Lecture 4: CNNs I - Architecture & Equivariance

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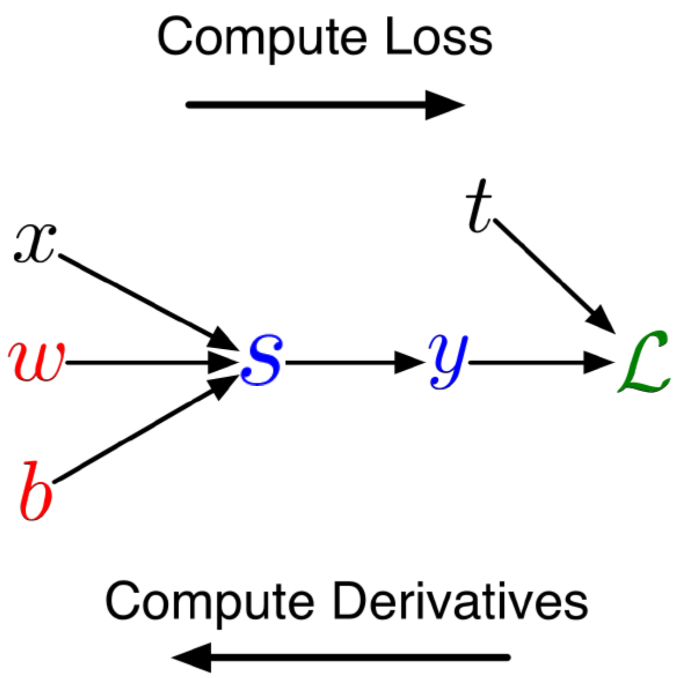
Computation graph

- Represent the computations using a computation graph
  - Nodes: inputs & computed quantities
  - Edges: which nodes are computed directly as function of which other nodes



General Backpropagation

- Given a computation graph

Let $v_1, \ldots, v_N$ be a topological ordering of the computation graph (i.e. parents come before children.)

v_N denotes the variable we're trying to compute derivatives of (e.g. loss)

forward pass

For $i = 1, \ldots, N$

Compute v_i as a function of $\mathrm{Pa}(v_i)$

backward pass

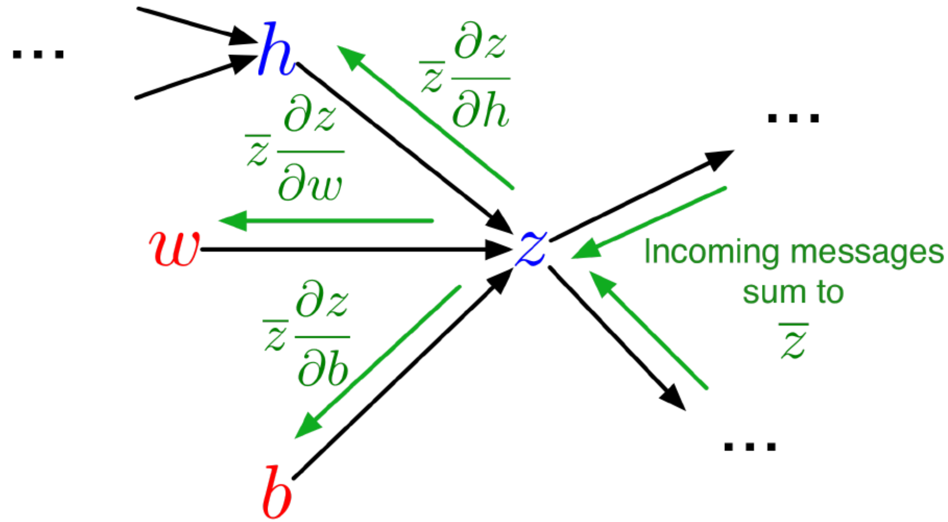
$\delta_{v_N} = 1$

For $i = N-1, \ldots, 1$

$\delta_{v_i} = \sum_{j \in \mathrm{Ch}(v_i)} \delta_{v_j} \frac{\partial v_j}{\partial v_i}$

General Backpropagation

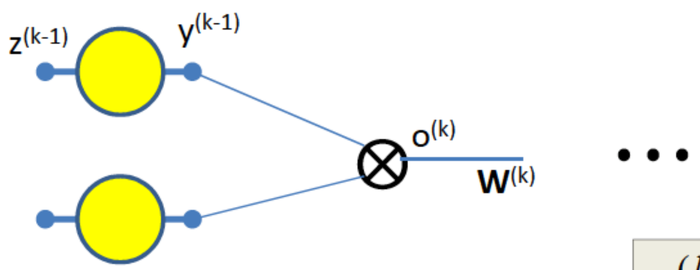
- Backprop as message passing:



  - Each node receives a set of messages from its children, which are aggregated into its error signal, then it passes messages to its parents
  - Modularity: each node only has to know how to compute derivatives w.r.t. its arguments – local computation in the graph

Patterns in backward flow

- Multiplicative node

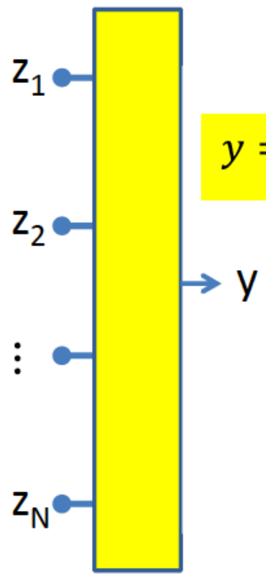


Forward: $\boxed{o_i^{(k)} = y_j^{(k-1)} y_l^{(k-1)}}$

$$\frac{\partial L}{\partial y_j^{(k-1)}} = \frac{\partial L}{\partial o_i^{(k)}} \frac{\partial o_i^{(k)}}{\partial y_j^{(k-1)}} = y_l^{(k-1)} \frac{\partial L}{\partial o_i^{(k)}}$$

Patterns in backward flow

- Max node



$$y = \max_j z_j$$

$$\frac{\partial y}{\partial z_i} = \begin{cases} 1, & i = \operatorname{argmax}_j z_j \\ 0, & otherwise \end{cases}$$

- Vector equivalent of subgradient
  - 1 w.r.t. the largest incoming input
    - Incremental changes in this input will change the output
  - 0 for the rest
    - Incremental changes to these inputs will not change the output

Vector form of BackProp

- Review: Jacobian of vector functions

$$\mathbf{J} = \left[\frac{\partial \mathbf{f}}{\partial x_1} \quad \cdots \quad \frac{\partial \mathbf{f}}{\partial x_n} \right] = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}.$$

- Vectorized chain rule

$$\mathbf{x} \in \mathbb{R}^m, \mathbf{y} \in \mathbb{R}^n$$

$$g : \mathbb{R}^m \to \mathbb{R}^n, \mathbf{y} = g(\mathbf{x})$$

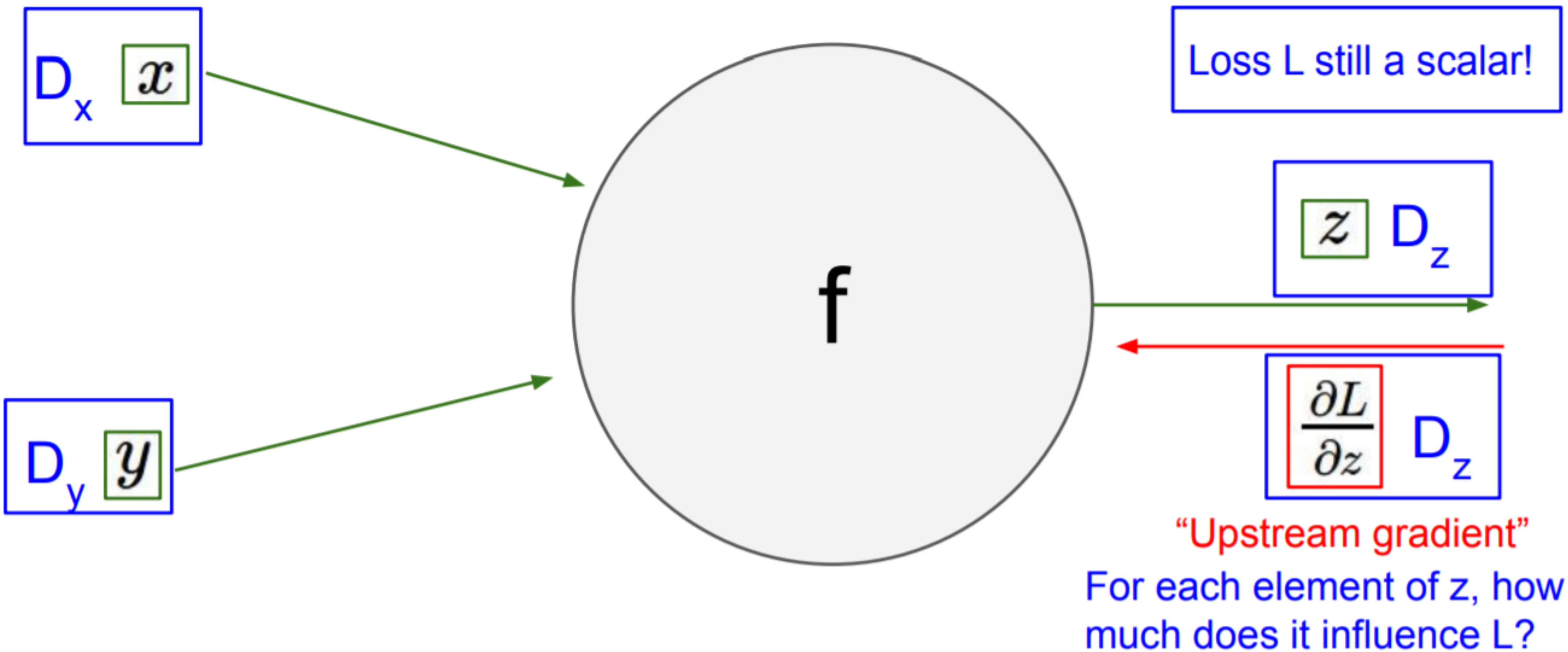
$$f : \mathbb{R}^n \to \mathbb{R}, z = f(\mathbf{y})$$

$$\frac{\partial z}{\partial \mathbf{x}_i} = \sum_{j=1}^{n} \frac{\partial z}{\partial \mathbf{y}_j} \frac{\partial \mathbf{y}_j}{\partial \mathbf{x}_i}$$

$$\nabla_{\mathbf{x}} z = \left[\frac{\partial \mathbf{y}_j}{\partial \mathbf{x}_i} \right] \nabla_{\mathbf{y}} z = \left(\frac{\partial \mathbf{y}}{\partial \mathbf{x}} \right)^T \nabla_{\mathbf{y}} z$$

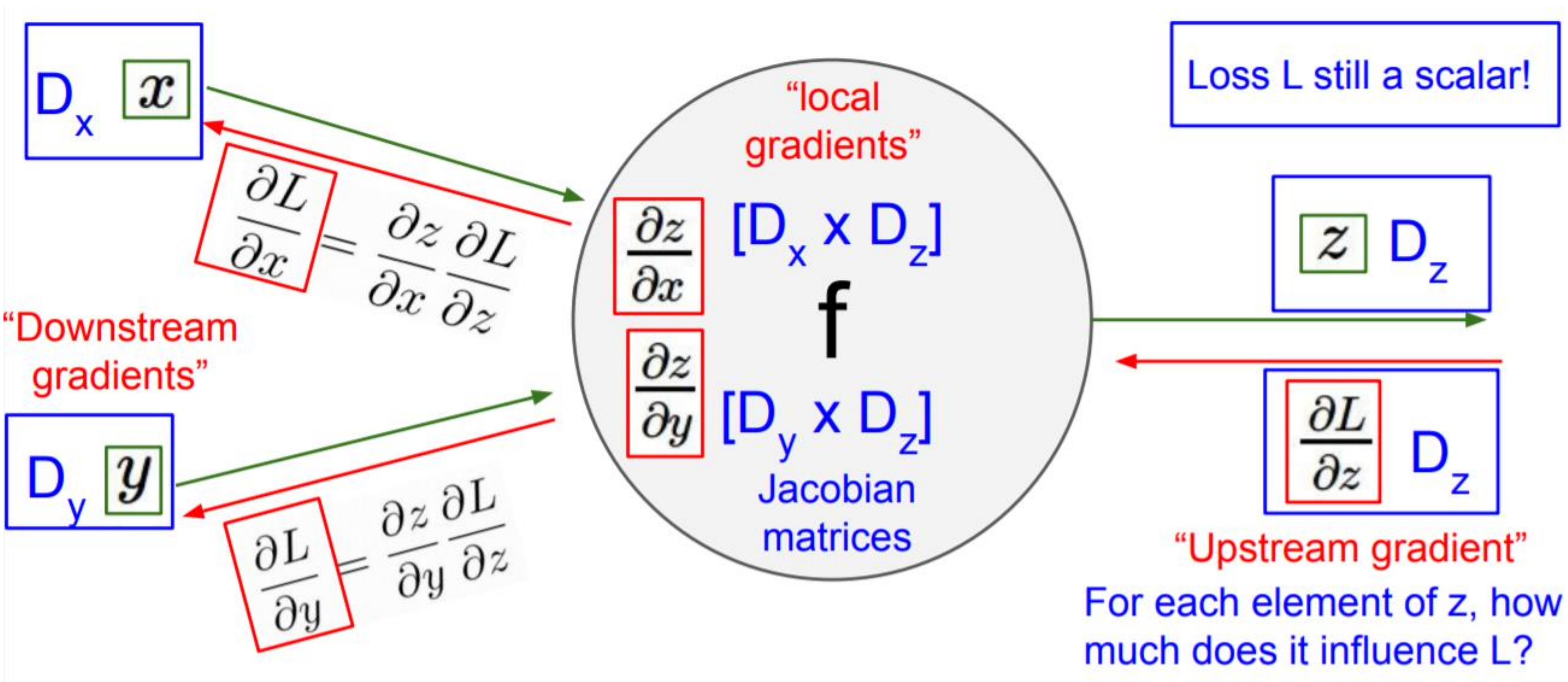
Vector form of BackProp

- Forward pass with vectors



Vector form of BackProp

- Note: here the Jacobian matrices are actually the transpose of the standard version.



Matrix form of BackProp

- Often used in mini-batches
  - N is the batch size, for instance.

x: [N×D]

[2 1 -3]
[-3 4 2]

w: [D×M]

[3 2 1 -1]
[2 1 3 2]
[3 2 1 -2]

Matrix Multiply

$$y_{n,m} = \sum_{d} x_{n,d} w_{d,m}$$

y: [N×M]

[13 9 -2 -6]
[5 2 17 1]

dL/dy: [N×M]

[2 3 -3 9]
[-8 1 4 6]

Matrix form of BackProp

- Often used in mini-batches
  - N is the batch size, for instance.

x: [N×D]

$$\begin{bmatrix} 2 & 1 & -3 \\ -3 & 4 & 2 \end{bmatrix}$$

w: [D×M]

$$\begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

Matrix Multiply

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

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dL/dy: [N×M]

$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

Jacobians:
dy/dx: [(N×D)×(N×M)]
dy/dw: [(D×M)×(N×M)]

For a neural net we may have
N=64, D=M=4096
Each Jacobian takes 256 GB of memory!
Must work with them implicitly!

Matrix form of BackProp

- Often used in mini-batches
  - N is the batch size, for instance.

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$$\begin{bmatrix} 2 & 1 & -3 \\ -3 & 4 & 2 \end{bmatrix}$$

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Matrix Multiply

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[N×D] [N×M] [M×D]

$$\boxed{\frac{\partial L}{\partial x} = \left(\frac{\partial L}{\partial y}\right) w^T}$$

$$\frac{\partial L}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} \frac{\partial y_{n,m}}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} w_{d,m}$$

Matrix form of BackProp

- Often used in mini-batches
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x: [N×D]

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Matrix Multiply

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dL/dy: [N×M]

$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

[N×D] [N×M] [M×D]

$$\boxed{\frac{\partial L}{\partial x} = \left(\frac{\partial L}{\partial y}\right) w^T}$$

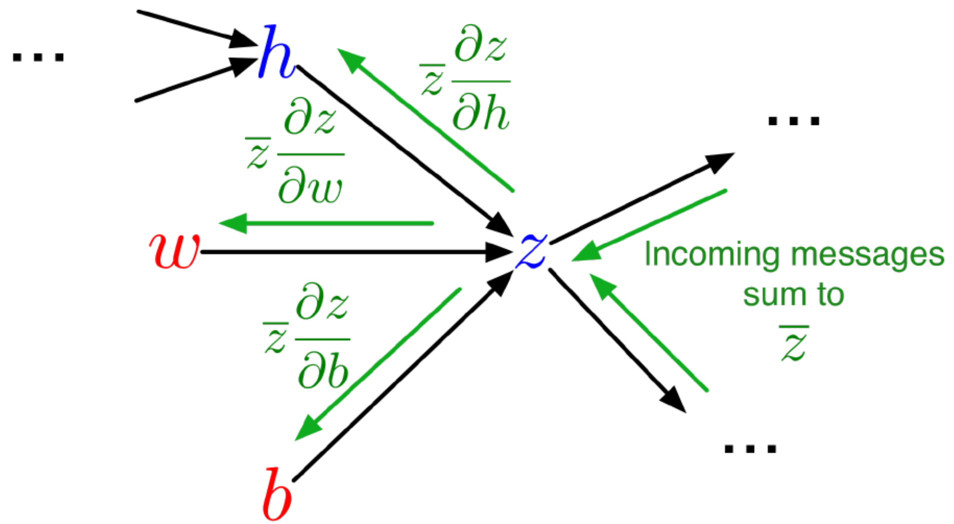
[D×M] [D×N] [N×M]

$$\boxed{\frac{\partial L}{\partial w} = x^T \left(\frac{\partial L}{\partial y}\right)}$$

These formulas are easy to remember: they are the only way to make shapes match up!

Computation cost

- Forward pass: one add-multiply operation per weight
- Backward pass: two add-multiply operations per weight



- For a multilayer network, the cost is linear in the number of layers, quadratic in the number of units per layer

Backpropagation

- Backprop is used to train the majority of neural nets
  - Even generative network learning, or advanced optimization algorithms (second-order) use backprop to compute the update of weights
- However, backprop seems biologically implausible
  - No evidence for biological signals analogous to error derivatives
  - All the existing biologically plausible alternatives learn much more slowly on computers.
  - So how on earth does the brain learn???

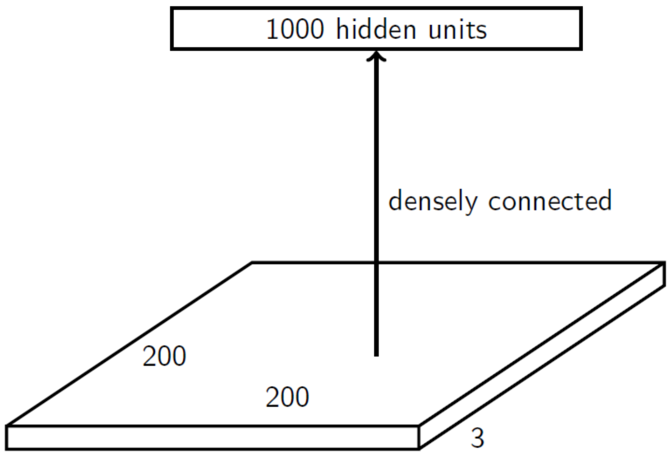
Outline

- Why Convolutional Neural Network (CNN)?
  - Motivation and overview
- What is the CNN?
  - Convolution layers & model complexity
  - Closer look at activation functions
  - Pooling layers & model complexity
  - Math properties
- Examples of CNNs

Acknowledgement: Roger Grosse@UofT & Feifei Li's cs231n notes

Motivation

- Visual recognition
  - Suppose we aim to train a network that takes a 200x200 RGB image as input



  - What is the problem with have full connections in the first layer?
    - Too many parameters! 200x200x3x1000 = 120 million
    - What happens if the object in the image shifts a little?

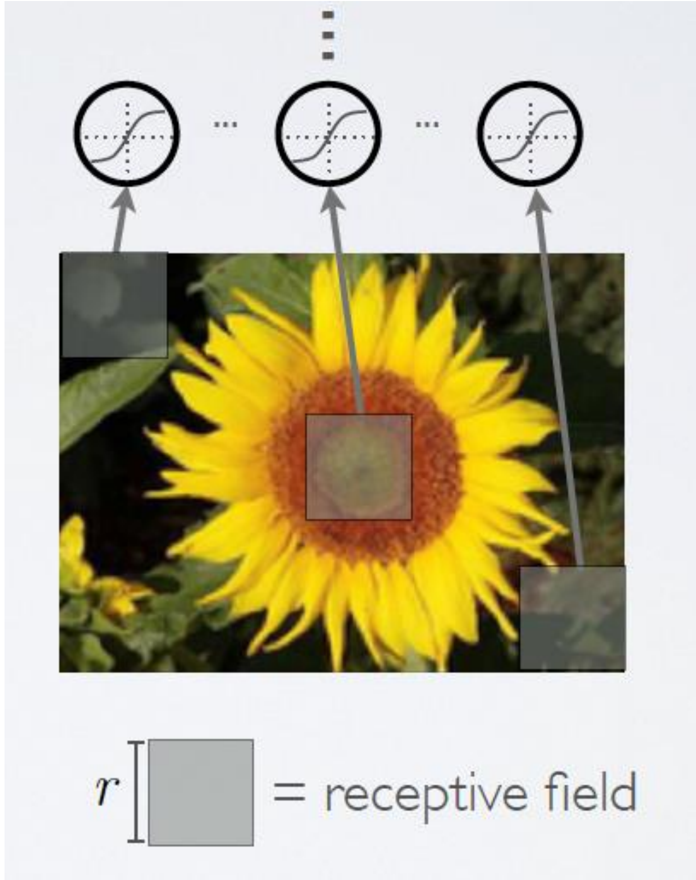
Our goal

- Visual Recognition: Design a neural network that
  - Much deal with very high-dimensional inputs
  - Can exploit the 2D topology of pixels in images
  - Can build in invariance/equivariance to certain variations we can expect
    - Translation, small deformations, illumination, etc.

- Convolution networks leverage these ideas
  - Local connectivity
  - Parameter sharing
  - Pooling/subsampling hidden units

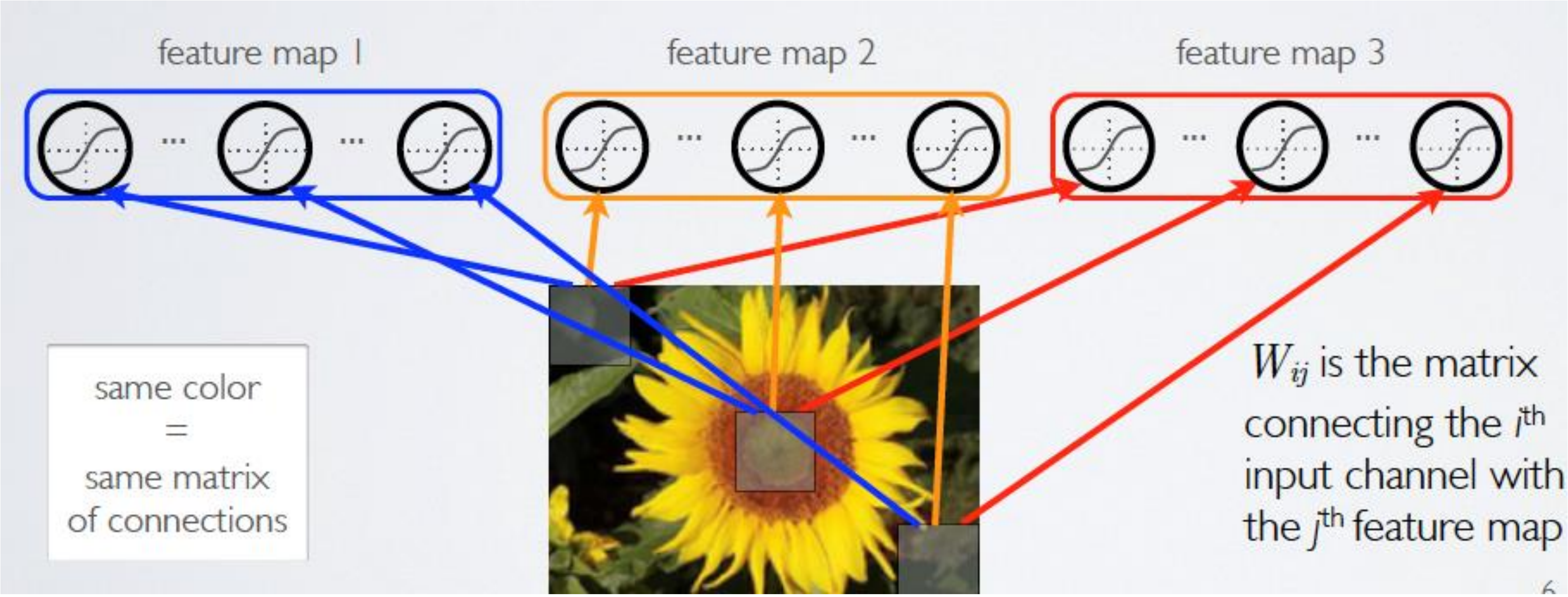
Overview of CNNs

- First idea: Use a local connectivity of hidden units
  - Each hidden unit is connected only to a subregion (patch) of the input image
  - Usually it is connected to all channels
  - Each neuron has a local receptive field



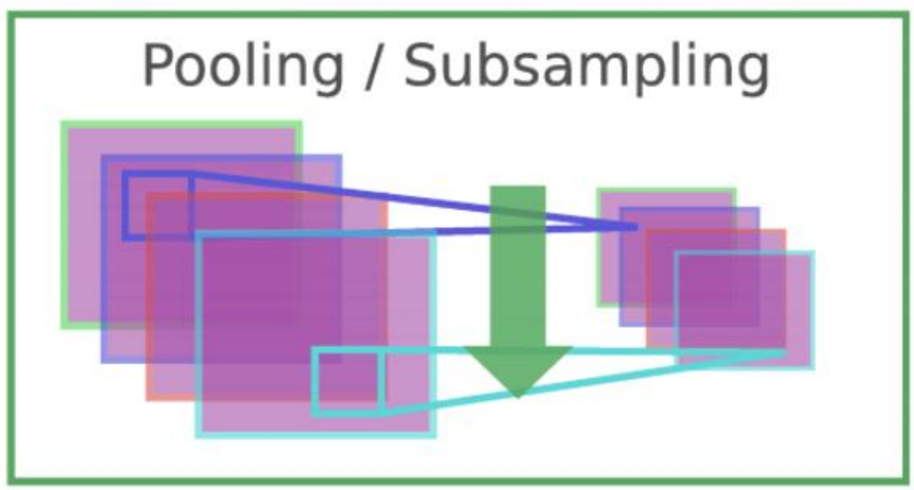
Overview of CNNs

- Second idea: share weights across certain units
  - Units organized into the same “feature map” share weight parameters
  - Hidden units within a feature map cover different positions in the image



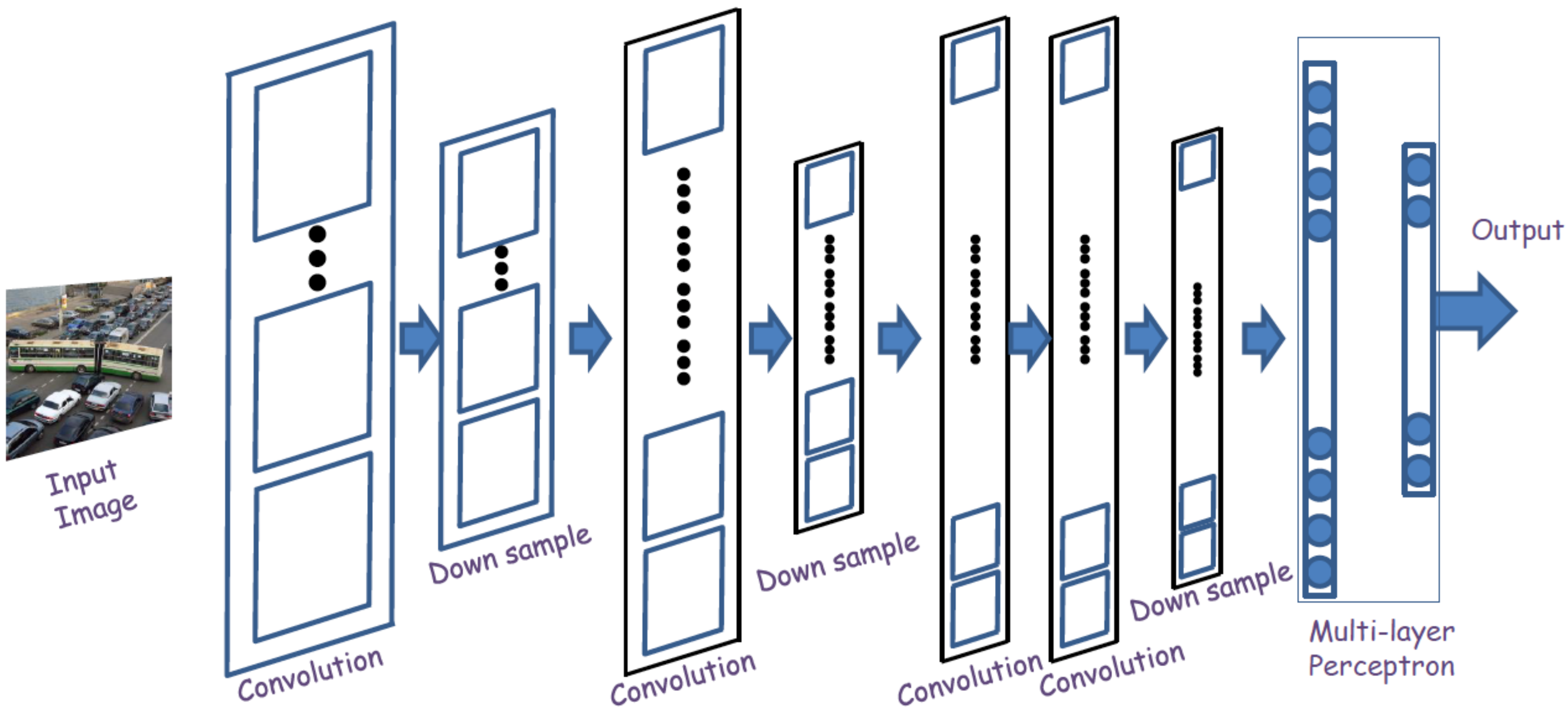
Overview of CNNs

- Third idea: pool hidden units in the same neighborhood
  - Averaging or Discarding location information in a small region
  - Robust toward small deformations in object shapes by ignoring details.



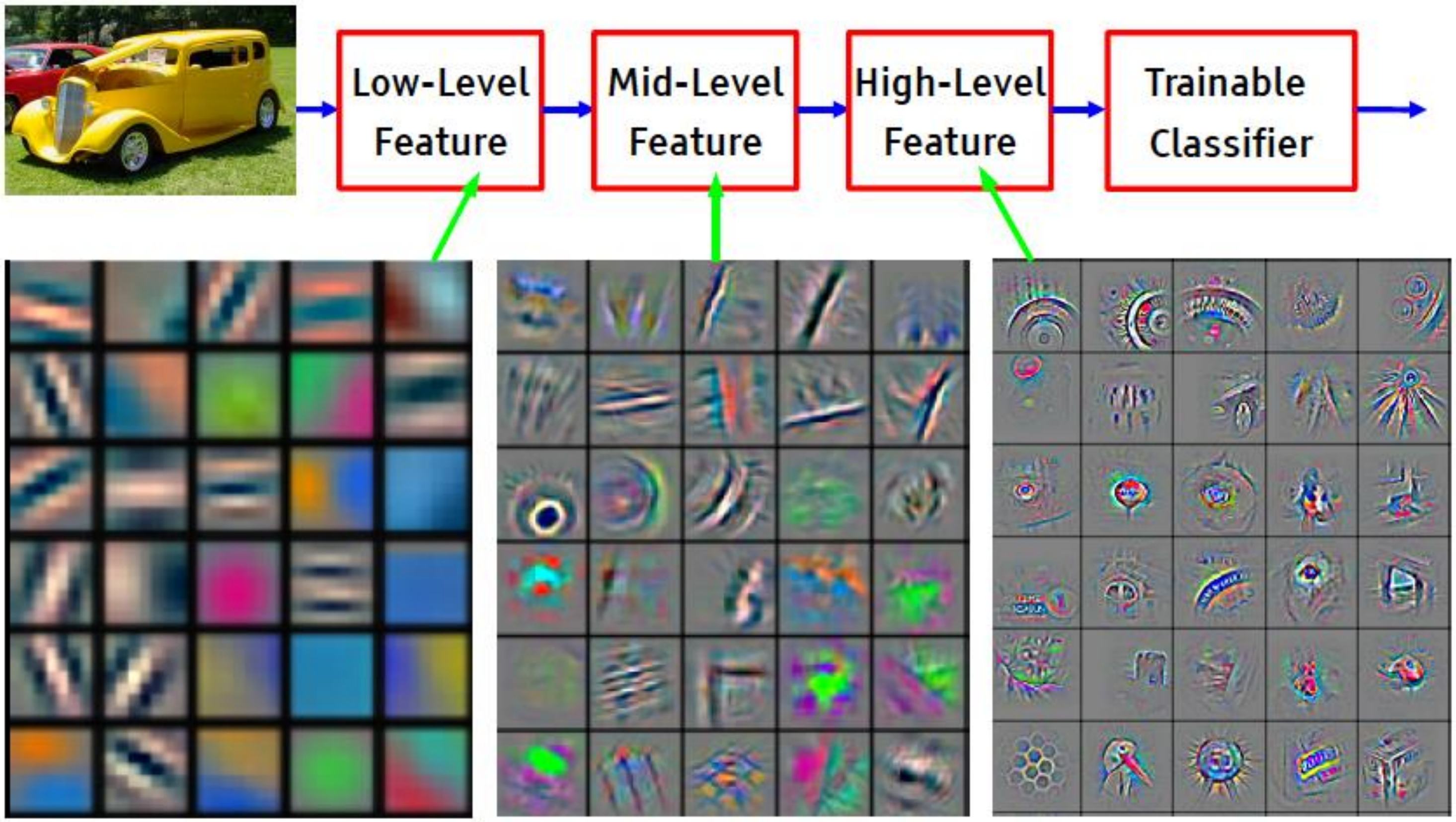
Overview of CNNs

- Fourth idea: Interleaving feature extraction and pooling operations
  - Extracting abstract, compositional features for representing semantic object classes



Overview of CNNs

- Artificial visual pathway: from images to semantic concepts (Representation learning)



Feature visualization of convolutional net trained on ImageNet from [Zeiler & Fergus 2013]

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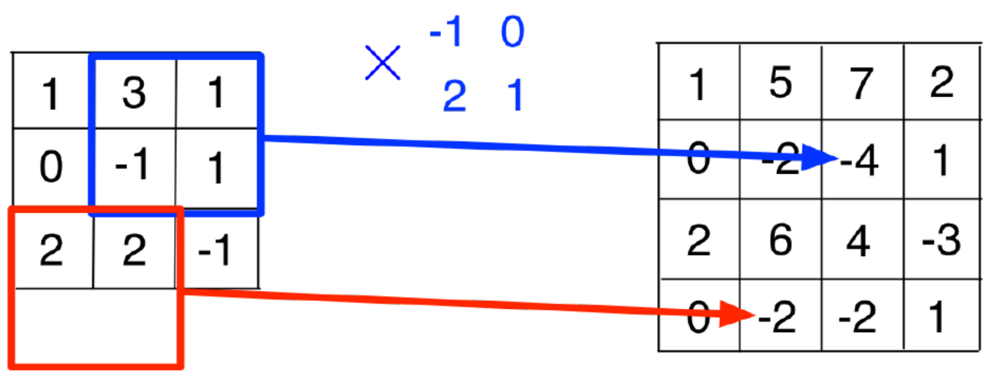
2D Convolution

If A and B are two 2-D arrays, then:

$$(A * B)_{ij} = \sum_s \sum_t A_{st} B_{i-s,j-t}.$$

$$\begin{array}{|c|c|c|}\hline 1 & 3 & 1 \\ \hline 0 & -1 & 1 \\ \hline 2 & 2 & -1 \\ \hline \end{array} \ast \begin{array}{|c|c|}\hline 1 & 2 \\ \hline 0 & -1 \\ \hline \end{array}$$



2D Convolution

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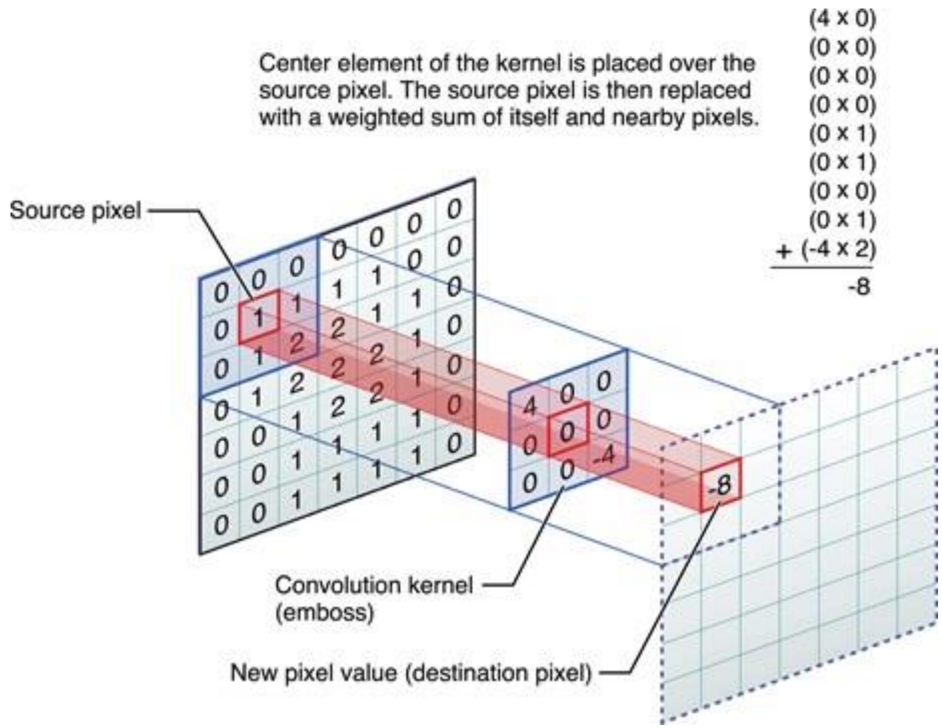
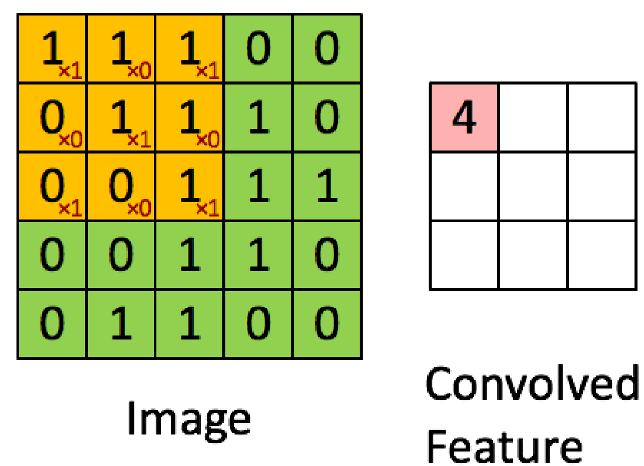
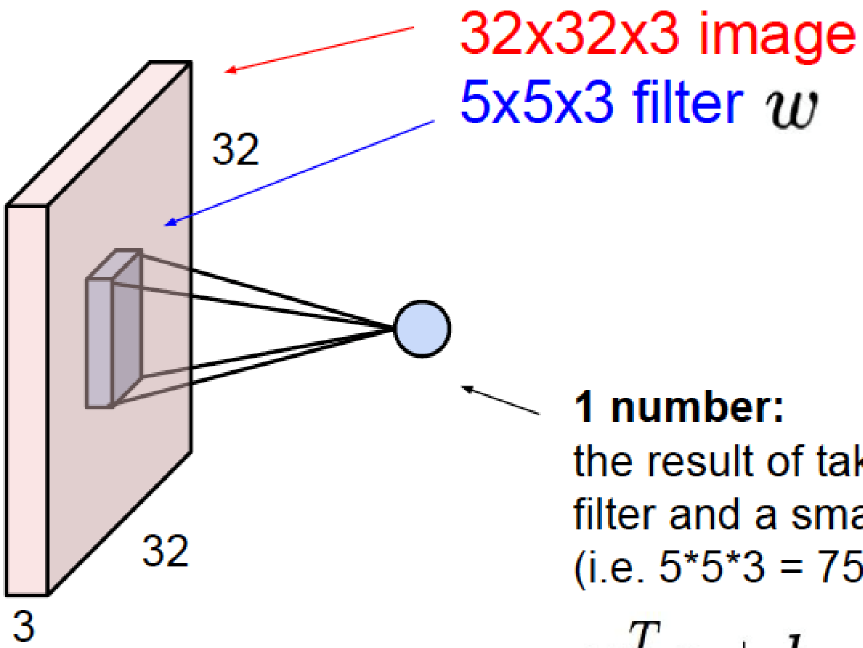




Picture Courtesy: developer.apple.com

Convolution Layers

- Formal definition

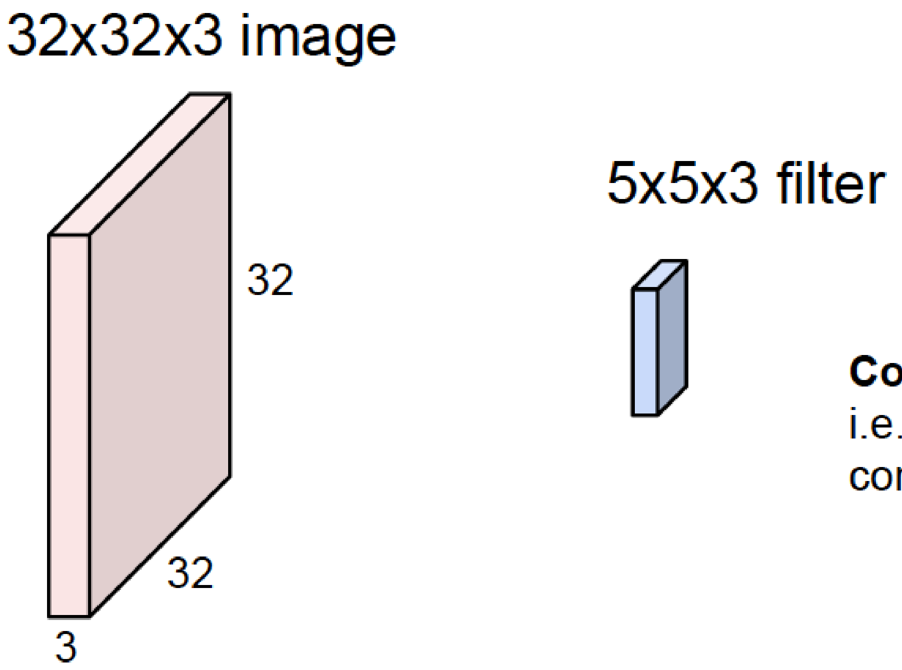


1 number:
the result of taking a dot product between the filter and a small 5x5x3 chunk of the image
(i.e. 5*5*3 = 75-dimensional dot product + bias)

$$w^T x + b$$

Convolution Layers

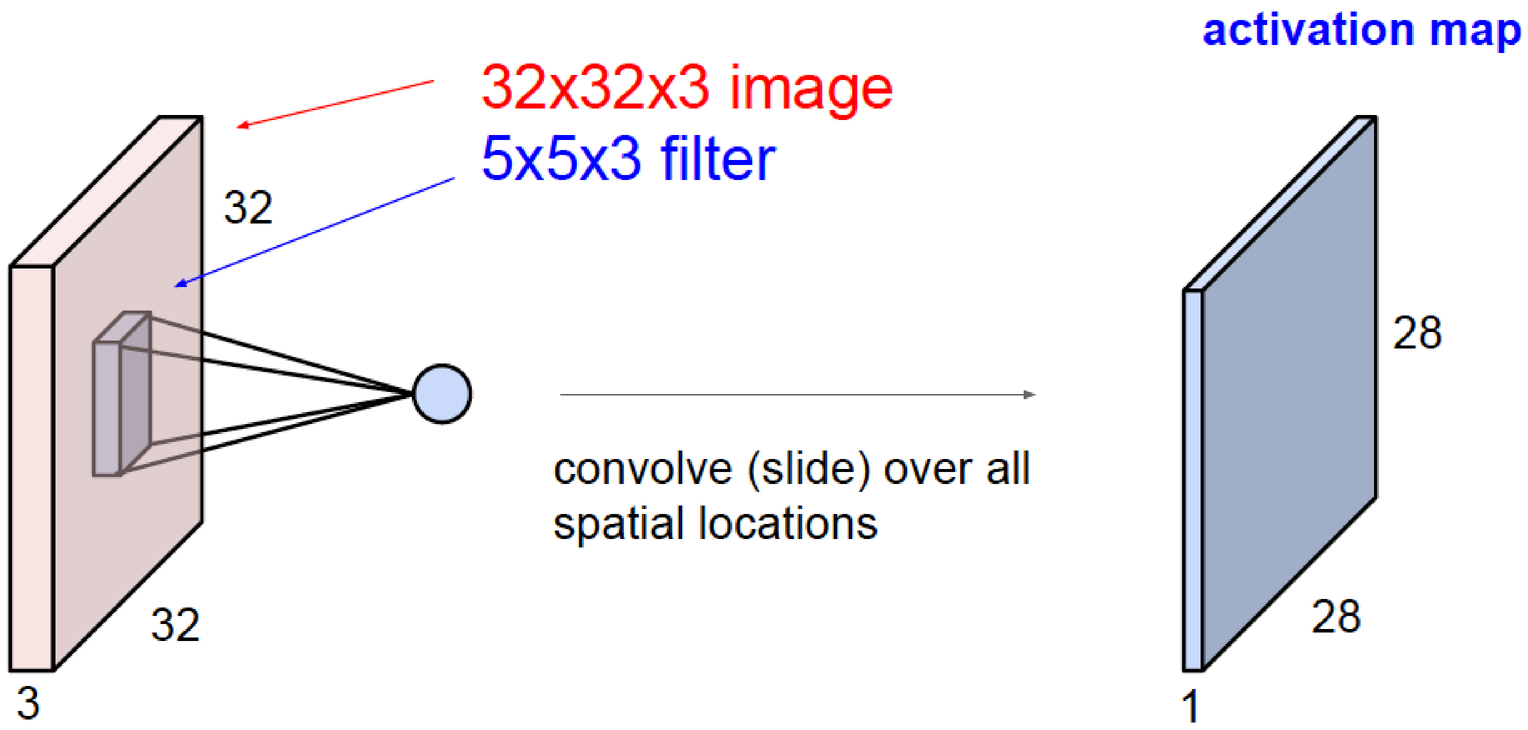
- Define a neuron corresponding to a 5x5 filter



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

Convolution Layers

- Convolution operation
  - Parameter sharing
  - Spatial information



Convolution Layers

- Convolution operation
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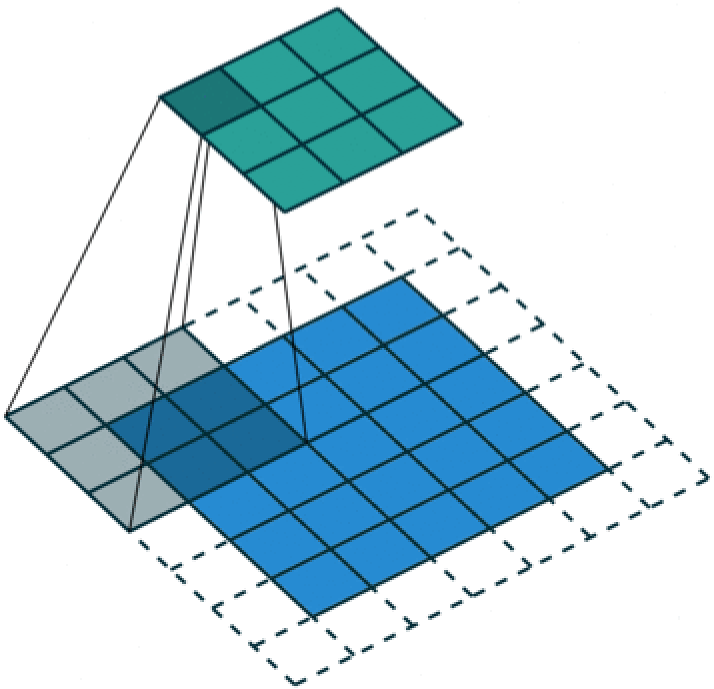
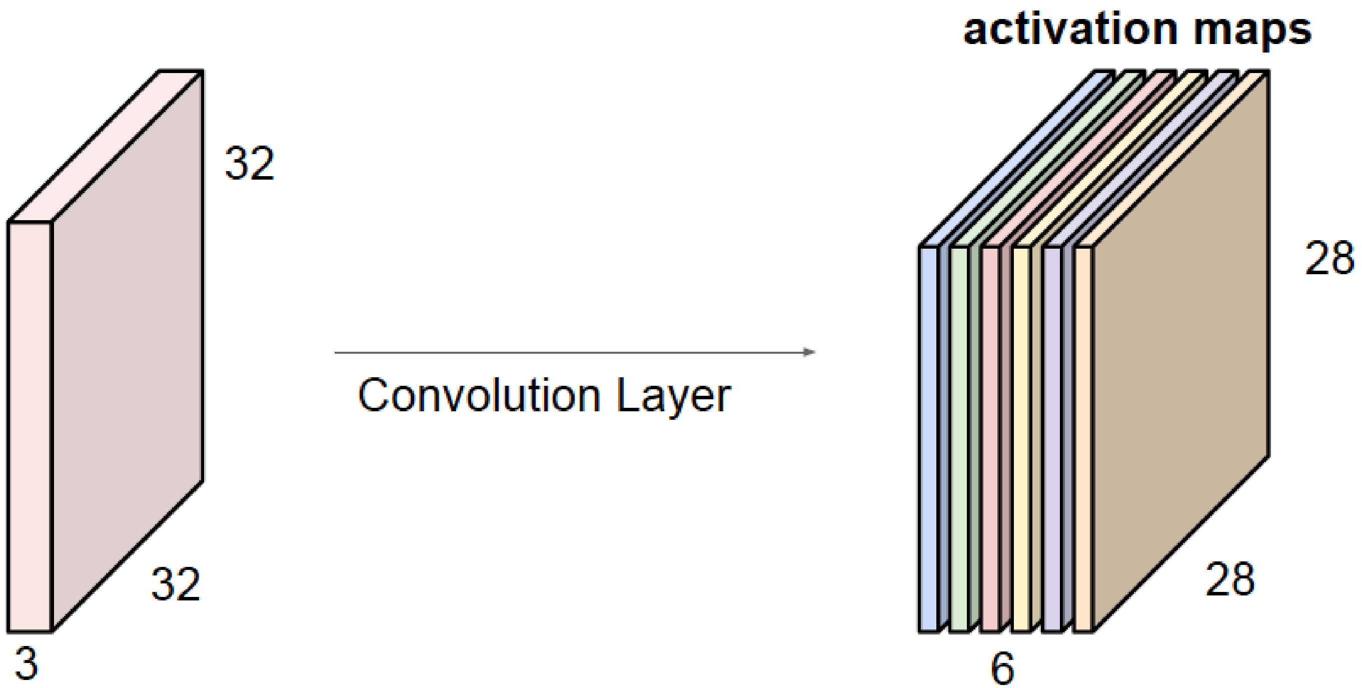
  - Spatial information



Convolution Layers

- Multiple kernels/filters

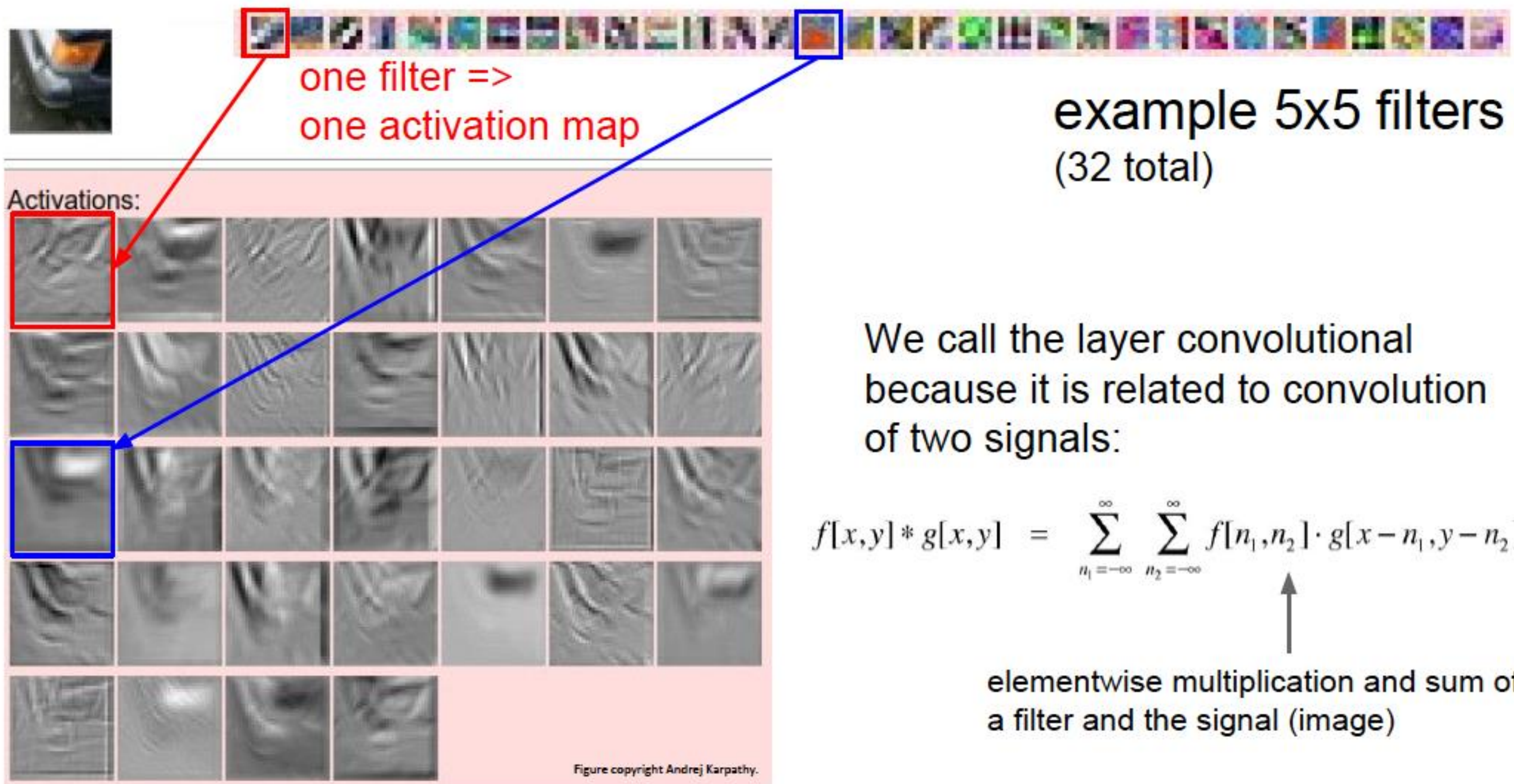
For example, if we had 6 5x5 filters, we'll get 6 separate activation maps:



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

Convolution Layers

- Visualizing the filters and their outputs



example 5x5 filters
(32 total)

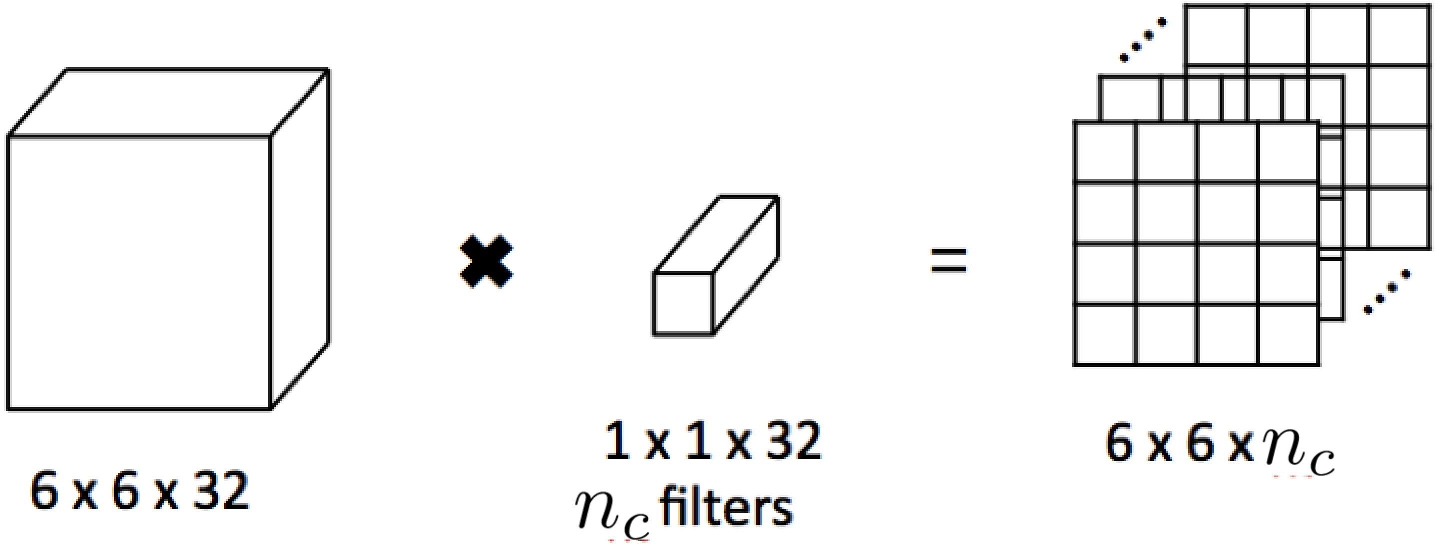
We call the layer convolutional because it is related to convolution of two signals:

$$f[x,y] * g[x,y] = \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} f[n_1,n_2] \cdot g[x-n_1, y-n_2]$$

elementwise multiplication and sum of a filter and the signal (image)

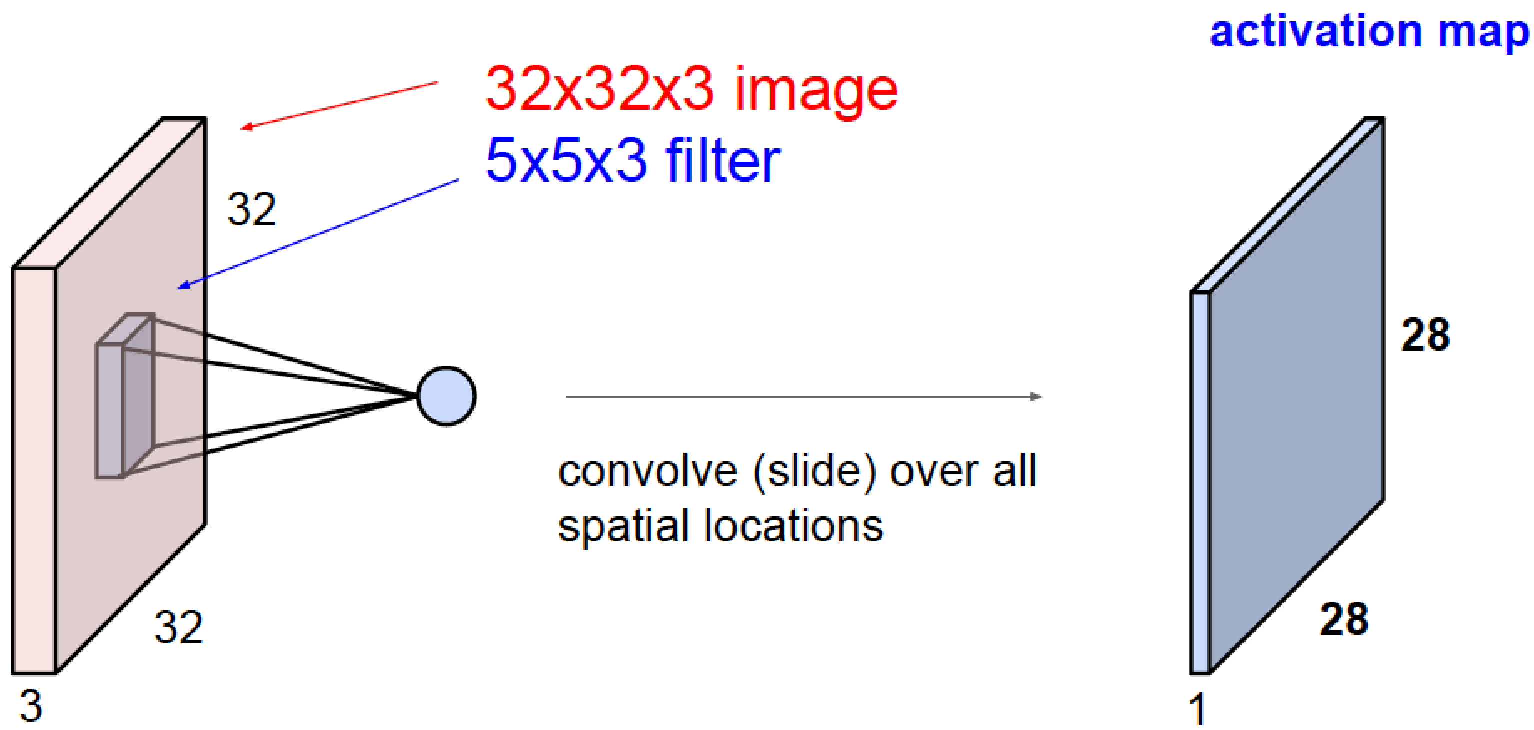
Special Convolutions

- 1x1 convolutions
  - Used in Network-in-network, GoogleNet
  - Reduce or increase dimensionality
  - Can be considered as 'feature pooling"



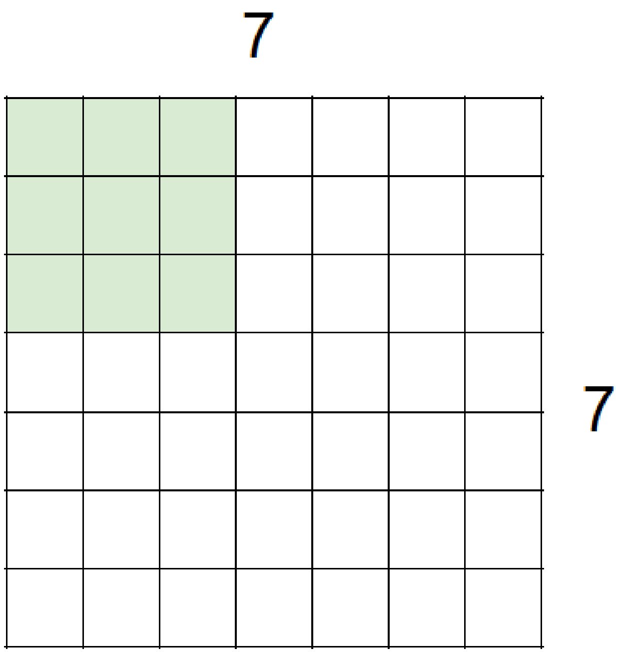
Complexity of Convolution Layers

- Sizes of activation maps and number of parameters



Complexity of Convolution Layers

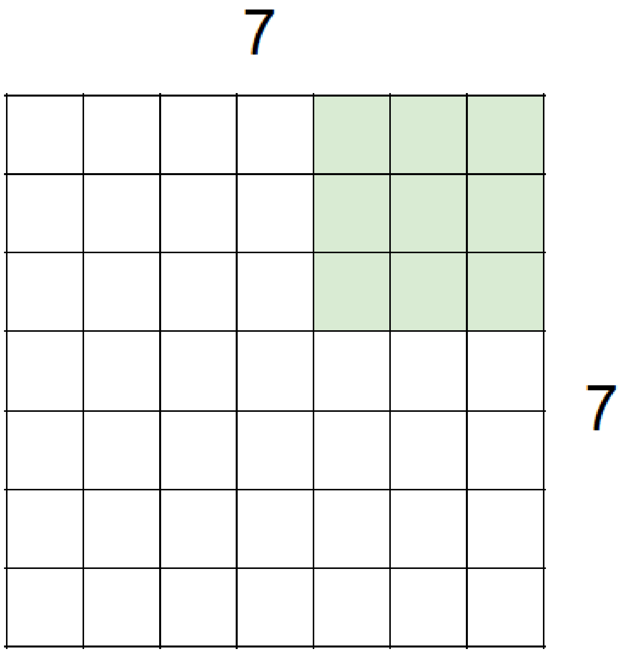
- Size of activation maps



7x7 input (spatially)
assume 3x3 filter

Complexity of Convolution Layers

- Size of activation maps

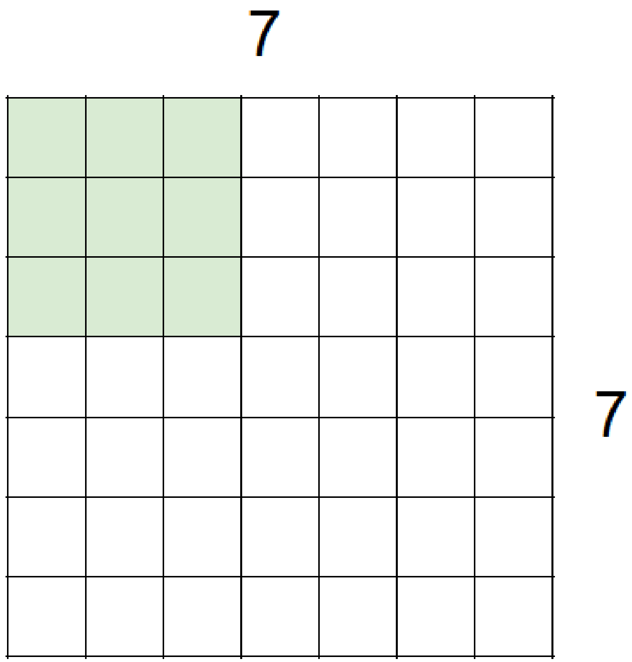


7x7 input (spatially)
assume 3x3 filter

=> 5x5 output

Complexity of Convolution Layers

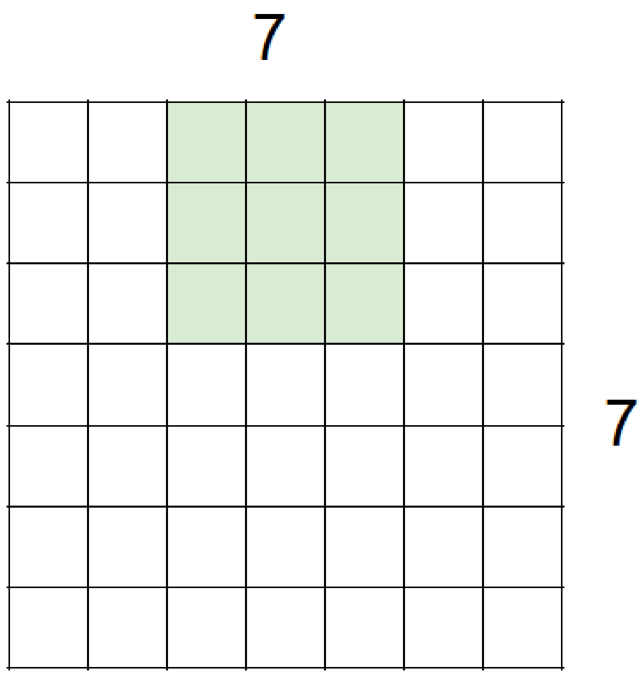
- Case: Stride > 1



7x7 input (spatially)
assume 3x3 filter
applied **with stride 2**

Complexity of Convolution Layers

- Case: Stride > 1



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Complexity of Convolution Layers

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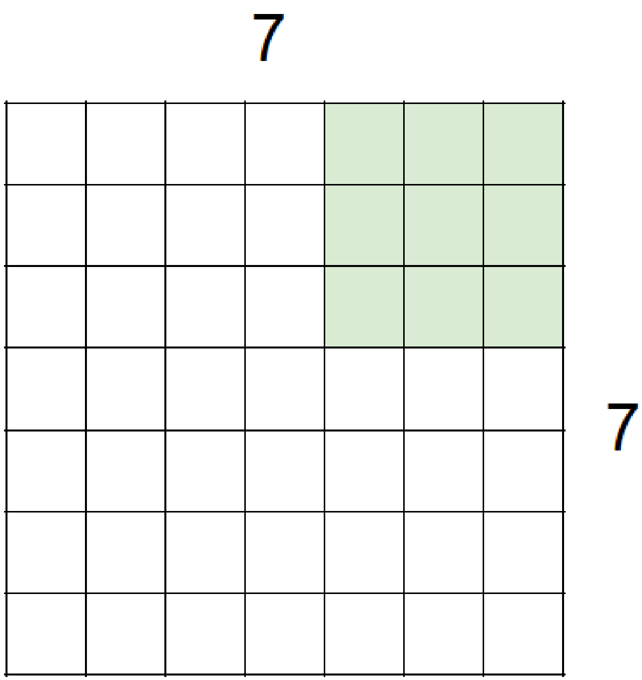
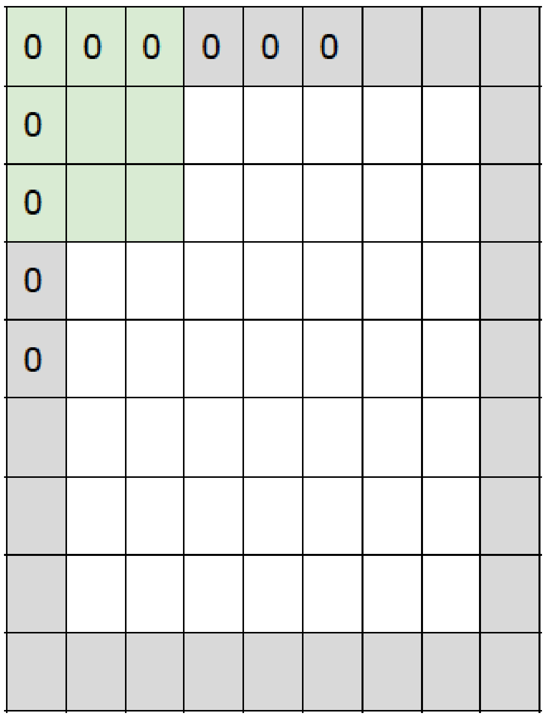


7x7 input (spatially)
assume 3x3 filter
applied **with stride 2**
=> 3x3 output!

Complexity of Convolution Layers

- Zero padding to handle non-integer cases or control the output sizes



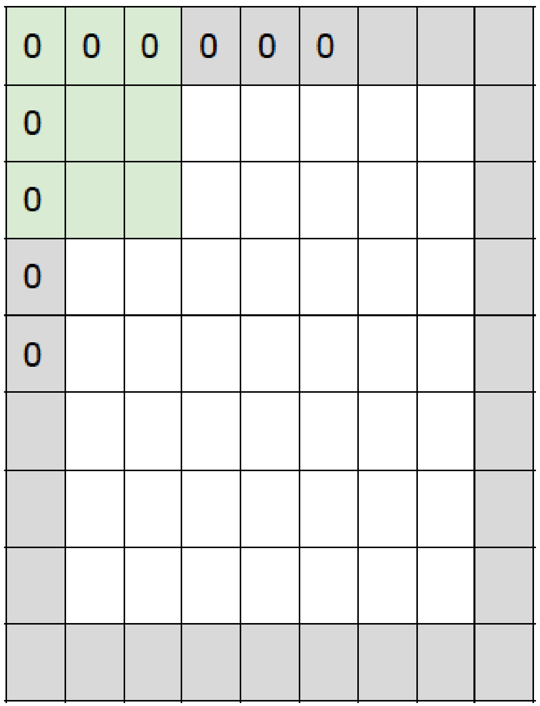
e.g. input 7x7
3x3 filter, applied with **stride 1**
pad with 1 pixel border => what is the output?

7x7 output!

(recall:)
(N - F) / stride + 1

Complexity of Convolution Layers

- Zero padding to handle non-integer cases or control the output sizes

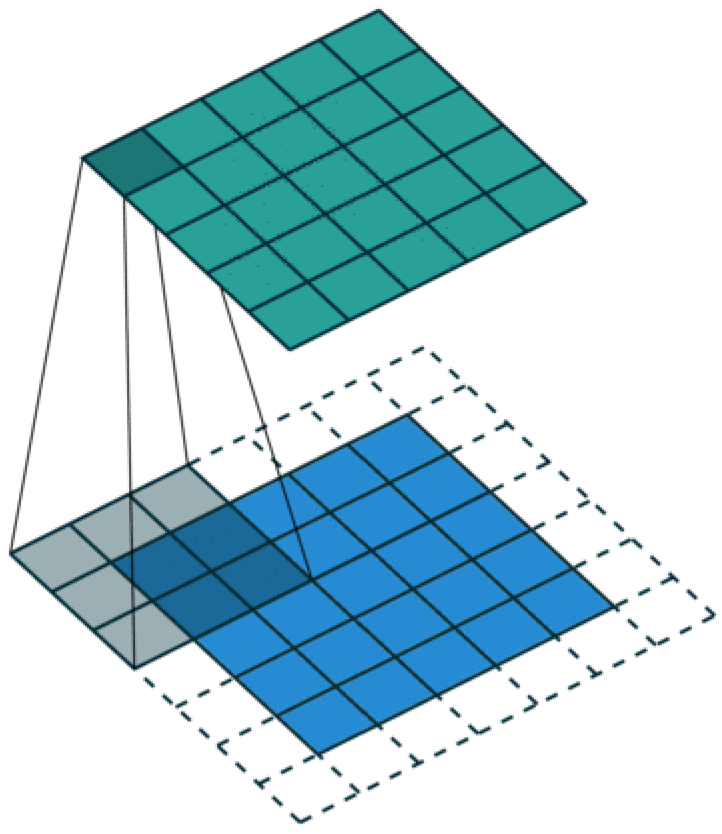


e.g. input 7x7
3x3 filter, applied with **stride 1**
pad with 1 pixel border => what is the output?

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

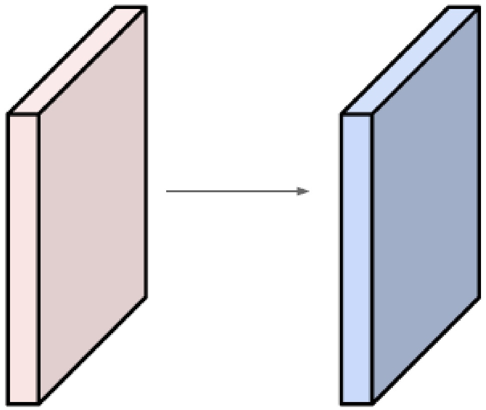
Complexity of Convolution Layers

- Zero padding to handle non-integer cases or control the output sizes



Complexity of Convolution Layers

Examples time:

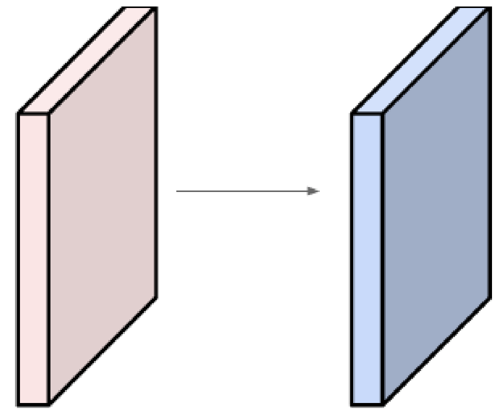


Input volume: **32x32x3**
10 5x5 filters with stride 1, pad 2

Output volume size:
(32+2*2-5)/1+1 = 32 spatially, so
32x32x10

Complexity of Convolution Layers

Examples time:



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**

Complexity of Convolution Layers

- Summary

- 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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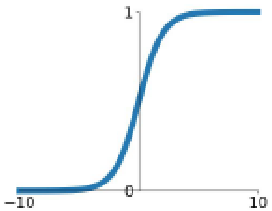
Review: Activation Function

- Zoo of Activation functions

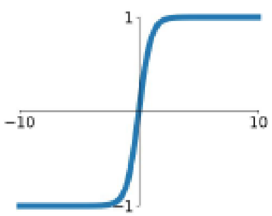
Sigmoid

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



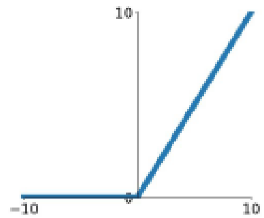
tanh

$\tanh(x)$



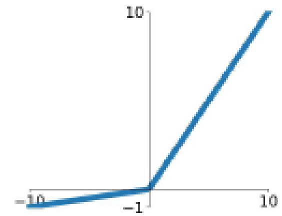
ReLU

$\max(0, x)$



Leaky ReLU

$\max(0.1x, x)$

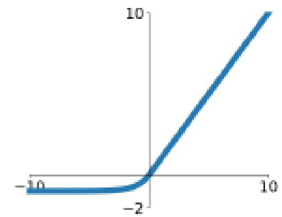


Maxout

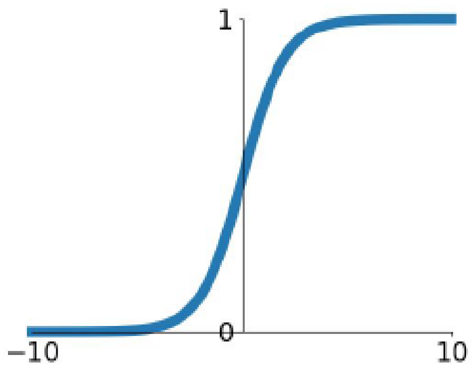
$\max(w_1^T x + b_1, w_2^T x + b_2)$

ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



Sigmoid function



Sigmoid

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

- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating "firing rate" of a neuron

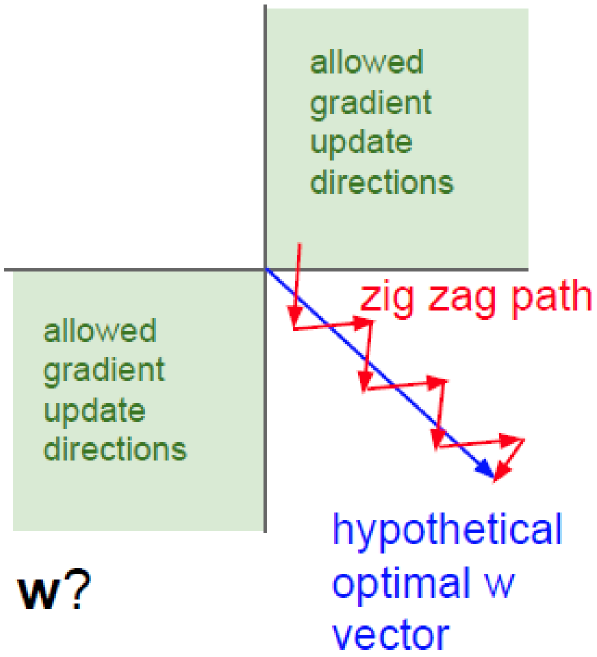
3 problems:

1. Saturated neurons "kill" the gradients
2. Sigmoid outputs are not zero-centered
3. exp() is a bit compute expensive

Sigmoid function

Consider what happens when the input to a neuron is always positive...

$$f\left(\sum_i w_i x_i + b\right)$$

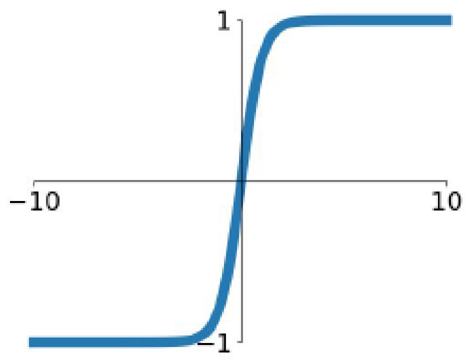


What can we say about the gradients on **w**?

Always all positive or all negative :(

(this is also why you want zero-mean data!)

Tanh function



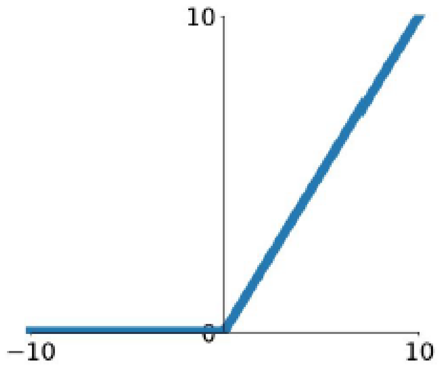
tanh(x)

- Squashes numbers to range [-1,1]
- zero centered (nice)
- still kills gradients when saturated :(

[LeCun et al., 1991]

- Recurrent neural networks: LSTM, GRU

Rectified Linear Unit



ReLU
(Rectified Linear Unit)

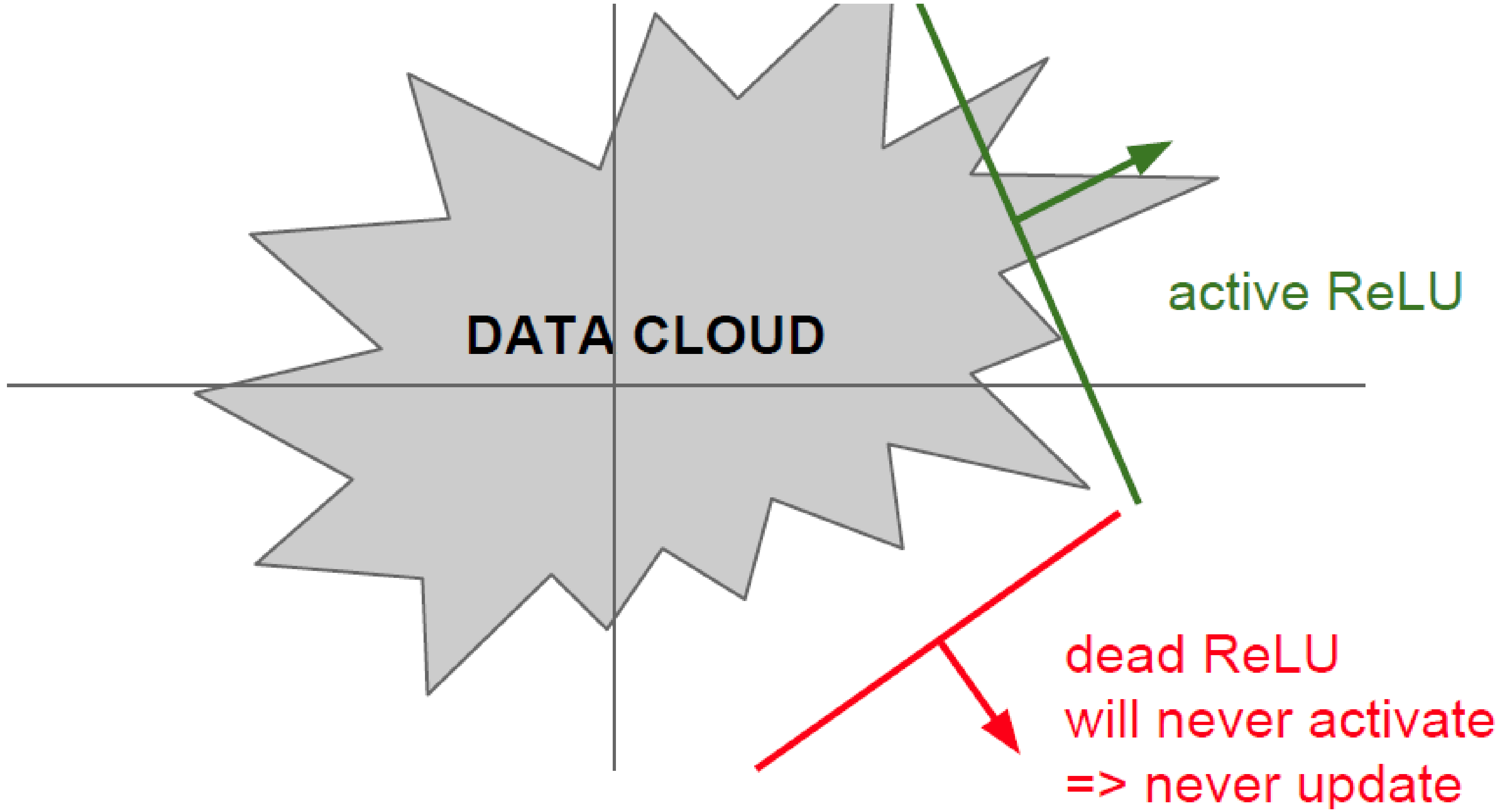
- Computes **f(x) = max(0,x)**

- Does not saturate (in +region)
- Very computationally efficient
- Converges much faster than sigmoid/tanh in practice (e.g. 6x)
- Actually more biologically plausible than sigmoid

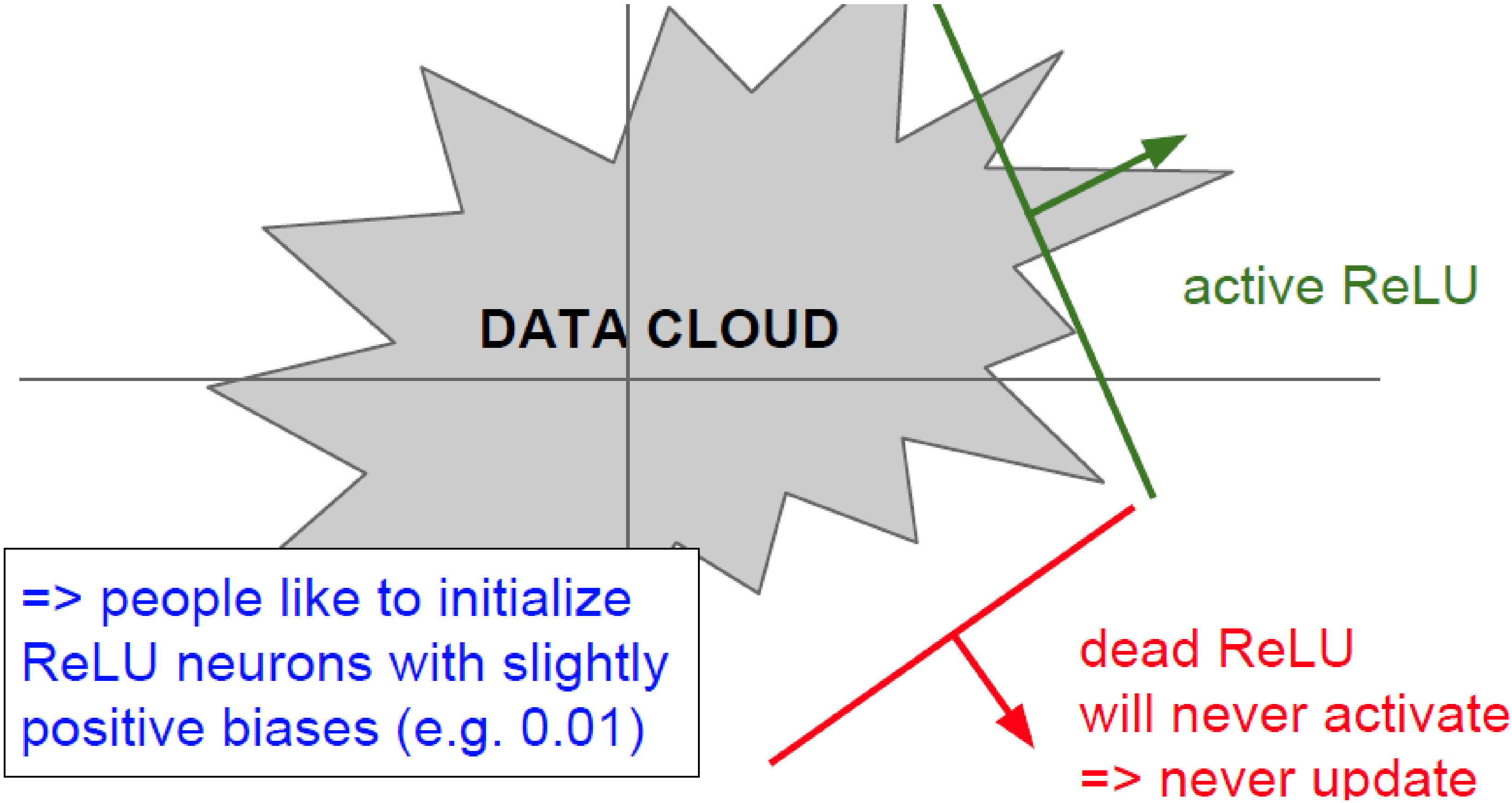
- Not zero-centered output
- An annoyance:

hint: what is the gradient when x < 0?

Rectified Linear Unit



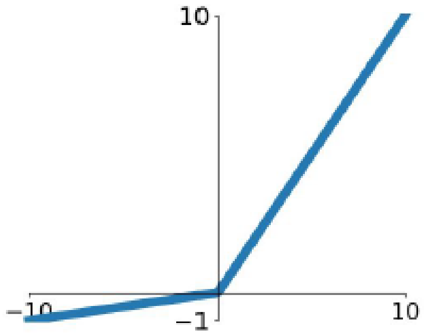
Rectified Linear Unit



=> people like to initialize ReLU neurons with slightly positive biases (e.g. 0.01)

Leaky ReLU

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



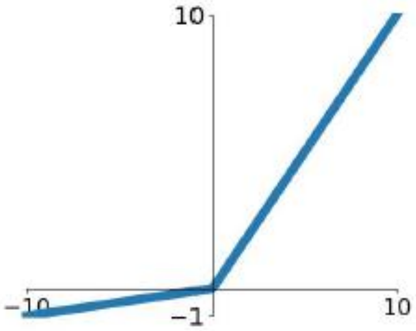
- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- **will not "die".**

Leaky ReLU

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

Leaky ReLU

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



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

Leaky ReLU

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

Parametric Rectifier (PReLU)

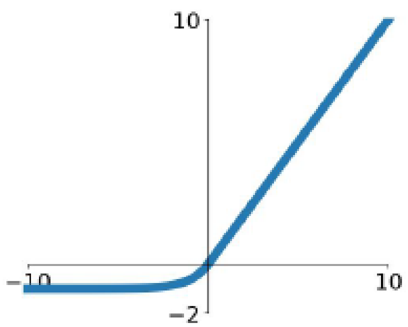
$$f(x) = \max(\alpha x, x)$$

backprop into \alpha
(parameter)

Exponential Linear Units (ELU)

[Clevert et al., 2015]

Exponential Linear Units (ELU)



- All benefits of ReLU
- Closer to zero mean outputs
- Negative saturation regime compared with Leaky ReLU adds some robustness to noise

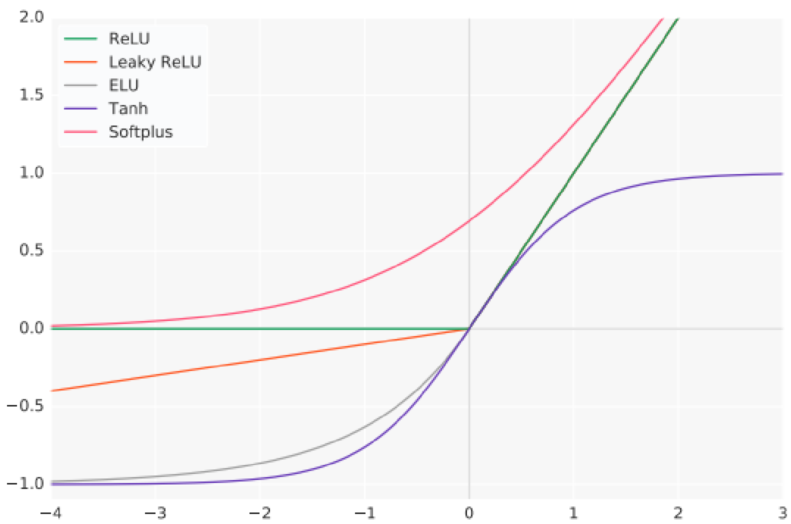
$$f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha\,(\exp(x) - 1) & \text{if } x \le 0 \end{cases}$$

- Computation requires exp()

Summary: Activation function

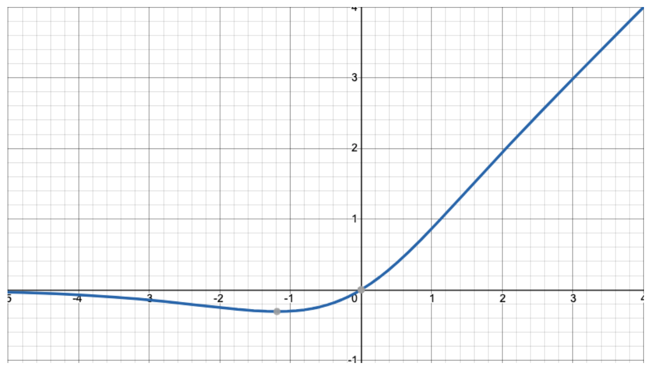
- For internal layers in CNNs
  - Use ReLU. Be careful with your learning rates
  - Try out Leaky ReLU / Maxout / ELU
  - Try out tanh but don't expect much
  - Don't use sigmoid

- For output layers
  - Task dependent
  - Related to your loss function



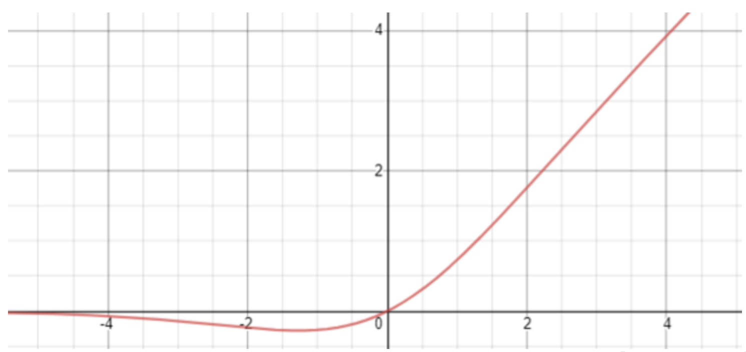
Summary: Activation function

- Recent progresses
  - Mish $f(x) = x \cdot \tanh(\varsigma(x))$, $\varsigma(x) = \ln(1+e^x)$,



https://arxiv.org/abs/1908.08681

  - Swish $f(x) = x * (1 + \exp(-x))^{-1}$



https://arxiv.org/abs/1710.05941

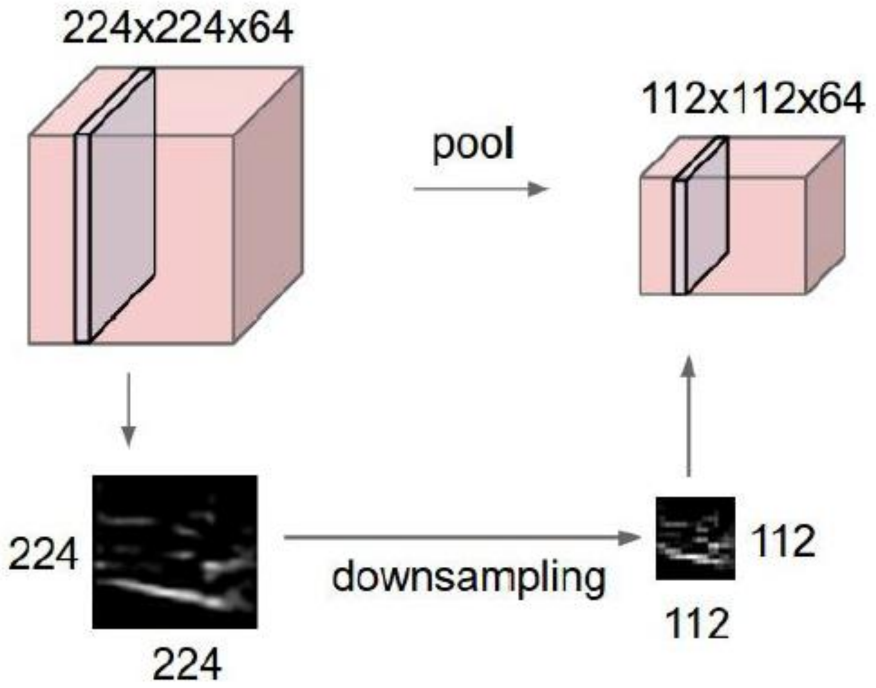
Outline

- Why Convolutional Neural Network (CNN)?
  - Motivation and overview
- What is the CNN?
  - Convolution layers & model complexity
  - Closer look at activation functions
  - Pooling layers & model complexity
  - Math properties
- Examples of CNNs

Acknowledgement: Roger Grosse@UofT & Feifei Li's cs231n notes

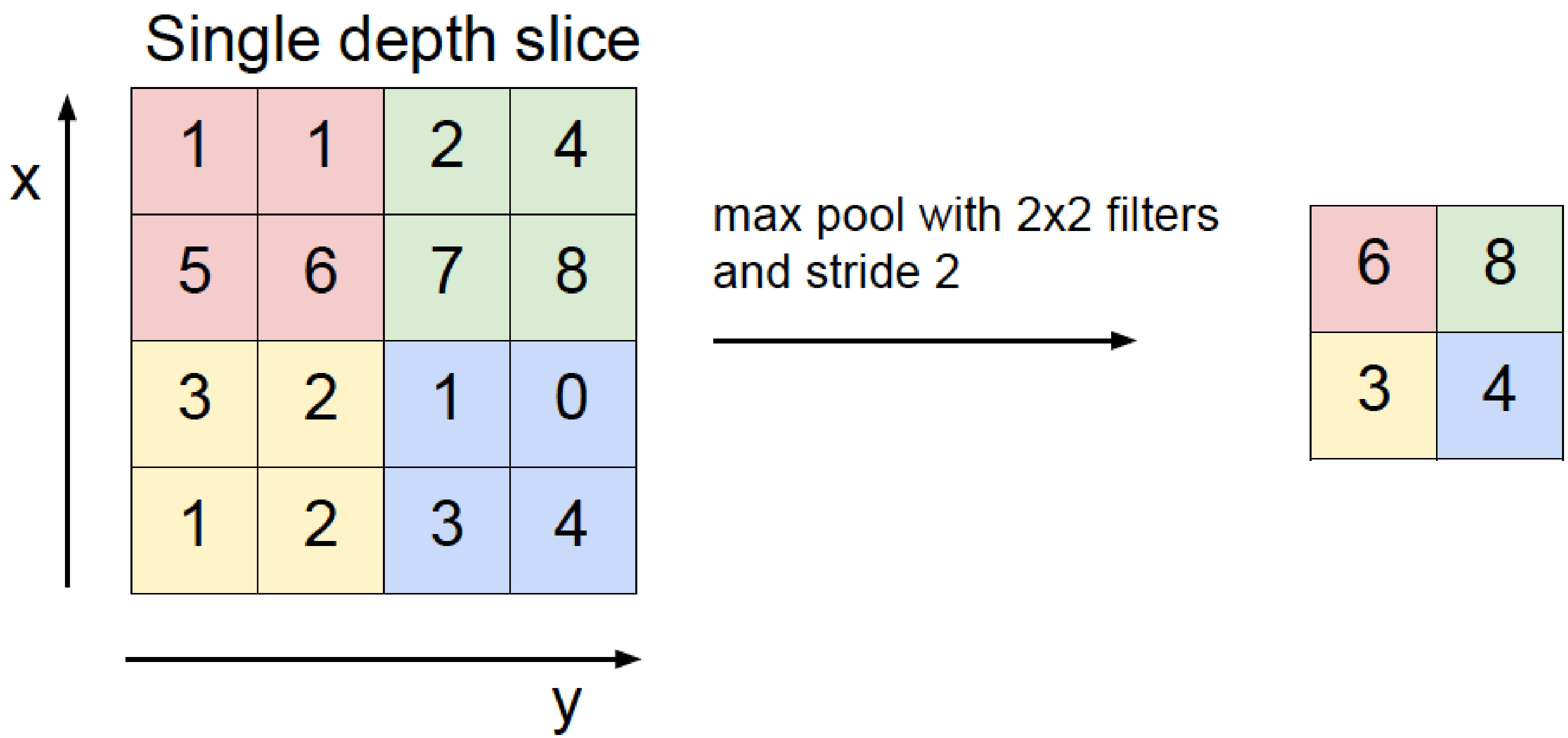
Pooling Layers

- Reducing the spatial size of the feature maps
  - Smaller representations
  - On each activation map independently
  - Low resolution means fewer details



Pooling Layers

- Example: max pooling



Complexity of Pooling Layers

- Summary

  - 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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Math Properties of CNNs

- What representations a CNN can capture in general?
- Consider a representation ϕ as an abstract function

$$\phi : \mathbf{x} \rightarrow \phi(\mathbf{x}) \in \mathbb{R}^d$$

- We want to look at how the representation changes upon transformations of input image.
  - Transformations represent the potential variations in the natural images
  - Translation, scale change, rotation, local deformation etc.

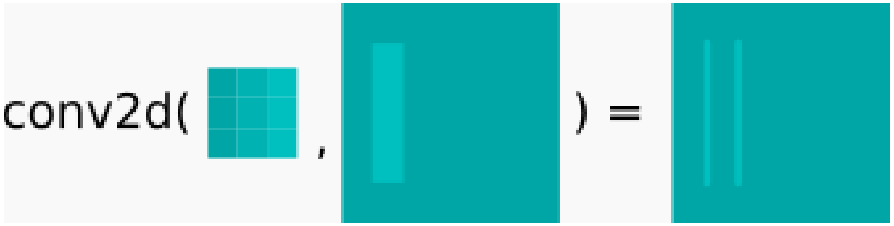
Math Properties of CNNs

- Two key properties of representations
  - Equivariance

    A representation ϕ is equivariant with a transformation g if the transformation can be transferred to the representation output.

$$\exists \text{ a map } M_g : \mathbb{R}^d \to \mathbb{R}^d \text{ such that:}$$
$$\forall \mathbf{x} \in \mathcal{X} : \phi(g\mathbf{x}) \approx M_g \phi(\mathbf{x})$$

  - Example: convolution w.r.t. translation



Math Properties of CNNs

- Two key properties of representations
  - Invariance

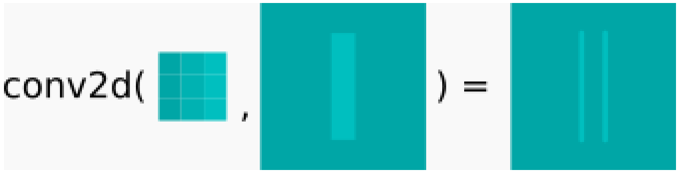
    A representation ϕ is invariant with a transformation g if the transformation has no effect on the representation output.

$$\forall \mathbf{x} \in \mathcal{X} : \phi(g\mathbf{x}) \approx \phi(\mathbf{x})$$

  - Example: convolution+pooling+FC w.r.t. translation

Math Properties of CNNs

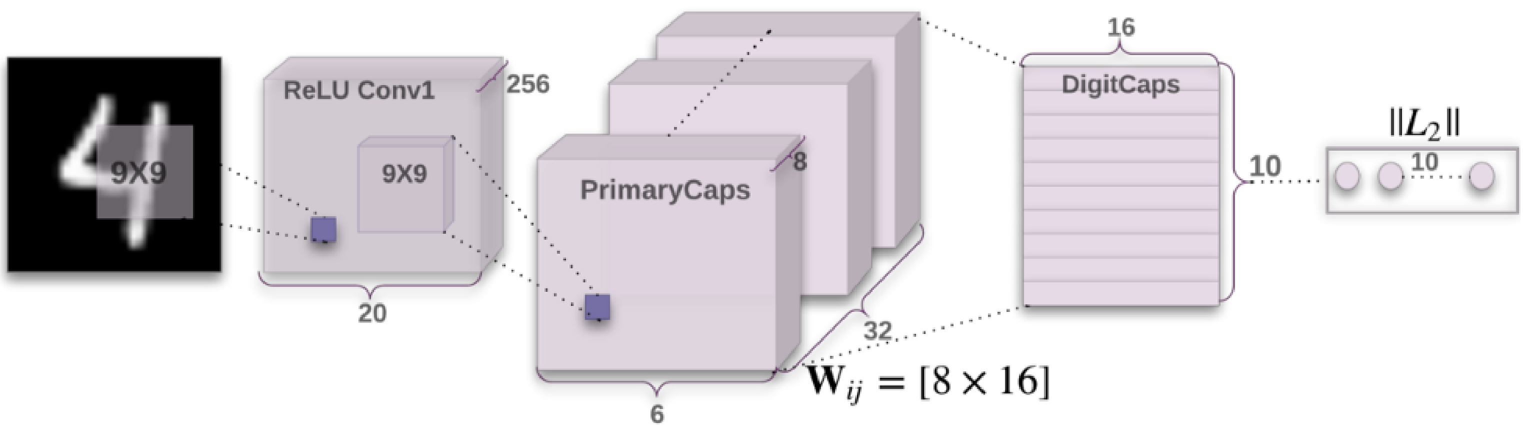
- Recent results on convolution layers
  - Convolutions are equivariant to translation
  - Convolutions are not equivariant to other isometries of the sampling lattice, e.g., rotation



  - What if a CNN learns rotated copies of the same filter?
    - The stack of feature maps is equivariant to rotation.

Math Properties of CNNs

- Recent results on convolution layers
  - Ordinary CNNs can be generalized to Group Equivariant Networks (Cohen and Welling ICML'16, Kondor and Trivedi ICML'18)
    - Redefining the convolution and pooling operations
    - Equivariant to more general transformation from some group *G*
  - Replacing pooling by other network designs
    - Capsule network (Sabour et al, 2017) https://arxiv.org/abs/1710.09829



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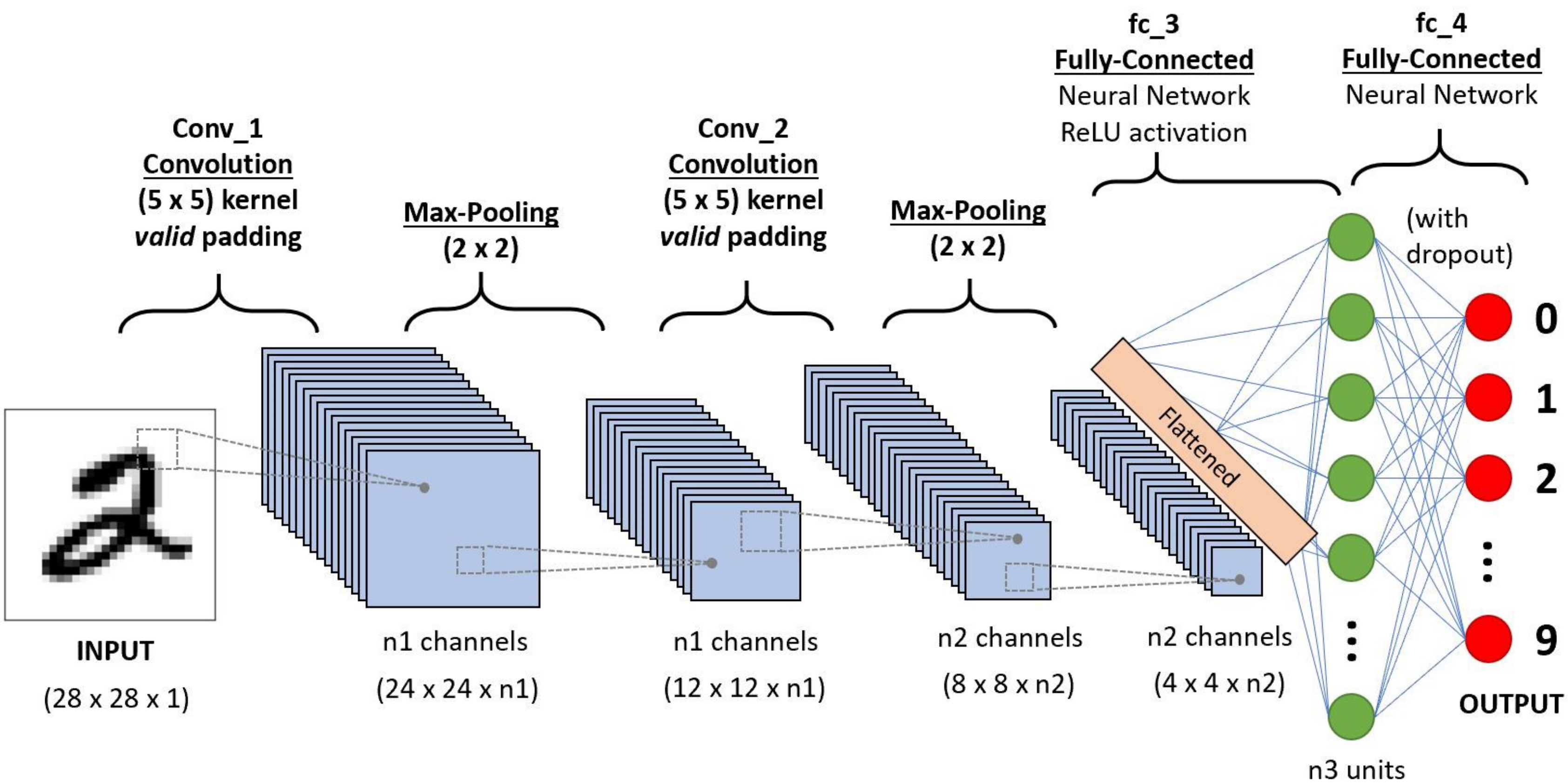
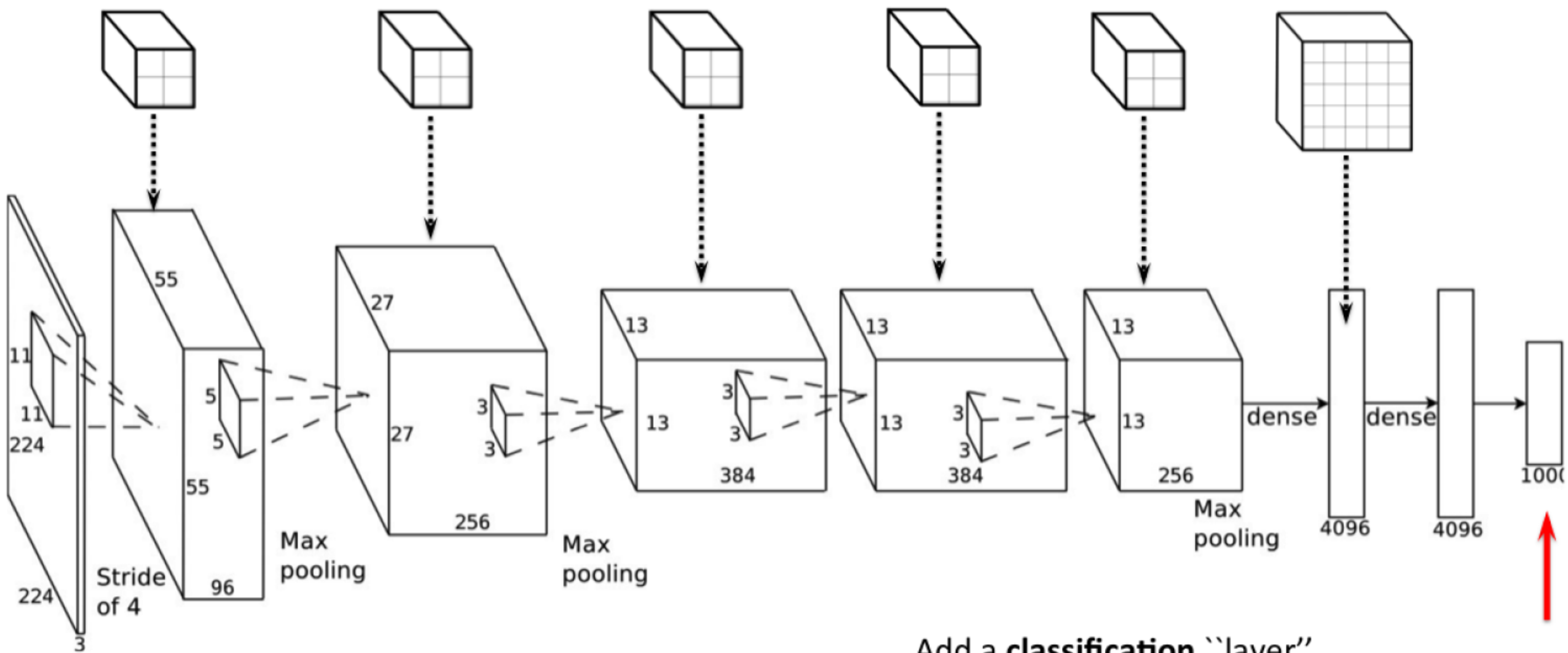
LeNet-5

- Handwritten digit recognition



AlexNet

- Deeper network structure



Add a **classification** ``layer''.

For an input image, the value in a particular dimension of this vector tells you the probability of the corresponding object class.

Summary of CNNs

- CNN properties [Bronstein et al., 2018]
  - Convolutional (Translation invariance)
  - Scale Separation (Compositionality)
  - Filters localized in space (Deformation Stability)
  - O(1) parameters per filter (independent of input image size n)
  - O(n) complexity per layer (filtering done in the spatial domain)
  - O(log n) layers in classification tasks
- Next time …
  - Structure design of Modern CNNs
- Reference
  - CS231n course notes http://cs231n.github.io/convolutional-networks/
  - D2L Chapter 6 + DLBook Chapter 9