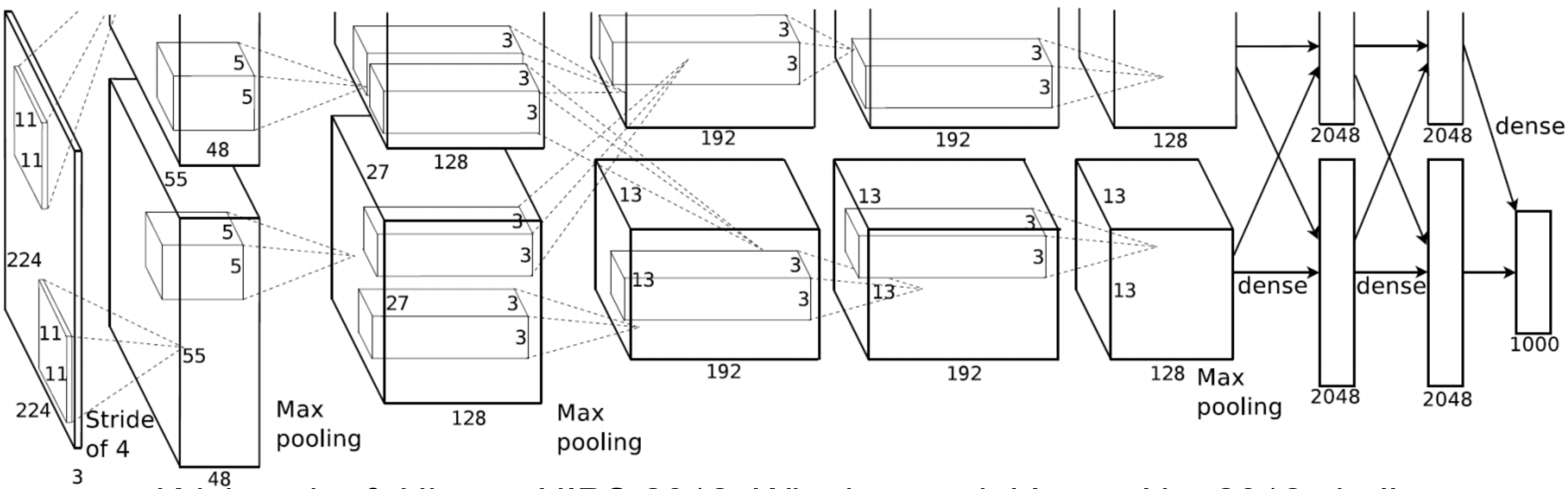


Figure: Kaiming He

Convolutional neural network architectures

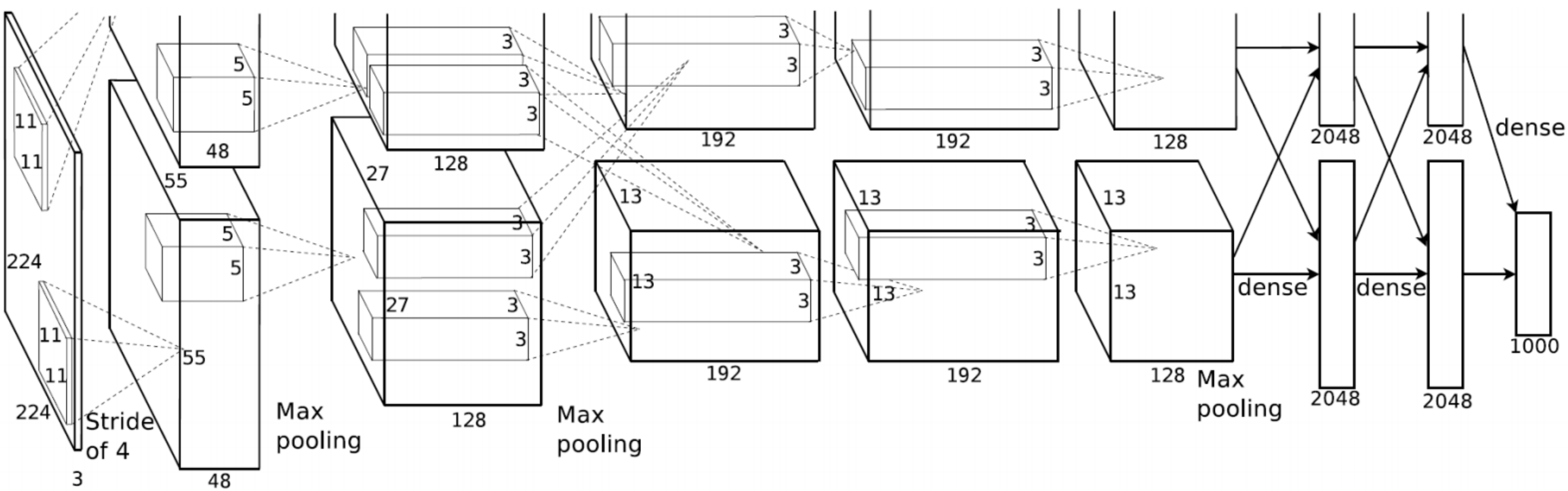
- Recent success with deeper networks
  - 19 layers in Simonyan & Zisserman, ICLR 2015
  - Hundreds of layers in residual networks, He et al. ECCV 2016
- More filters per layer: hundreds to thousands instead of tens
- More parameters: tens or hundreds of millions



Krizhevsky & Hinton, NIPS 2012, Winning model ImageNet 2012 challenge

Other factors that matter

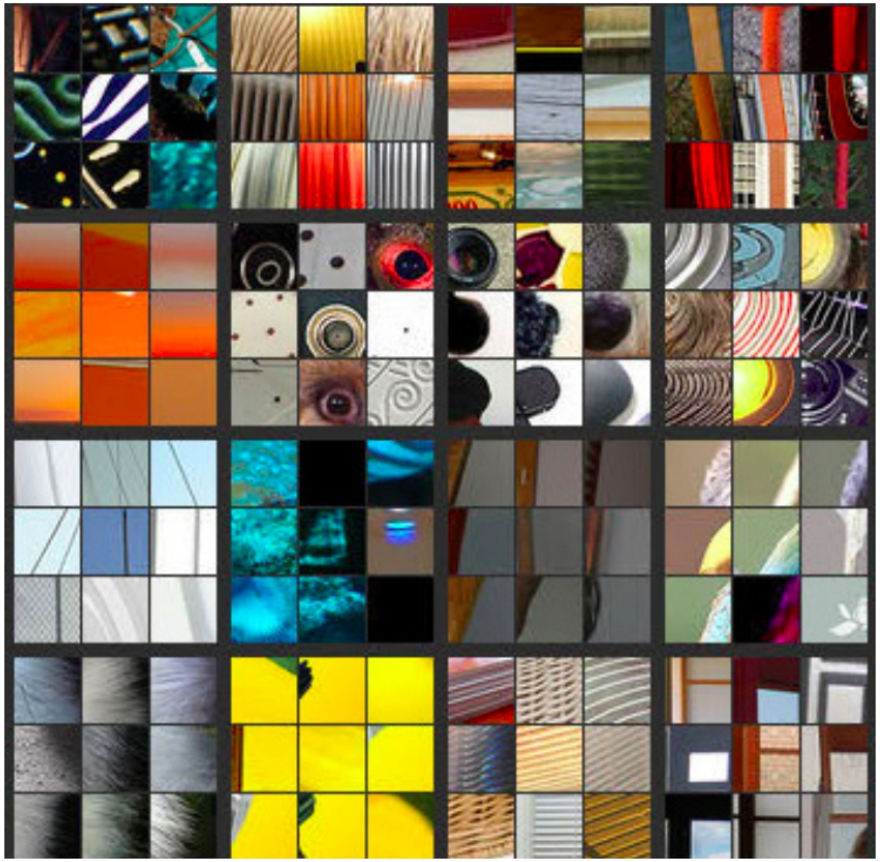
- More training data
  - 1.2 millions of 1000 classes in ImageNet challenge
  - 200 million faces in Schroff et al, CVPR 2015
- GPU-based implementations
  - Massively parallel computation of convolutions
  - Krizhevsky & Hinton, 2012: six days of training on two GPUs
  - Rapid progress in GPU compute performance



Krizhevsky & Hinton, NIPS 2012, Winning model ImageNet 2012 challenge

Understanding convolutional neural network activations

- Patches generating highest response for a selection of convolutional filters,
  - Showing 9 patches per filter
  - Zeiler and Fergus, ECCV 2014
- Layer 1: simple edges and color detectors



- Layer 2: corners, center-surround, ...

Understanding convolutional neural network activations

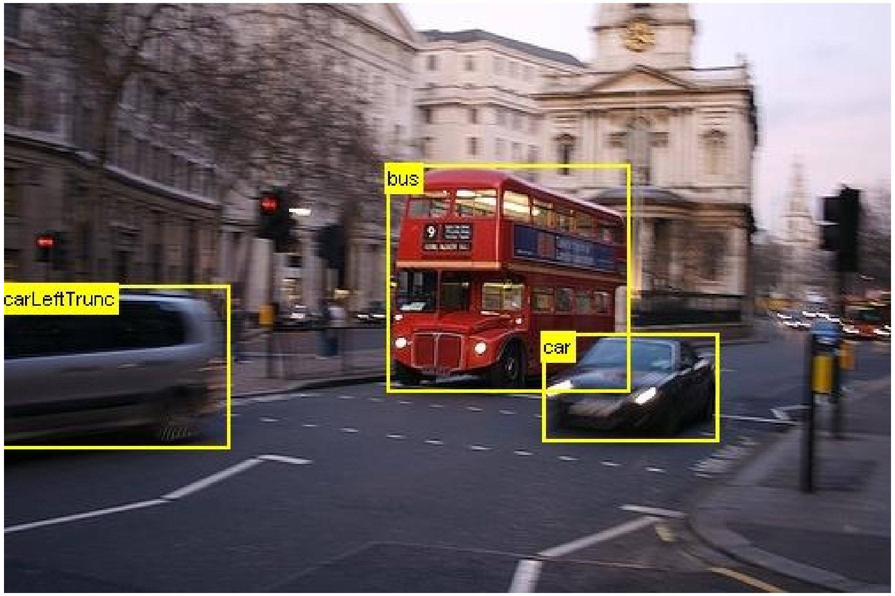
- Layer 3: various object parts

Understanding convolutional neural network activations

- Layer 4+5: selective units for entire objects or large parts of them

Convolutional neural networks for other tasks

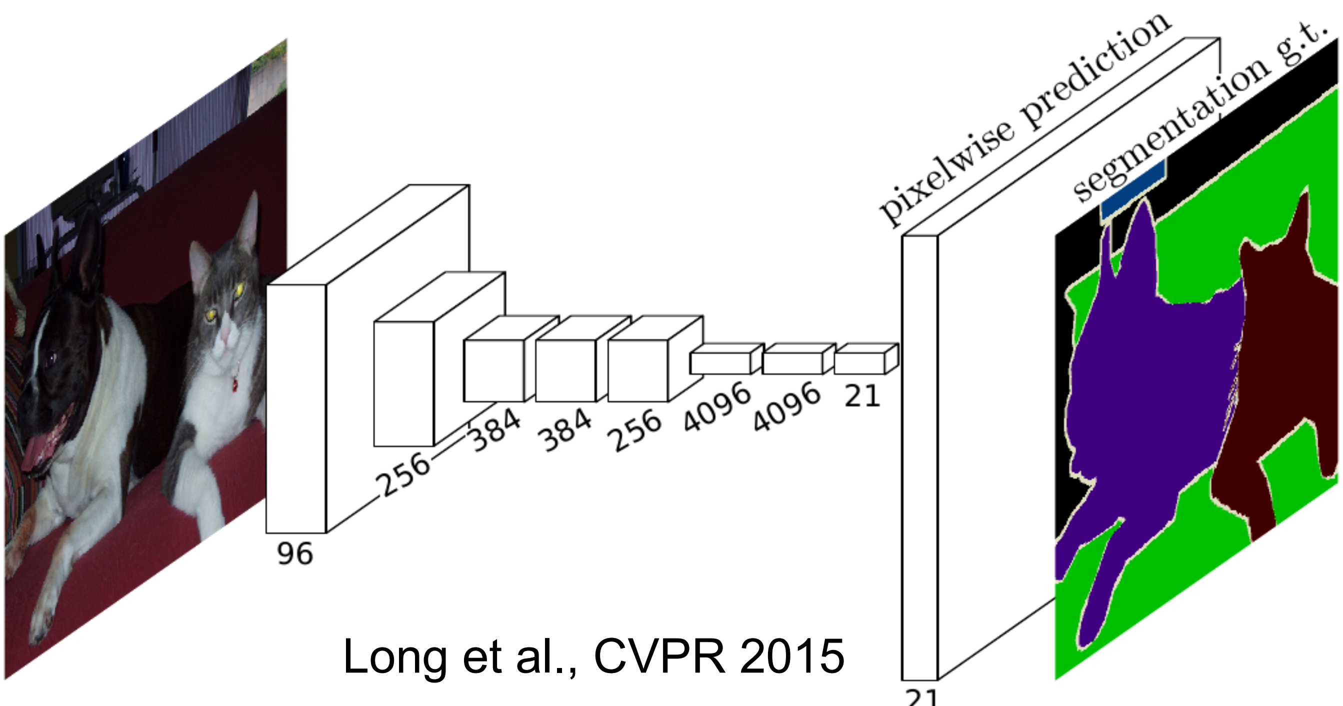
- Object category localization



- **Semantic segmentation**

Application to semantic segmentation

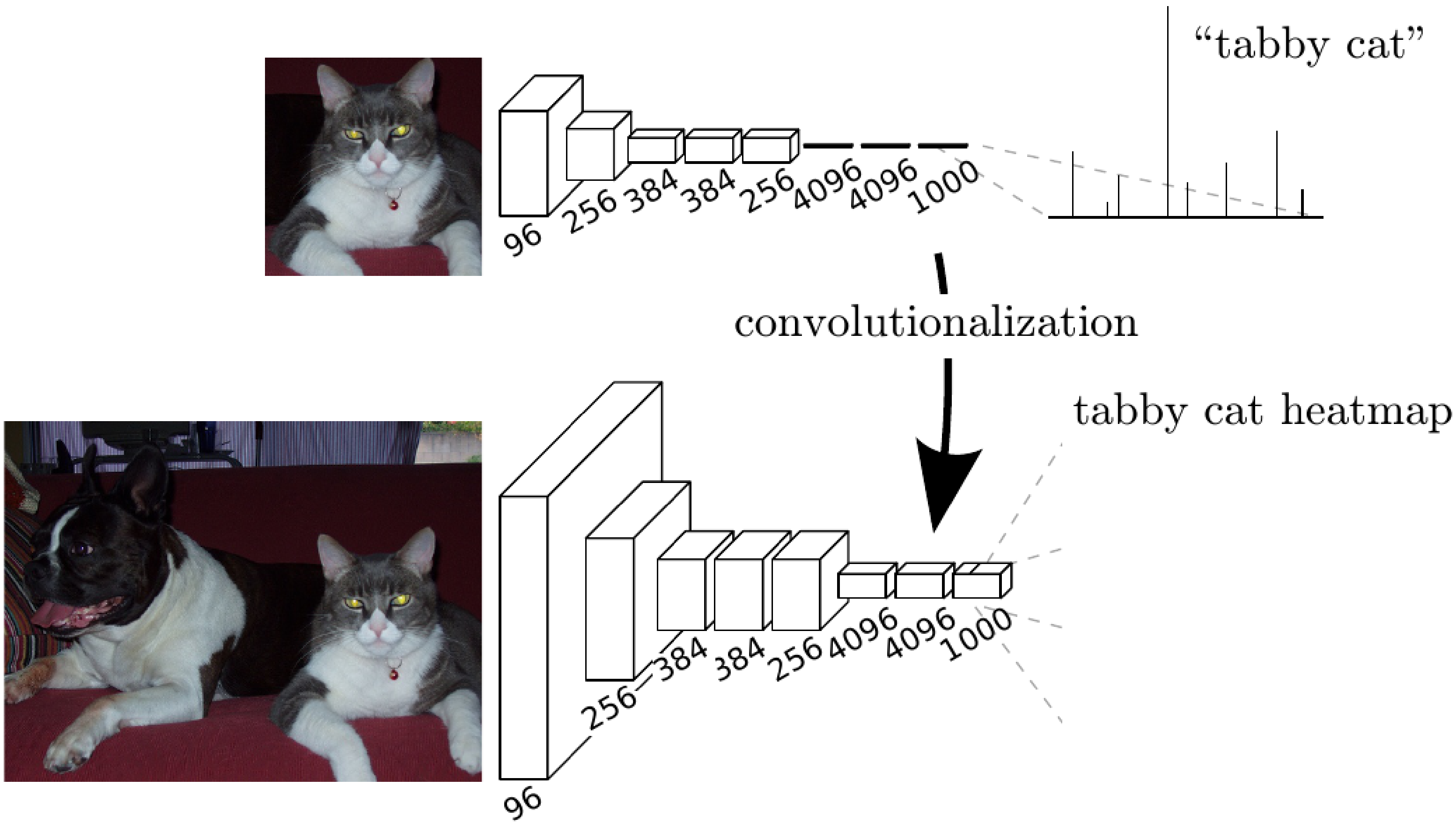
- Assign each pixel to an object or background category
  - Consider running CNN on small image patch to determine its category
  - Train by optimizing per-pixel classification loss
- Similar to SPP-net: want to avoid wasteful computation of convolutional filters
  - Compute convolutional layers once per image
  - Here all local image patches are at the same scale
  - Many more local regions: dense, at every pixel



Long et al., CVPR 2015

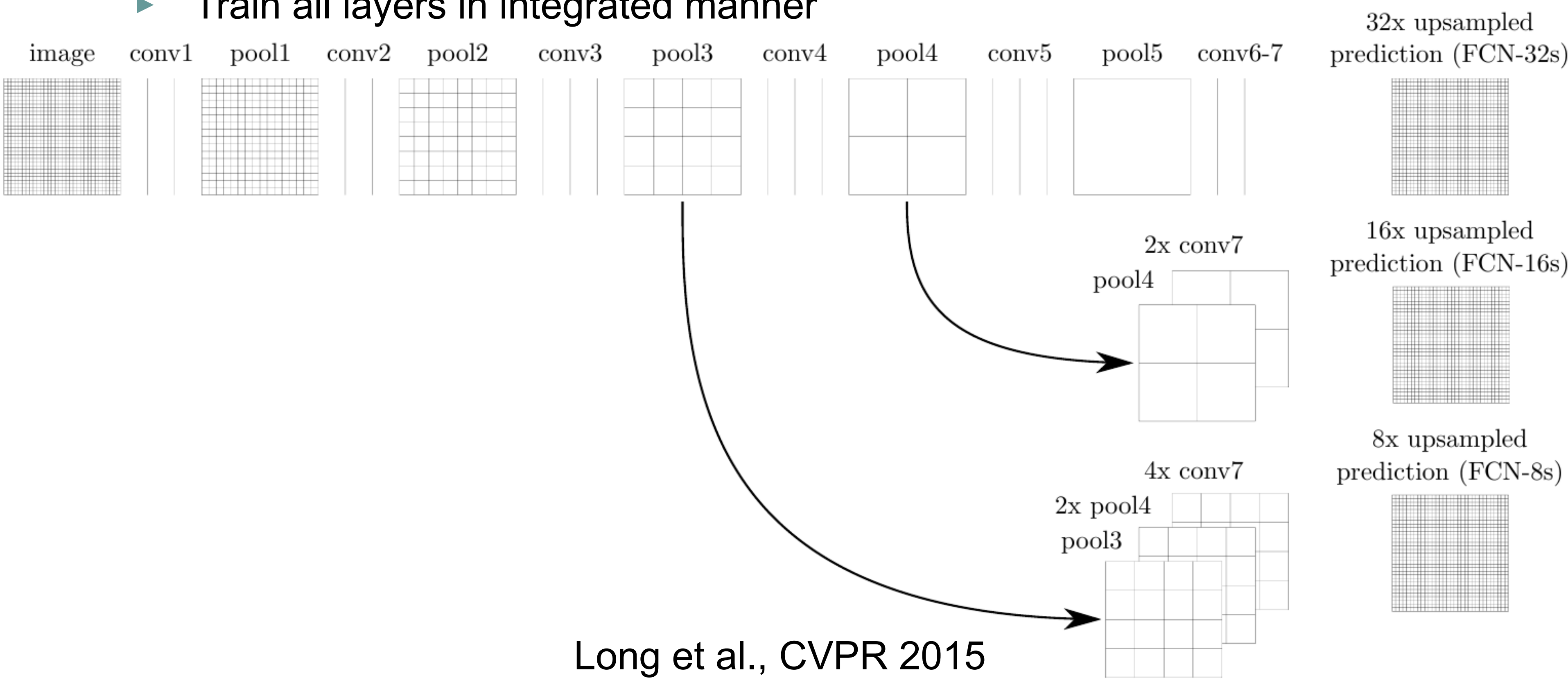
Application to semantic segmentation

- Interpret fully connected layers as 1x1 sized convolutions
  - Function of features in previous layer, but only at own position
  - Still same function is applied across all positions
- Five sub-sampling layers reduce the resolution of output map by factor 32



Application to semantic segmentation

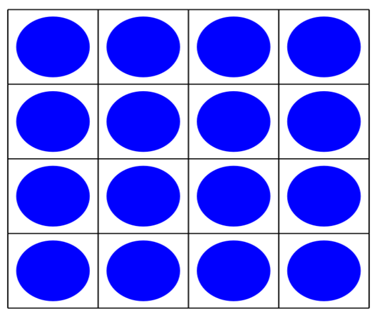
- Idea 1: up-sampling via bi-linear interpolation
  - Gives blurry predictions
- Idea 2: weighted sum of response maps at different resolutions
  - Upsampling of the later and coarser layer
  - Concatenate fine layers and upsampled coarser ones for prediction
  - Train all layers in integrated manner

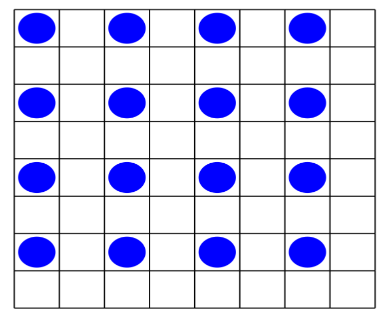


Long et al., CVPR 2015

Upsampling of coarse activation maps

- Simplest form: use bilinear interpolation or nearest neighbor interpolation
  - Note that these can be seen as upsampling by zero-padding, followed by convolution with specific filters, no channel interactions
- Idea can be generalized by learning the convolutional filter
  - No need to hand-pick the interpolation scheme
  - Can include channel interactions, if those turn out be useful





$$\text{Bi-linear:} \quad \frac{1}{4}\begin{pmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{pmatrix} \qquad \text{Nearest neighbor:} \quad \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

- Resolution-increasing counterpart of strided convolution
  - Average and max pooling can be written in terms of convolutions
  - See: “Convolutional Neural Fabrics”, Saxena & Verbeek, NIPS 2016.

Application to semantic segmentation

- Results obtained at different resolutions
  - Detail better preserved at finer resolutions