Language Technologies Institute

Carnegie Mellon University

Advanced Multimodal Machine Learning

Lecture 3.1: Optimization and Convolutional Neural Networks

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* Original version co-developed with Tadas Baltrusaitis

Lecture Objectives

- Components of a neural network
- Learning the model
  - Optimization
  - Gradient computation
- Convolutional Neural networks
  - Convolution and pooling
  - Architectures
  - Training tricks

Linear Classification: 2) Loss Function - RECAP

(or cost function or objective)

Scores $f(x_i; W)$

Label $y_i = 2\ (dog)$

→ **Loss** $L_i = ?$

Image x_i

(Size: 32*32*3)

0 (duck) ?	-12.3
1 (cat) ?	45.6
2 (dog) ?	98.7
3 (pig) ?	12.2
4 (bird) ?	-45.3

How to assign only one number representing how "unhappy" we are about these scores?

Multi-class problem

The loss function quantifies the amount by which the prediction scores deviate from the actual values.

First Loss Function: Cross-Entropy Loss - RECAP

(or logistic loss)

Logistic function:

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

Logistic regression:
(two classes)

$$p(y_i = \text{"}dog\text{"} | x_i; w) = \sigma(w^T x_i)$$

= true
for two-class problem

Softmax function:
(multiple classes)

$$p(y_i | x_i; W) = \frac{e^{f_{y_i}}}{\sum_j e^{f_j}}$$

Second Loss Function: Hinge Loss

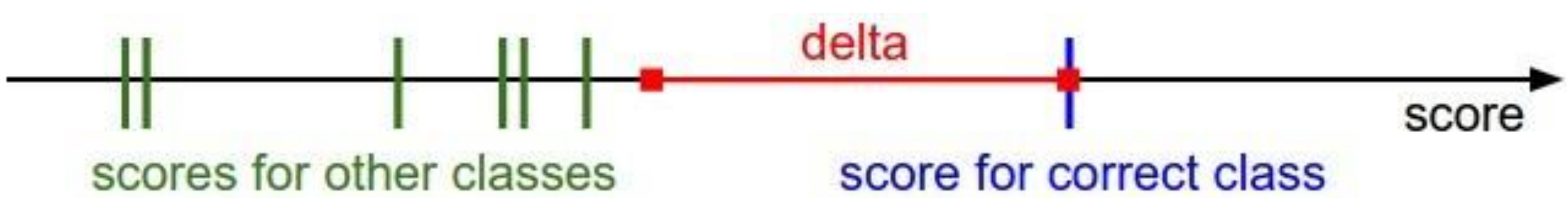
(or max-margin loss or Multi-class SVM loss)

$$L_i = \sum_{j \neq y_i} \max(0, f(x_i, W)_j - f(x_i, W)_{y_i} + \Delta)$$

loss due to example i

sum over all incorrect labels

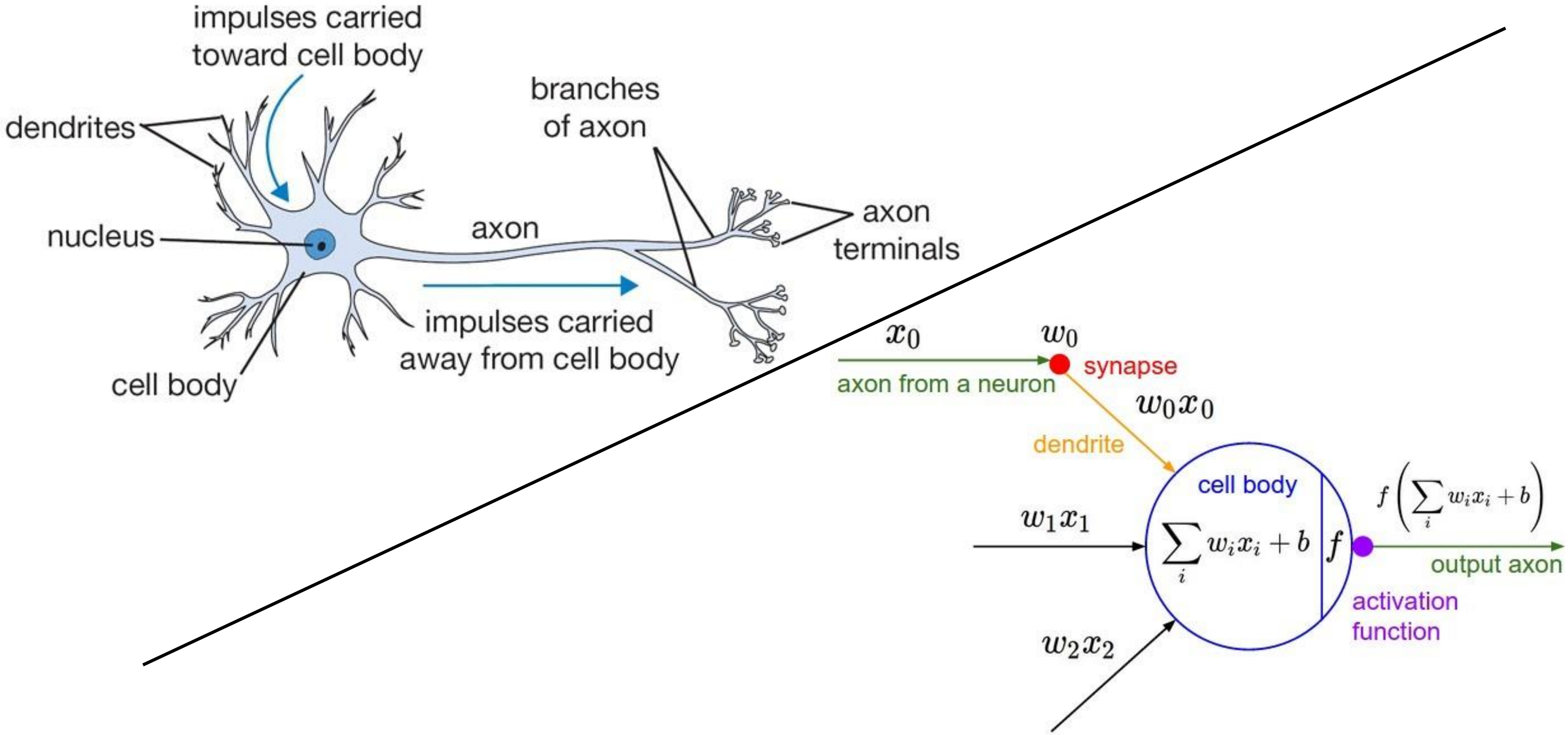
difference between the correct class score and incorrect class score



Basic Concepts: Neural Networks

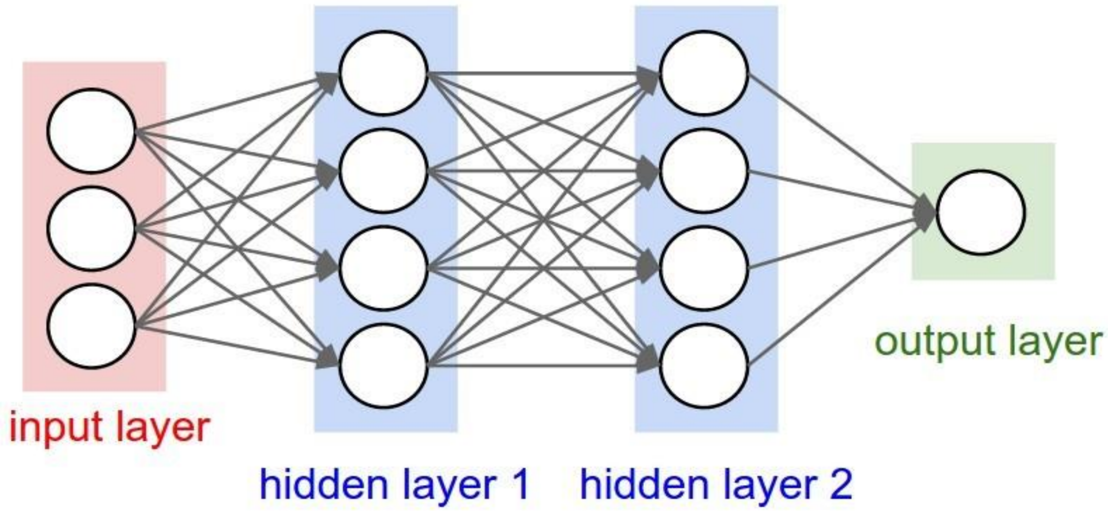
Neural Networks – inspiration

- Made up of artificial neurons



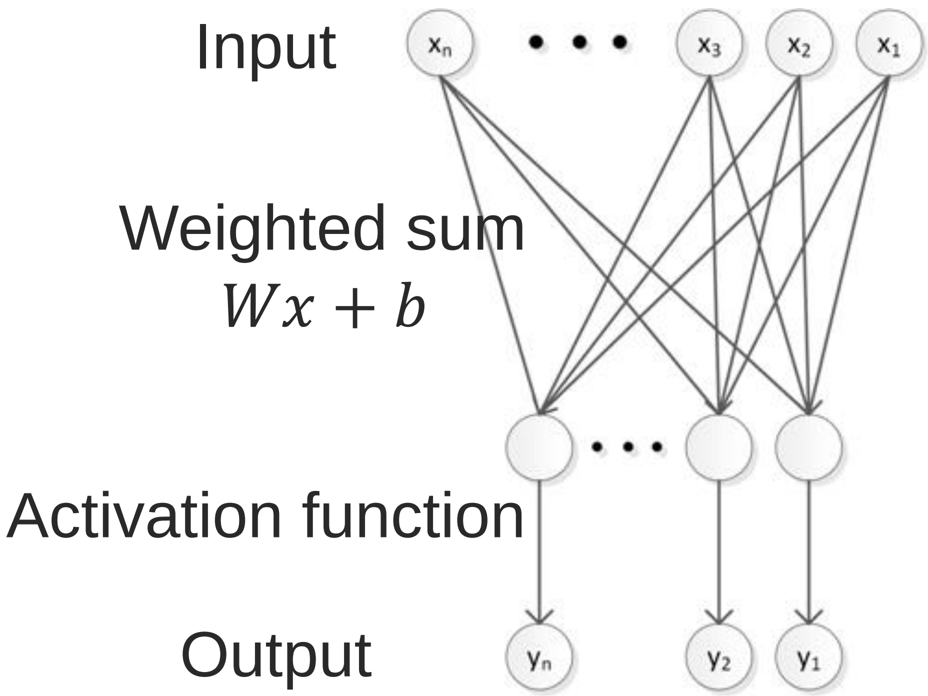
Neural Networks – score function

- Made up of artificial neurons
  - Linear function (dot product) followed by a nonlinear activation function
- Example a Multi Layer Perceptron



Basic NN building block

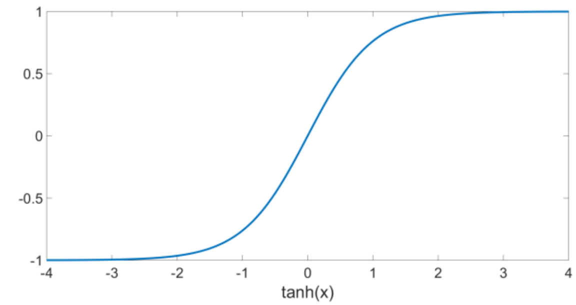
- Weighted sum followed by an activation function

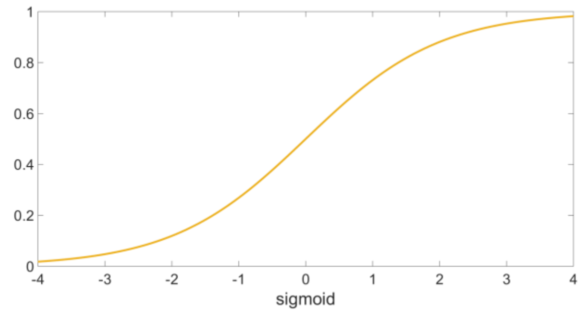


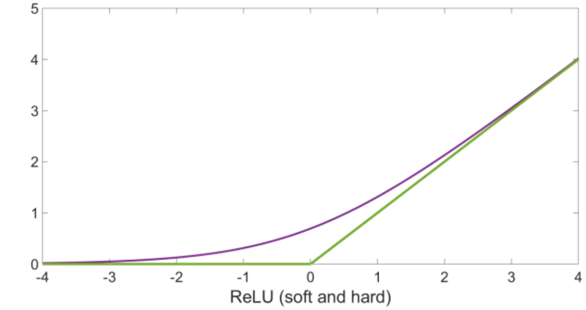
$$y = f(Wx + b)$$

Neural Networks – activation function

- $f(x) = \tanh(x)$
- Sigmoid - $f(x) = (1 + e^{-x})^{-1}$
- Linear – $f(x) = ax + b$
- ReLU $f(x) = \max(0, x) \sim \log(1 + \exp(x))$
  - Rectifier Linear Units
  - Faster training - no gradient vanishing
  - Induces sparsity







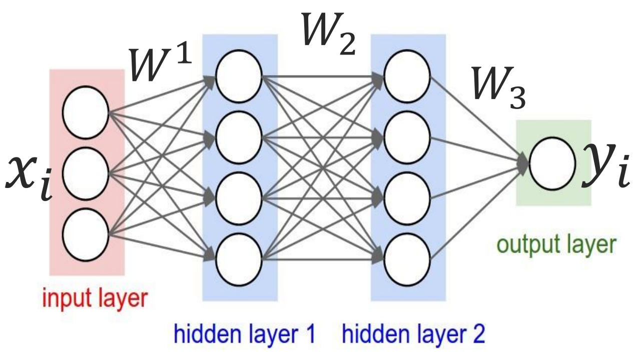
Multi-Layer Feedforward Network

Activation functions (individual layers)

$$f_{1;W_1}(x) = \sigma(W_1 x + b_1)$$

$$f_{2;W_2}(x) = \sigma(W_2 x + b_2)$$

$$f_{3;W_3}(x) = \sigma(W_3 x + b_3)$$



Score function

$$y_i = f(x_i) = f_{3;W_3}(f_{2;W_2}(f_{1;W_1}(x_i)))$$

Loss function (e.g., Euclidean loss)

$$L_i = (f(x_i) - y_i)^2 = (f_{3;W_3}(f_{2;W_2}(f_{1;W_1}(x_i))))^2$$

Neural Networks inference and learning

- Inference (Testing)
  - Use the score function ($y = f(\boldsymbol{x}; W)$)
  - Have a trained model (parameters W)
- Learning model parameters (Training)
  - Loss function (L)
  - Gradient
  - Optimization

Learning model parameters

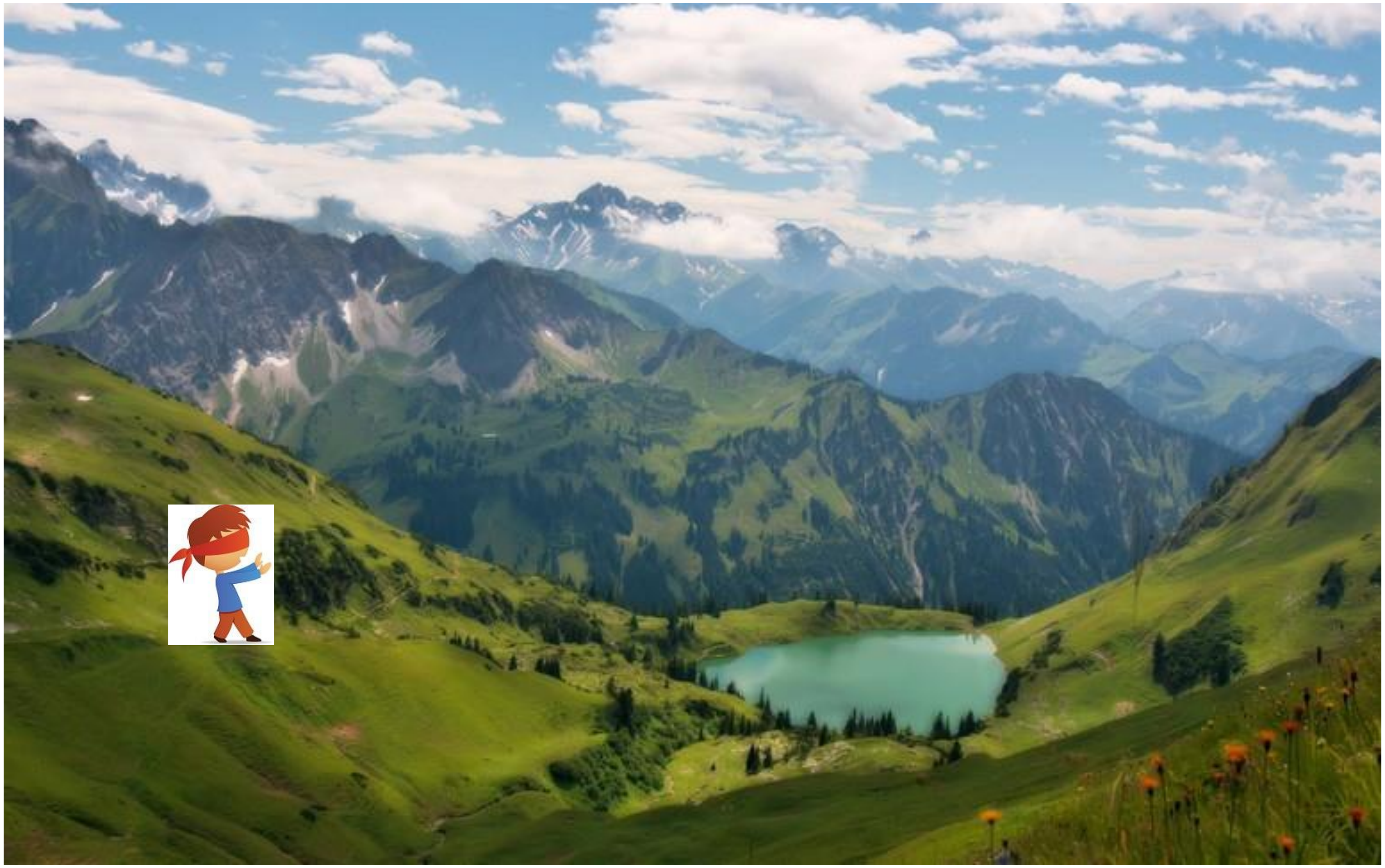
Learning model parameters

- We have our training data
  - $\mathrm{X} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_n\}$ (e.g. images, videos, text etc.)
  - $\mathrm{Y} = \{y_1, y_2, \dots, y_n\}$ (labels)
  - Fixed
- We want to learn the W (weights and biases) that leads to best loss

$$\operatorname*{argmin}_{W}[L(\mathrm{X}, \mathrm{Y}, W)]$$

- The notation means find W for which $L(\mathrm{X}, \mathrm{Y}, W)$ has the lowest value

Optimization



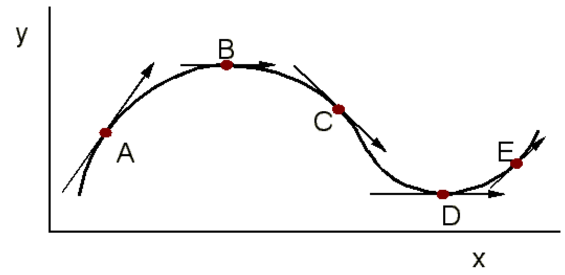
Optimizing a generic function

- We want to find a minimum of the loss function
- How do we do that?
  - Searching everywhere (global optimum) is computationally infeasible
  - We could search randomly from our starting point (mostly picked at random) and then refine the search region – impractical and not accurate
  - Instead we can follow the gradient

What is a gradient?

- Geometrically
  - Points in the direction of the greatest rate of increase of the function and its magnitude is the slope of the graph in that direction
- More formally in 1D

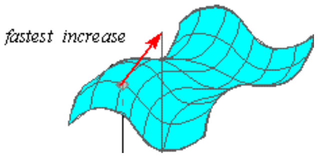
$$\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$



- In higher dimensions

$$\frac{\partial f}{\partial x_i}(a_1, \dots, a_n) = \lim_{h \to 0} \frac{f(a_1, \dots, a_i + h, \dots, a_n) - f(a_1, \dots, a_i, \dots, a_n)}{h}$$

> In multiple dimension, the **gradient** is the vector of (partial derivatives) and is called a **Jacobian**.



Numeric gradient

- Can set *h* to a very low number and compute:

$$\frac{df(x)}{dx} = \frac{f(x+h) - f(x)}{h}$$

- Slow and just an approximation
  - Need to compute score once (or even twice for central limit) for each parameter
  - Sensitive to choice of h
- h needs to be chosen as well - hyperparameter

Analytical gradient

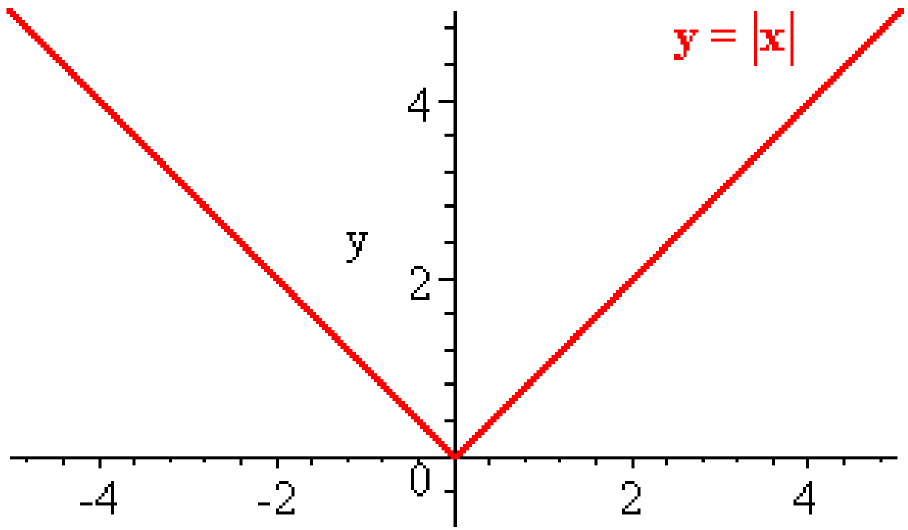
- If we know the function and it is **differentiable**
  - Derivative/gradient is defined at every point in *f*
  - Sometimes use differentiable approximations
  - Some are locally differentiable
- Use Calculus (or Wikipedia)!
- Examples:

$$f(x) = \frac{1}{1+e^{-x}};\ \frac{df}{dx} = (1 - f(x))f(x)$$

$$f(x) = (x-y)^2;\ \frac{df}{dx} = 2(x-y)$$

Analytical gradient

- If we know the function and it is **differentiable**
  - Derivative/gradient is defined at every point in *f*
  - Sometimes use differentiable approximations
  - Some are locally differentiable
- Use Cal
- Example



$f($ … $x)$

$f($ …

Which one should we use?

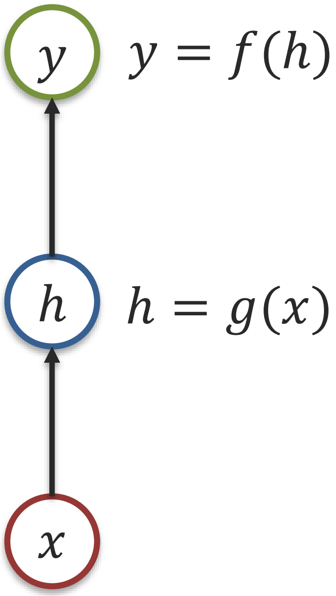
- Numeric
  - Slow
  - Approximate
- Analytical
  - More error prone to implement (need to get the gradient right)
  - Can use automated tools to help – Theano, autograd, Matlab symbolic toolbox
- Have both, use analytical for speed but check using numeric
- Why you should understand gradient

Neural Networks gradient

Gradient Computation

Chain rule:

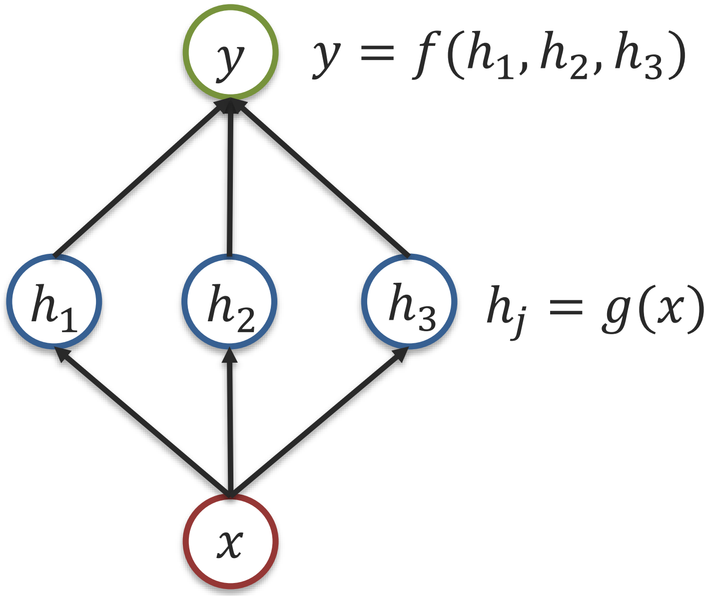
$$\frac{\partial y}{\partial x} = \frac{\partial y}{\partial h}\frac{\partial h}{\partial x}$$



Optimization: Gradient Computation

Multiple-path chain rule:

$$\frac{\partial y}{\partial x} = \sum_j \frac{\partial y}{\partial h_j} \frac{\partial h_j}{\partial x}$$



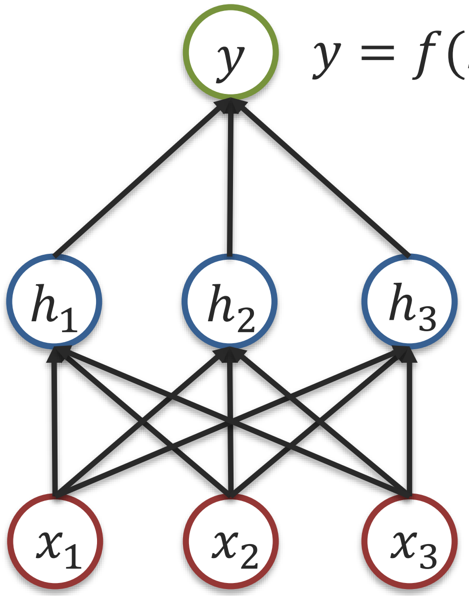
Optimization: Gradient Computation

Multiple-path chain rule:

$$\frac{\partial y}{\partial x_1} = \sum_j \frac{\partial y}{\partial h_j} \frac{\partial h_j}{\partial x_1}$$

$$\frac{\partial y}{\partial x_2} = \sum_j \frac{\partial y}{\partial h_j} \frac{\partial h_j}{\partial x_2}$$

$$\frac{\partial y}{\partial x_3} = \sum_j \frac{\partial y}{\partial h_j} \frac{\partial h_j}{\partial x_3}$$



$y = f(h_1, h_2, h_3)$

$h_j = g(\boldsymbol{x})$

Optimization: Gradient Computation

Vector representation:

$$\nabla_{\boldsymbol{x}}\, y = \left[\frac{\partial y}{\partial x_1}, \frac{\partial y}{\partial x_2}, \frac{\partial y}{\partial x_3}\right]$$

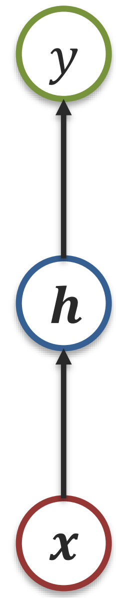
Gradient

$$\nabla_{\boldsymbol{x}}\, y = \left(\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{x}}\right)^T \nabla_{\boldsymbol{h}}\, y$$

"local" Jacobian

(matrix of size $|h| \times |x|$ computed using partial derivatives)

"backprop" Gradient



$y = f(\boldsymbol{h})$

$\boldsymbol{h} = g(\boldsymbol{x})$

Backpropagation Algorithm (efficient gradient)

Forward pass

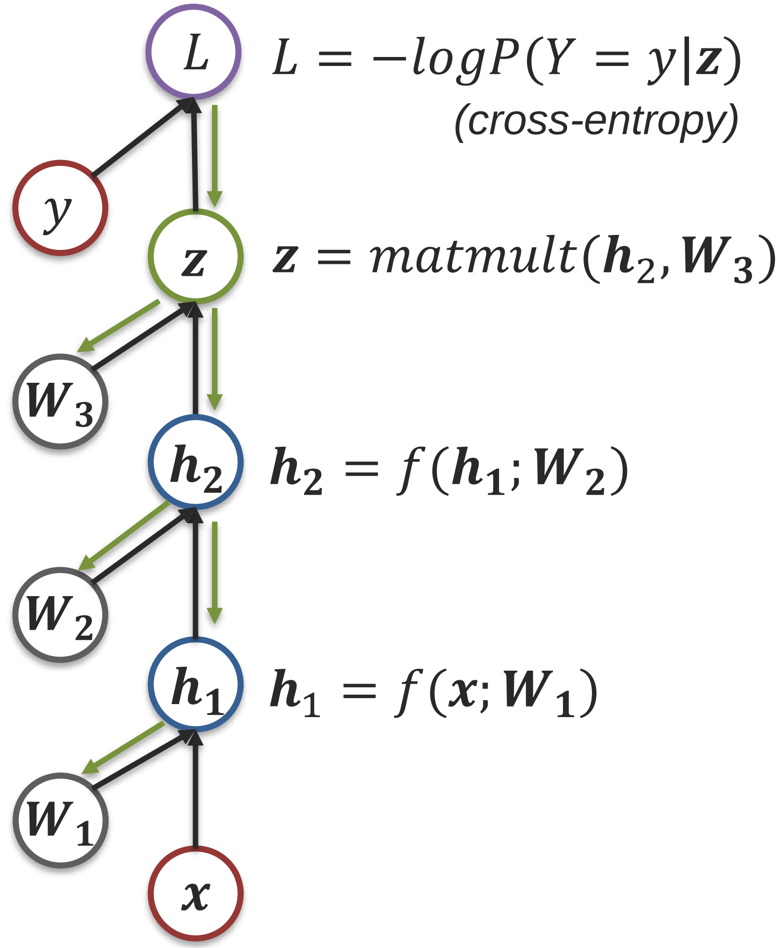
- Following the graph topology, compute value of each unit

Backpropagation pass

- Initialize output gradient = 1
- Compute "local" Jacobian matrix using values from forward pass
- Use the chain rule:

Gradient = "local" Jacobian x "backprop" gradient

- Why is this rule important?



Computational Graph: Multi-layer Feedforward Network

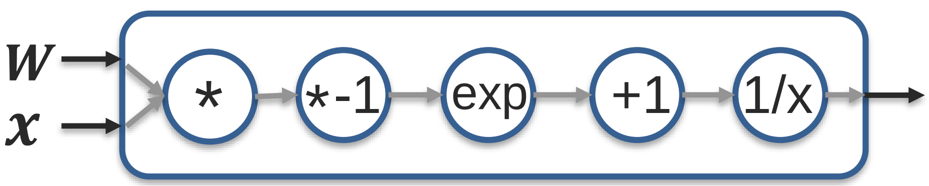
Computational unit:

$h = f(x; W)$

- Multiple input
- One output
- Vector/tensor

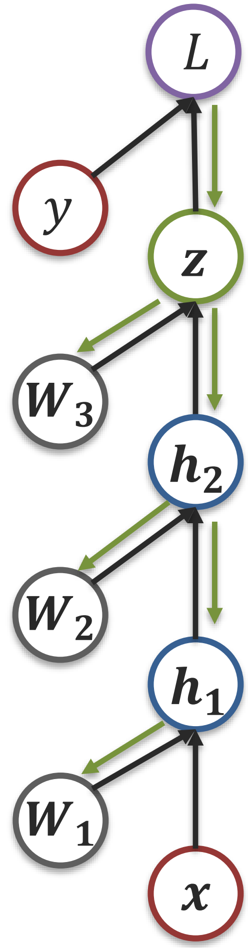
- Sigmoid unit:

$$h_j = (1 + e^{-W_j x})^{-1}$$



Differentiable "unit" function!

(or close approximation to compute "local Jacobian)



$L = -logP(Y = y|z)$ (cross-entropy)

$z = matmult(h_2, W_3)$

$h_2 = f(h_1; W_2)$

$h_1 = f(x; W_1)$

Gradient descent

How to follow the gradient

- Many methods for optimization
  - **Gradient Descent (actually the "simplest" one)**
  - Newton methods (use Hessian – second derivative)
  - Quasi-Newton (use approximate Hessian)
    - BFGS
    - LBFGS
    - Don't require learning rates (fewer hyperparameters)
    - But, do not work with stochastic and batch methods so rarely used to train modern Neural Networks
- **All of them look at the gradient**
  - Very few non gradient based optimization methods

Parameter Update Strategies

Gradient descent:

$$\theta^{(t+1)} = \theta^{t} - \epsilon_k \nabla_\theta L$$

Gradient of our loss function

New model parameters

Previous parameters

Learning rate at iteration *k*

$$\epsilon_k = (1-\alpha)\epsilon_0 + \alpha\epsilon_\tau$$

Decay learning rate linearly until iteration τ

Learning rate at iteration *k*

Decay

Initial learning rate

Extensions:

- Stochastic (“batch”)
- with momentum
- AdaGrad
- RMSProp

Vanilla Gradient Descent

- Compute gradient with respect to loss and keep updating weights till convergence

```
while not converged:
        # compute gradients
        weights_grad = compute_gradient(loss_fun, data, weights)
        # perform parameter update
        weights += - step_size * weights_grad
       # (optionally update step size)
```

Batch (stochastic) gradient descent

- Using all of data points might be tricky when computing a gradient
  - Uses lots of memory and slow to compute
- Instead use batch gradient descent
  - Take a subset of data when computing the gradient

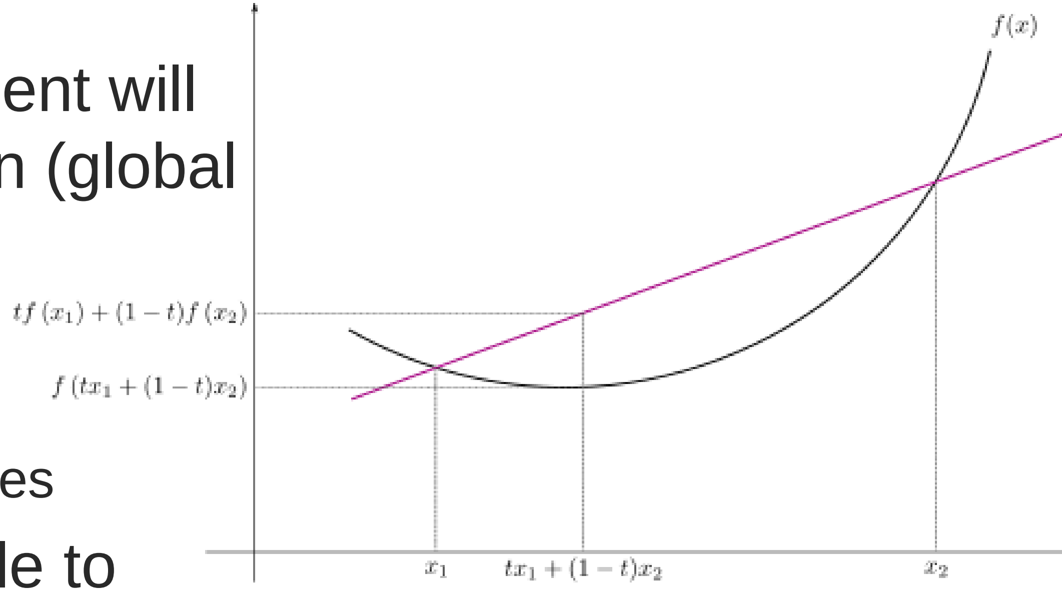
```
while not converged:
        # Shuffle data
        data = randomize(data)
        # Split data into batches and update each batch individual
        for data_batch in data:
                weights_grad = backpropagation(loss_fun, data_batch , weights)
                # perform parameter update
                weights += - step_size * weights_grad
```

Iteration

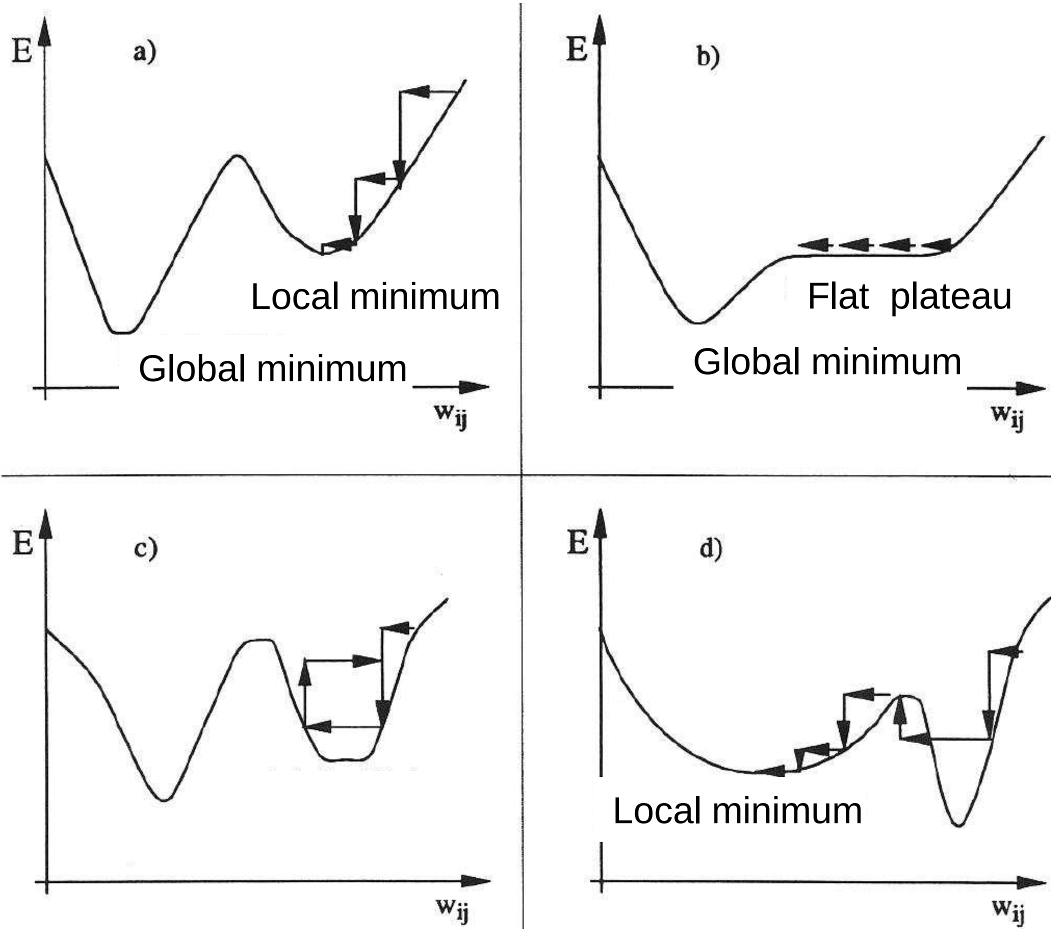
Epoch

Convex vs. non-convex functions and local minima

- Convex – gradient descent will lead to a perfect solution (global optimum)
  - Logistic regression
  - Least squares models
  - Support vector machines
- Non-convex – impossible to guarantee that the solution is the best – will lead to local-minima
  - Neural networks
  - Various graphical models



Potential issues

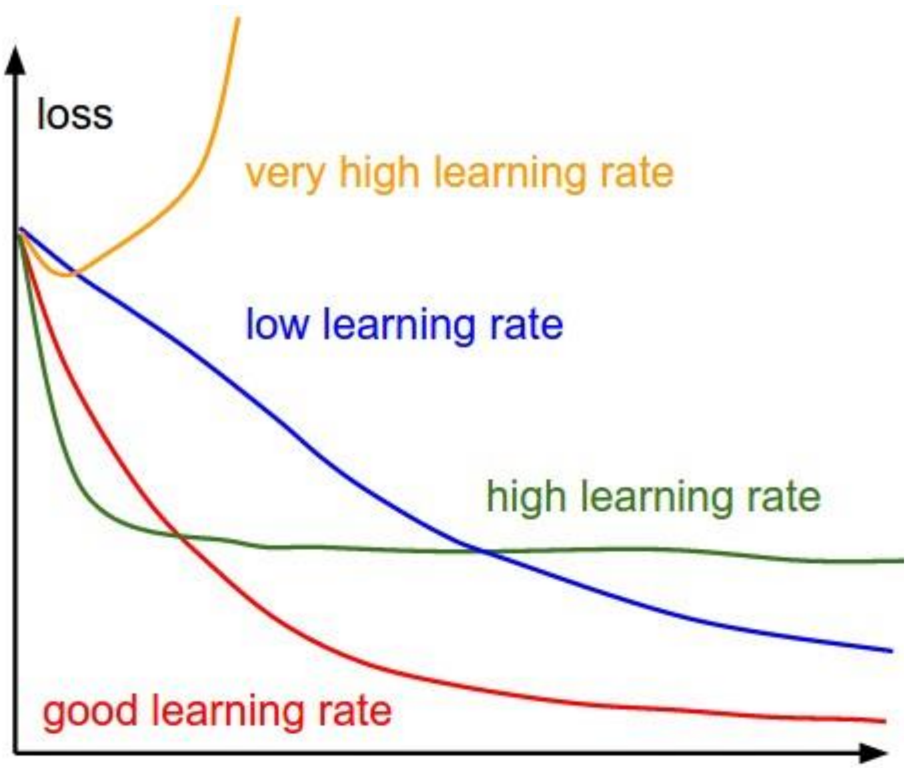


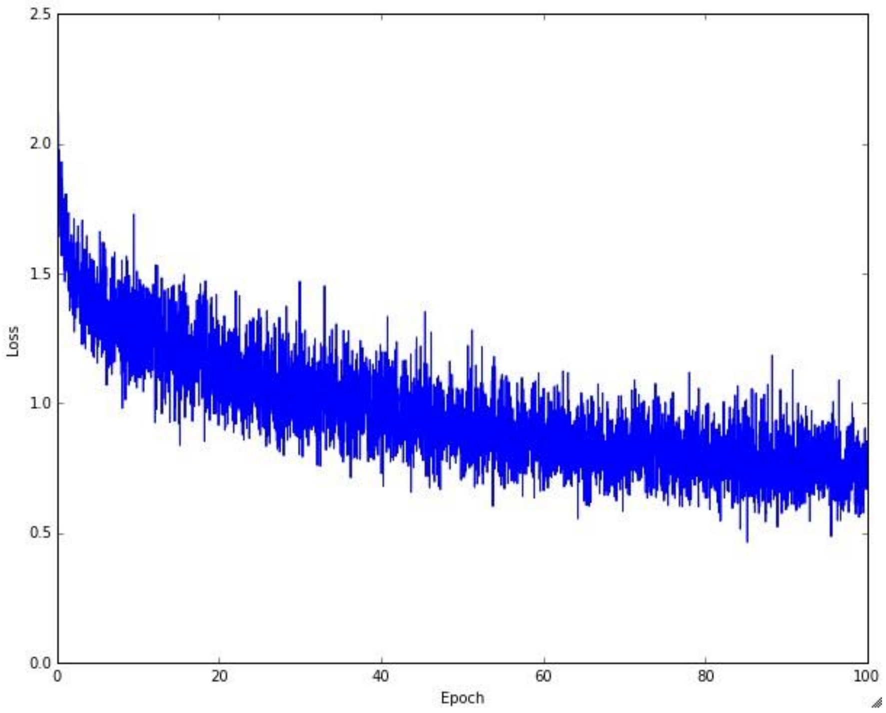
- Problems that can occur?
  - Getting stuck in local minima (global minimum is never found) (a)
  - Getting stuck on flat plateaus of the error-plane (b)
  - Oscillations in error rates (c)
  - Learning rate is critical (d)

Some observations:

- Small steps are likely to lead to consistent but slow progress.
- Large steps can lead to better progress but are more risky.
- Note that eventually, for a large step size we will overshoot and make the loss worse.

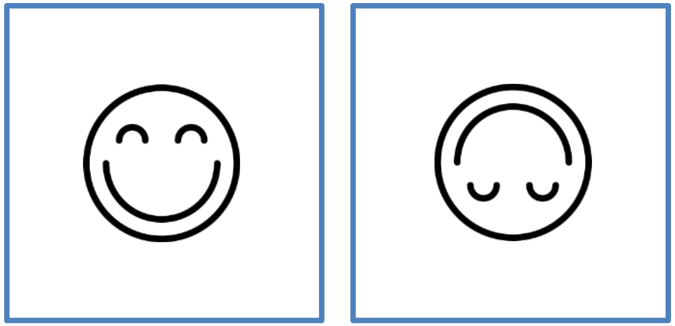
Interpreting learning rates



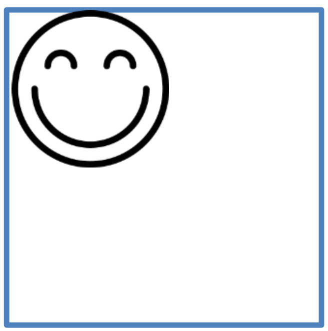


Convolutional Neural Networks

A Shortcoming of MLP



2 Data Points – detect which head is up!
Easily modeled using one neuron.
What is the best neuron to model this?

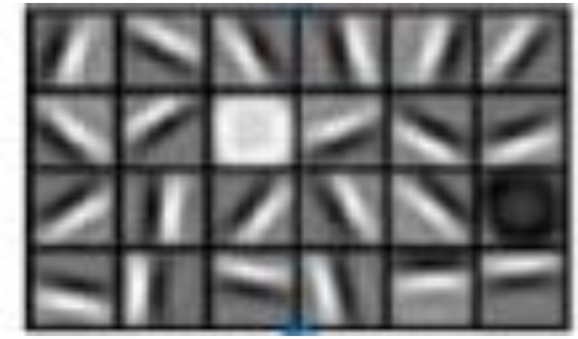


This head may or may not be up – what happened?

Solution: instead of modeling the entire image, model the important region.

Why not just use an MLP for images (1)?

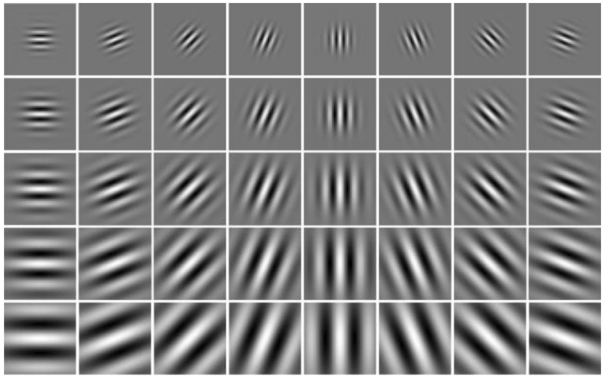
- MLP connects each pixel in an image to each neuron
- Does not exploit redundancy in image structure
  - Detecting edges, blobs
  - Don’t need to treat the top left of image differently from the center



- Too many parameters
  - For a small 200×200 pixel RGB image the first matrix would have $120000 \times n$ parameters for the first layer alone

Why not just use an MLP for images (2)?

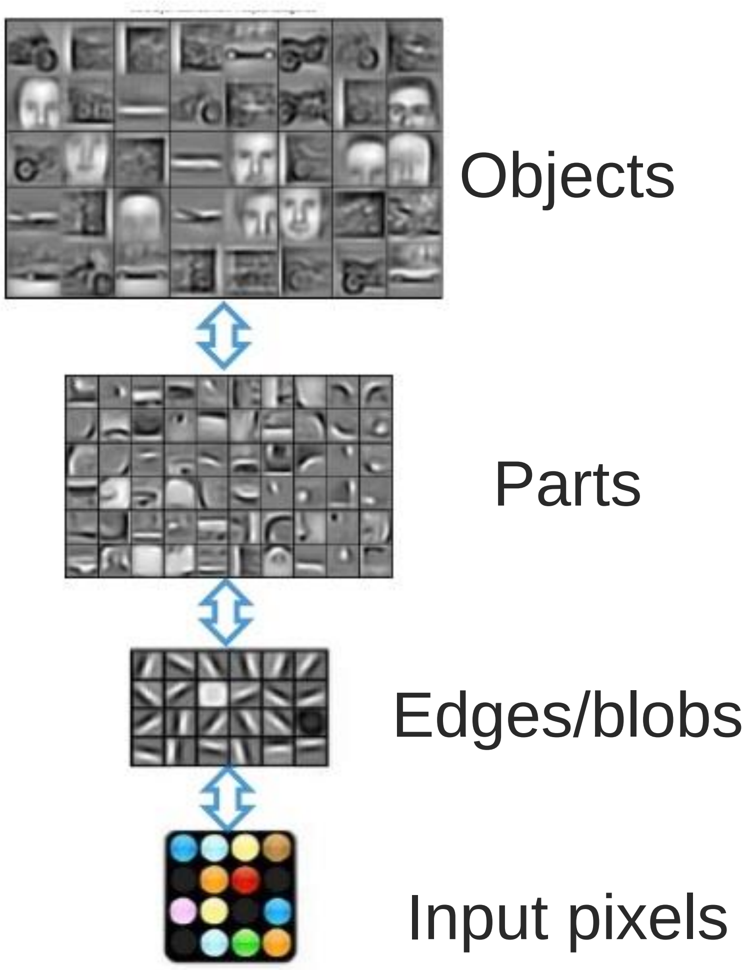
- Human visual system works in a filter fashion
  - First the eyes detect edges and change in light intensity
  - The visual cortex processing performs Gabor like filtering



- MLP does not exploit translation invariance
- MLP does not necessarily encourage visual abstraction

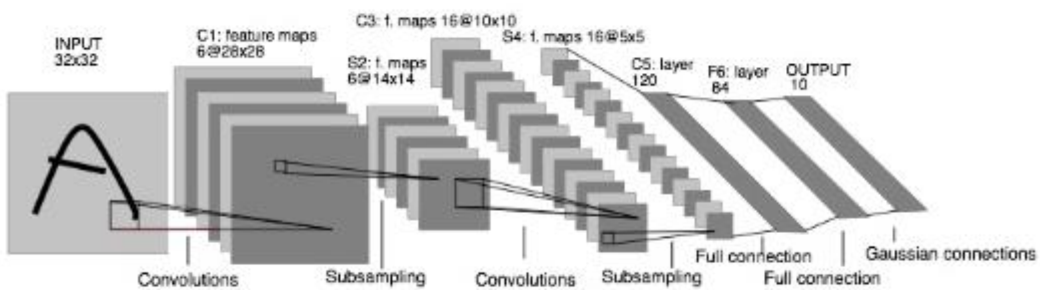
Why use Convolutional Neural Networks

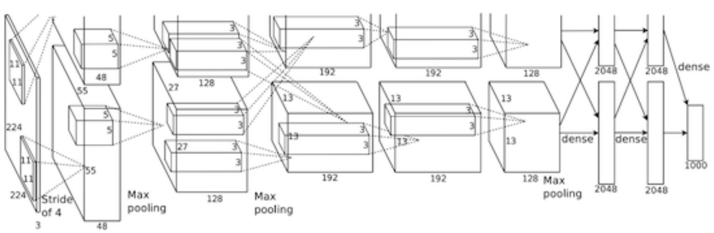
- Using basic Multi Layer Perceptrons does not work well for images
- Intention to build more abstract representation as we go up every layer

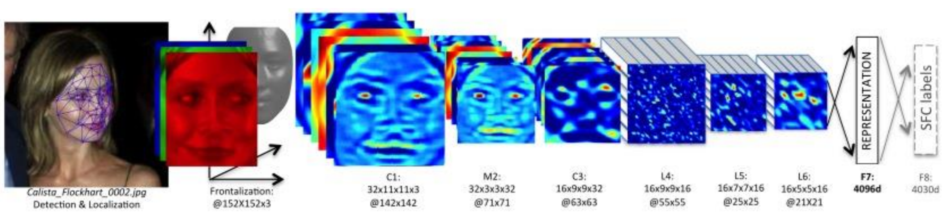


Convolutional Neural Networks

- They are everywhere that uses representation learning with images
- State of the art results – object recognition, face recognition, segmentation, OCR, visual emotion recognition
- Extensively used for multimodal tasks as well

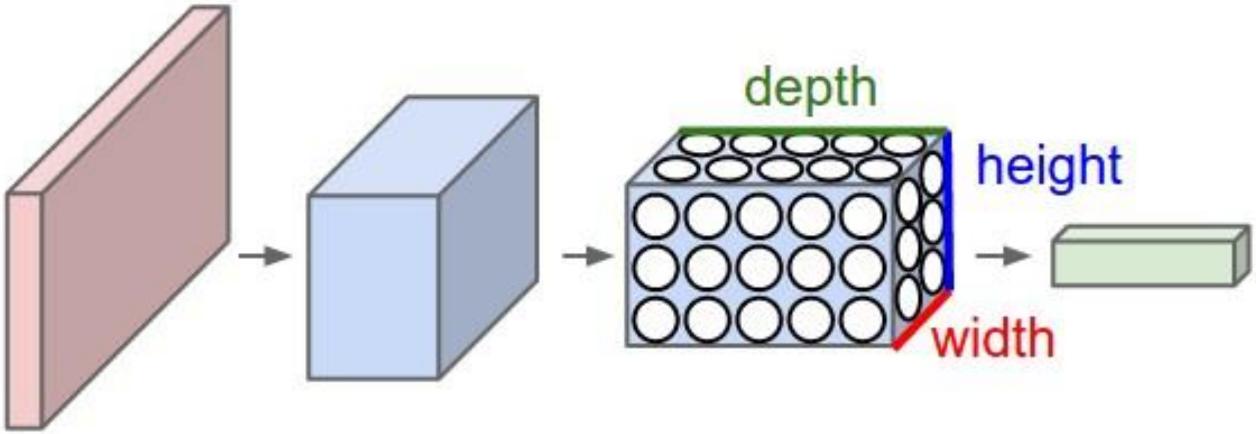






Main differences of CNN from MLP

- Addition of:
  - Convolution layer
  - Pooling layer
- Everything else is the same (loss, score and optimization)
- MLP layer is called Fully Connected layer



Convolution

Convolutional definition

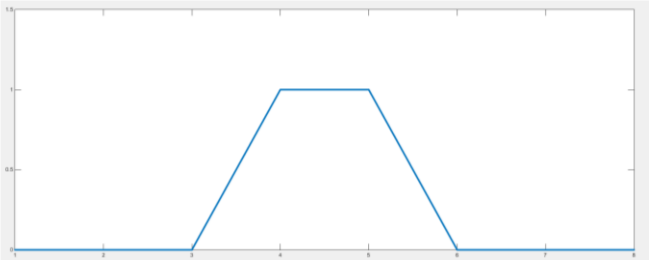
- A basic mathematical operation (that given two functions returns a function)

$$(f * g)[n] \stackrel{\text{def}}{=} \sum_{m=-\infty}^{\infty} f[m]g[n-m]$$

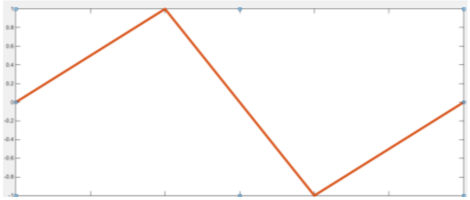
- Have a continuous and discrete versions (we focus on the latter)

Convolution in 1D

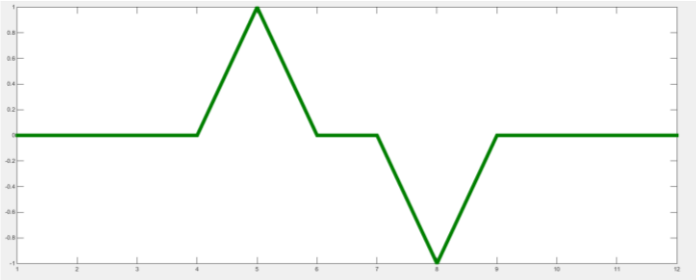
- Example
  - $f = [\dots, 0,1,1,1,0,0, \dots]$



  - $g = [\dots, 0,1,-1,0 \dots]$



- $f * g = [\dots, 0,1,0,0,-1,0,0, \dots]$



$$(f * g)[n] \stackrel{\text{def}}{=} \sum_{m=-\infty}^{\infty} f[m]g[n-m]$$

Convolution in practice

- In CNN we only consider functions with limited domain (not from $-\infty$ to ∞)
- Also only consider fully defined (valid) version
  - We have a signal of length N
  - Kernel of length K
  - Output will be length $\mathrm{N}-\mathrm{K}+1$
- $f=[1,2,1]$, $g=[1,-1]$, $f*g=[1,-1]$

Convolution in practice

- If we want output to be different size we can add padding to the signal
  - Just add 0s at the beginning and end
- $f = [0,0,1,2,1,0,0]$, $g = [1, -1]$, $f * g = [0,1,1,-1,-1,0]$

- Also have strided convolution (the filter jumps over pixels or signal)
  - With stride 2
  - $f = [0,0,1,2,1,0,0]$, $g = [1, -1]$, $f * g = [0,1,-1,0]$
  - Why is this a good idea? Where can this fail?

Convolution in 2D

- Example of image and a kernel

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Convolution kernel

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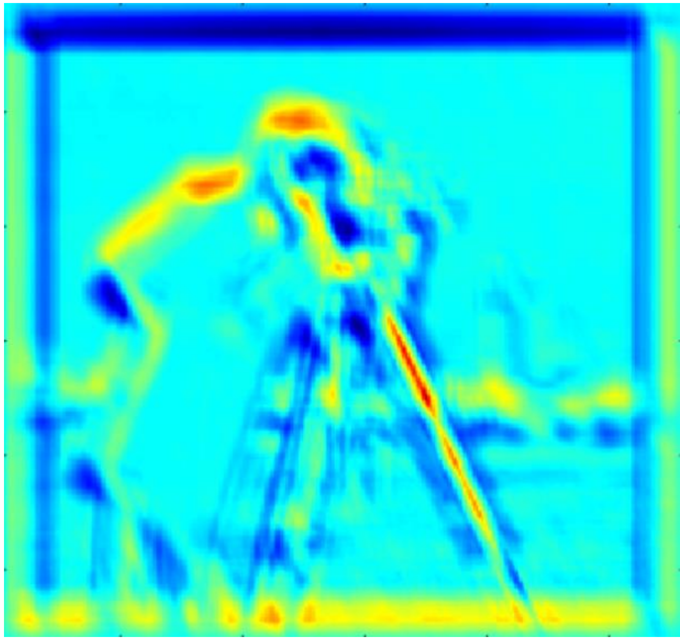
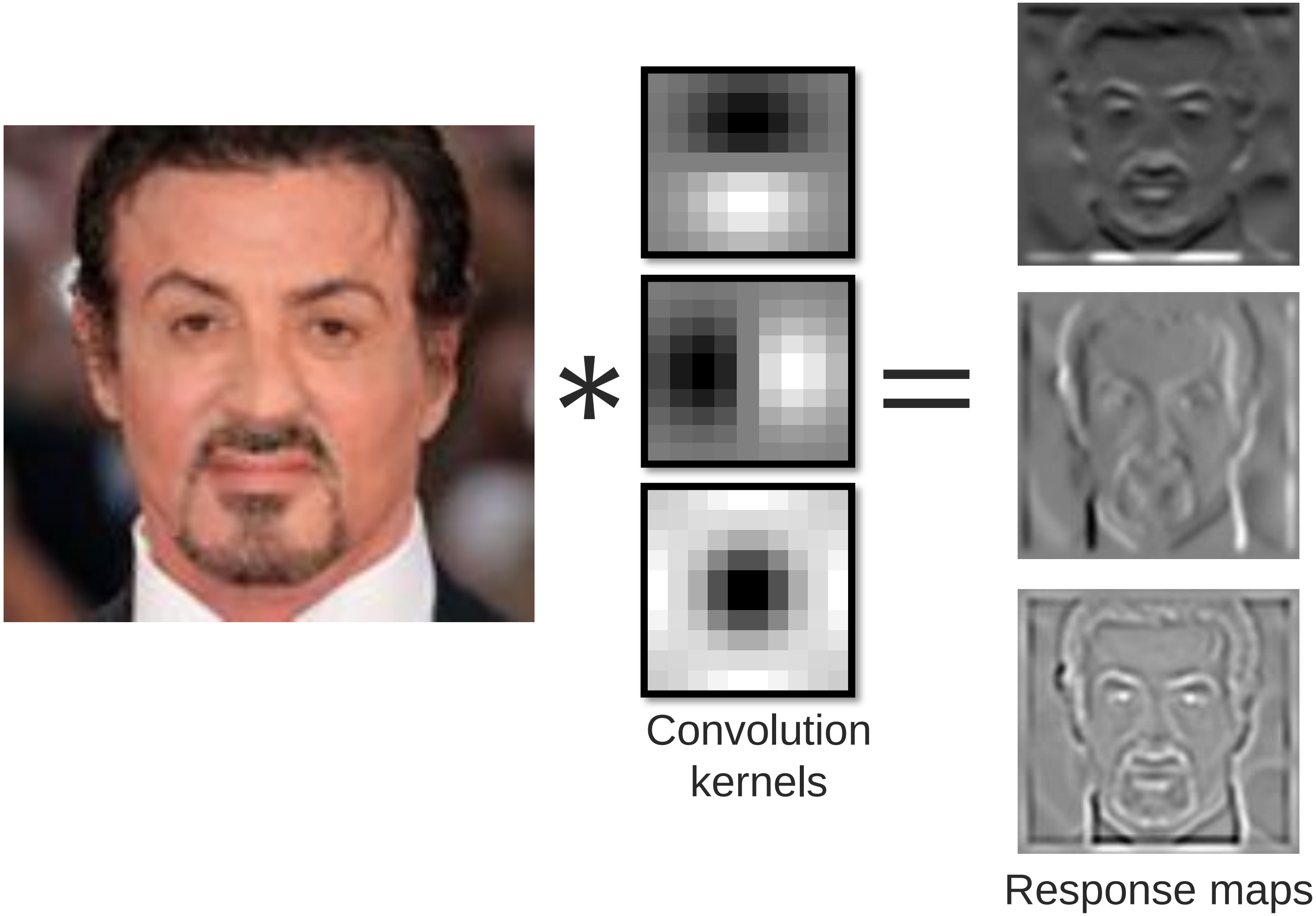


Response map

Convolution in 2D

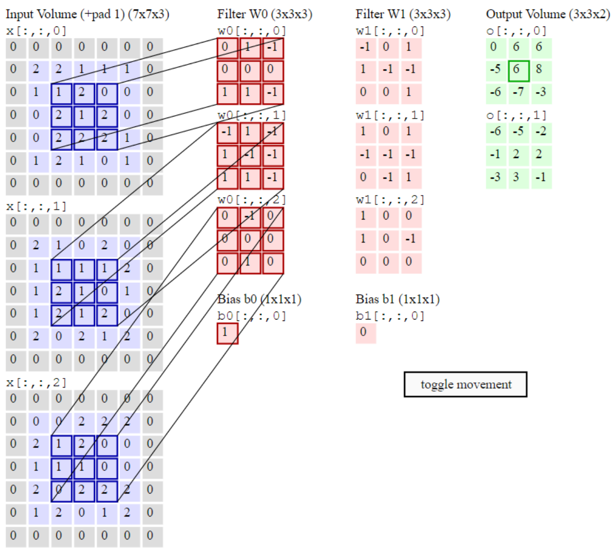


Convolution intuition

- Correlation/correspondence between two signals
  - Template matching
- Why are we interested in convolution
  - Allows to extract structure from signal or image
  - A very efficient operation on signals and images

Sample CNN convolution

- Great animated visualization of 2D convolution
- http://cs231n.github.io/convolutional-networks/



Convolution with MLP

Fully connected layer

- Weighted sum followed by an activation function

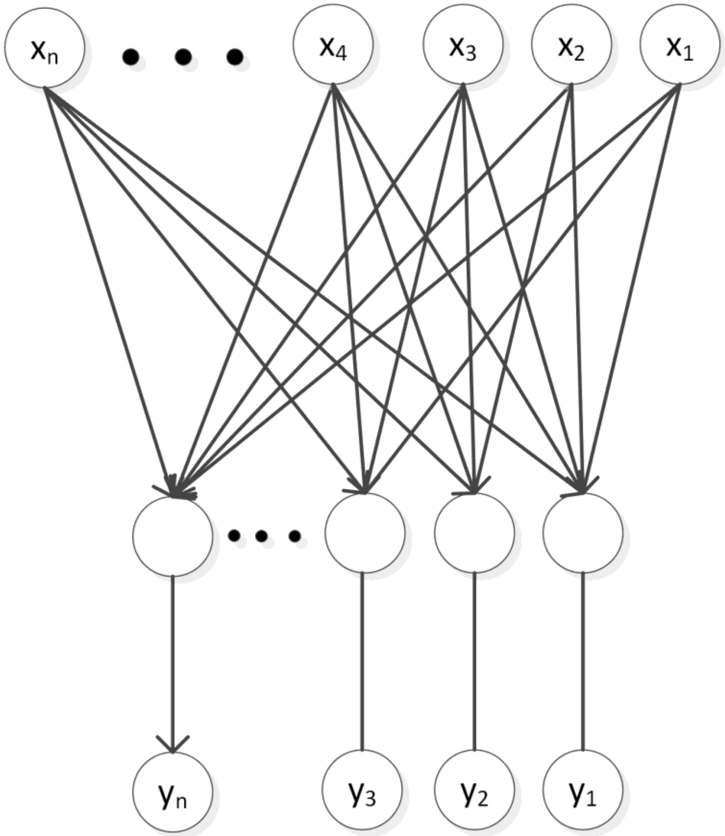
Input

Weighted sum
$Wx + b$

Activation function

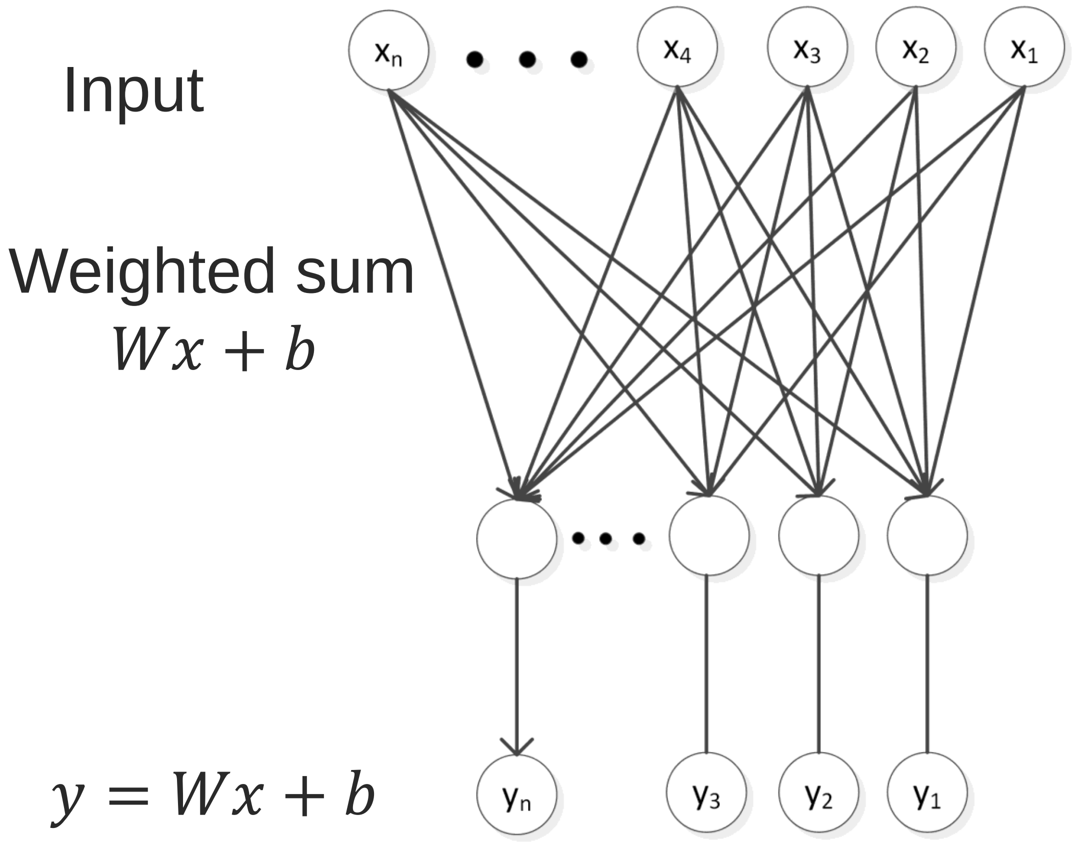
Output

$y = f(Wx + b)$



Convolution as MLP (1)

- Remove activation



Kernel	w_1	w_2	w_3

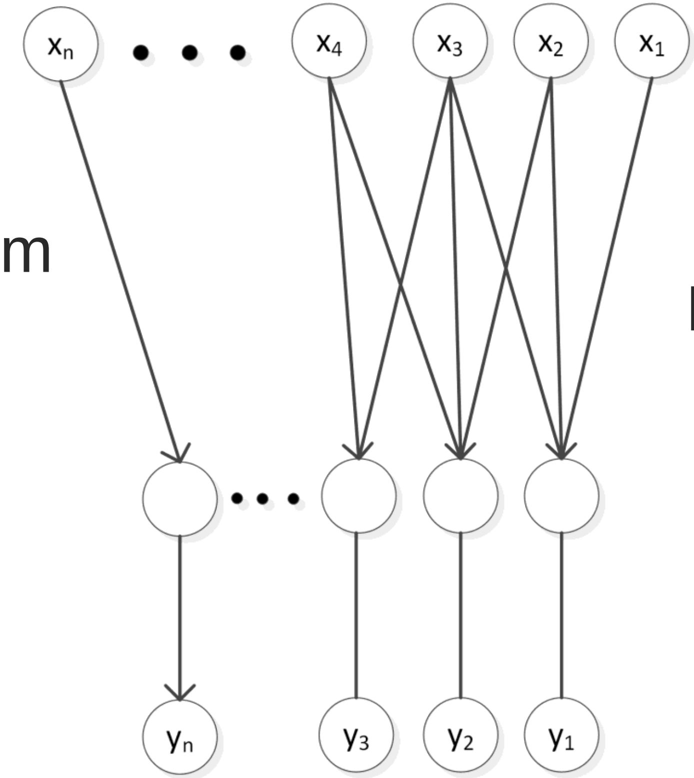
Convolution as MLP (2)

- Remove redundant links making the matrix W sparse (optionally remove the bias term)

Input

Weighted sum
Wx

$y = Wx$

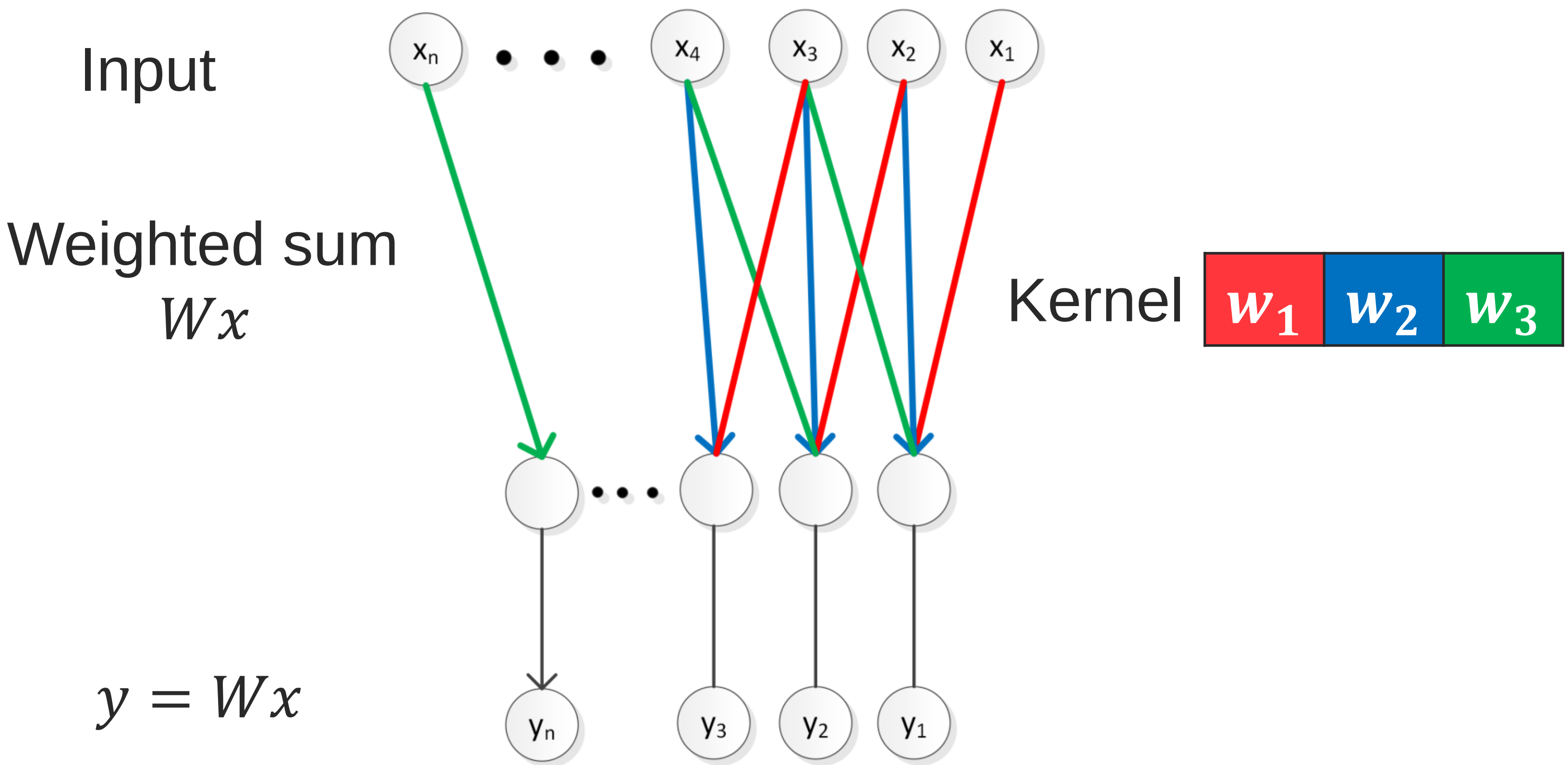


Kernel

$\boldsymbol{w_1}$	$\boldsymbol{w_2}$	$\boldsymbol{w_3}$

Convolution as MLP (3)

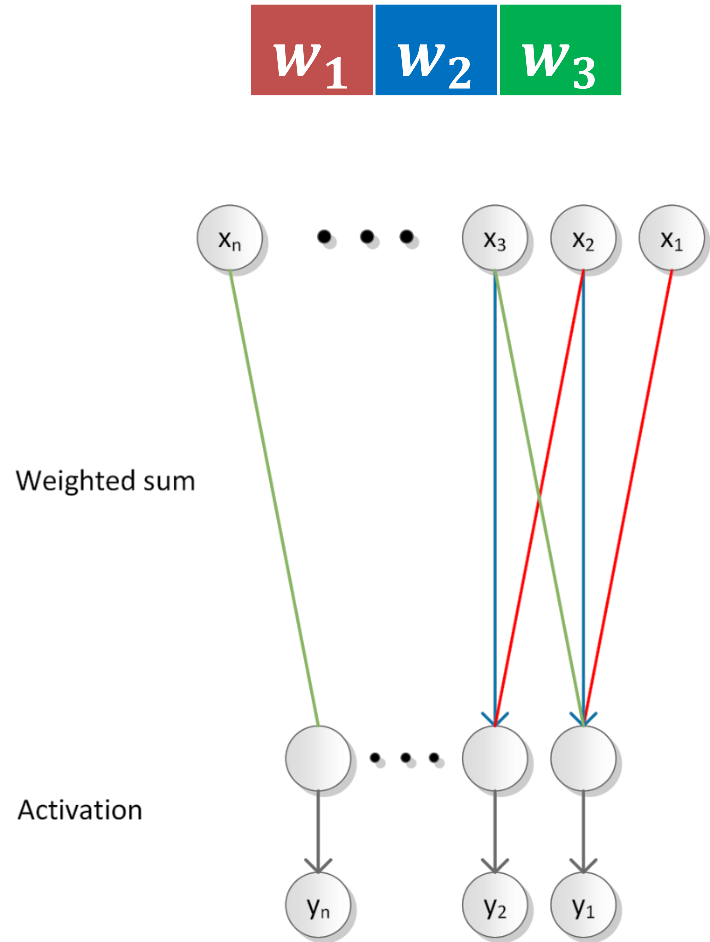
- We can also share the weights in matrix W not to do redundant computation



How do we do convolution in MLP recap

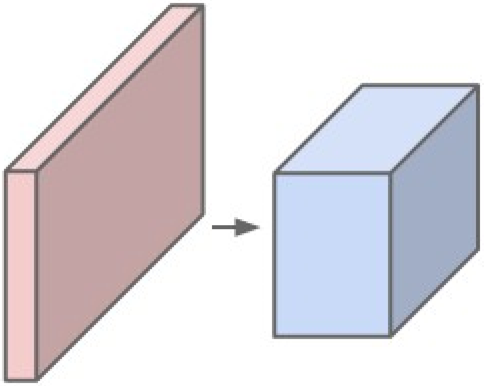
- Not a fully connected layer anymore
- Shared weights
  - Same colour indicates same (shared) weight

$$
W = \begin{pmatrix}
w_1 & w_2 & w_3 & & 0 & 0 & 0 \\
0 & w_1 & w_2 & \cdots & 0 & 0 & 0 \\
0 & 0 & w_1 & & 0 & 0 & 0 \\
 & \vdots & & \ddots & & \vdots & \\
0 & 0 & 0 & & w_3 & 0 & 0 \\
0 & 0 & 0 & \cdots & w_2 & w_3 & 0 \\
0 & 0 & 0 & & w_1 & w_2 & w_3
\end{pmatrix}
$$



More on convolution

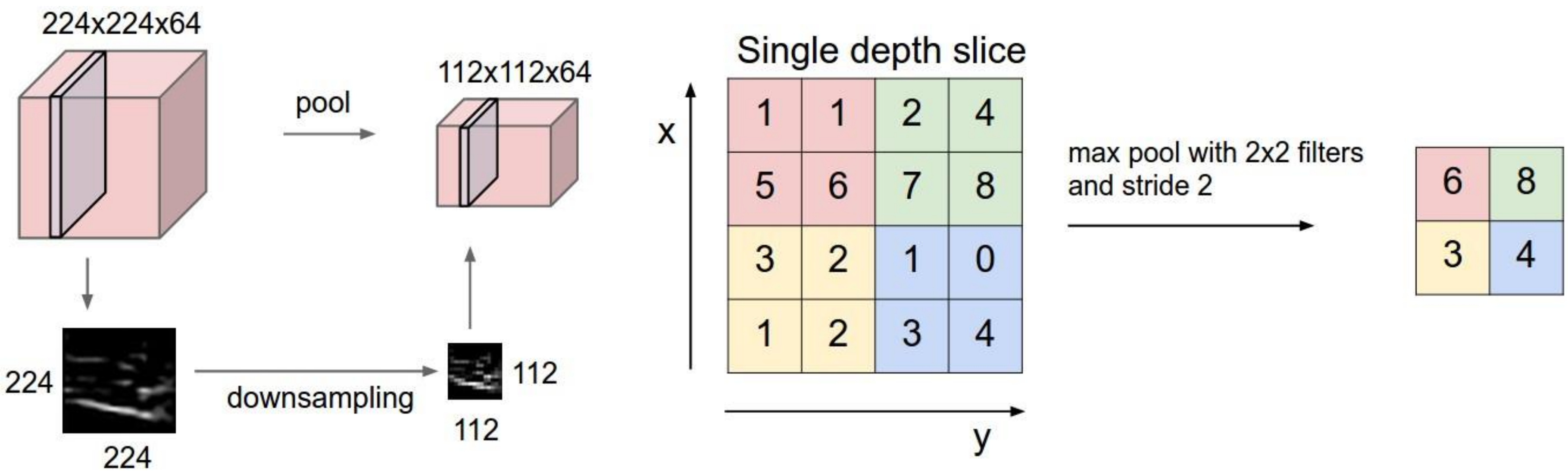
- Can expand this to 2D
  - Just need to make sure to link the right pixel with the right weight
- Can expand to multi-channel 2D
  - For RGB images
- Can expand to multiple kernels/filters
  - Output is not a single image anymore, but a **volume** (sometimes called a feature map)
  - Can be represented as a tensor (a 3D matrix)
- Usually also include a bias term and an activation



Pooling layer

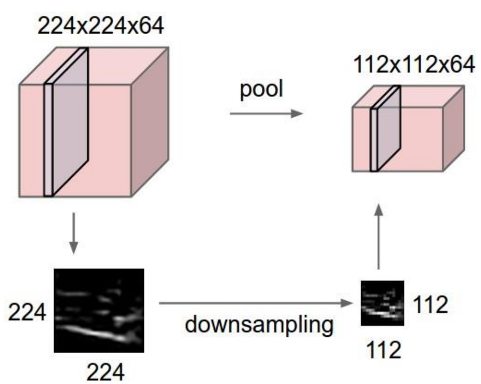
Pooling layer

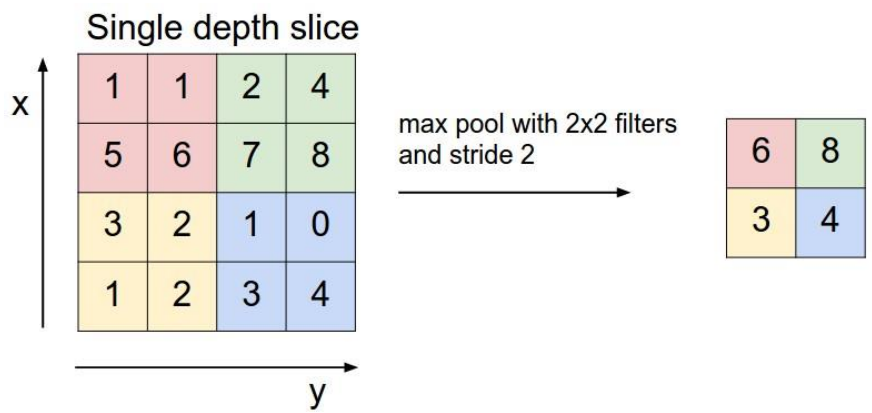
- Image subsampling



Pooling layer motivation

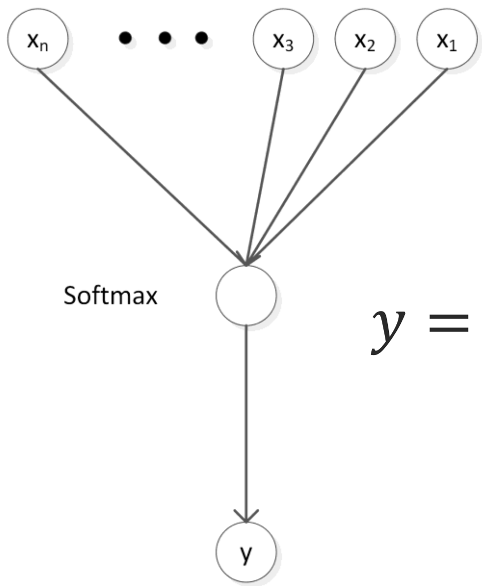
- Used for sub-sampling
  - Allows summarization of response
- Helps with translational invariance
- Have filter size and stride (hyperparameters)





Pooling layer gradient

1. Record during forward pass which pixel was picked and use the same in backward pass
2. Pick the maximum value from input using a smooth and differentiable approximation

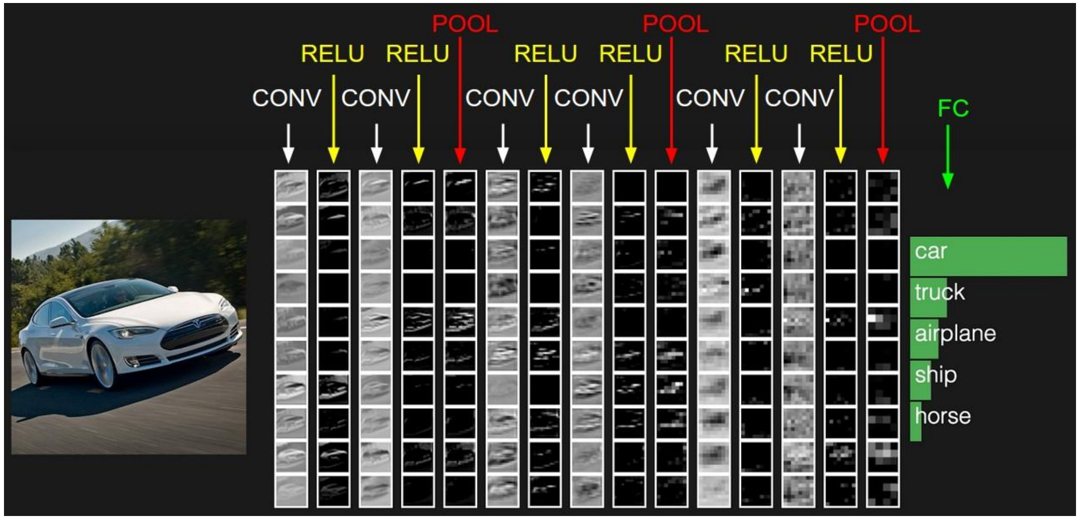


$$y = \frac{\sum_{i=1}^{n} x_i e^{\alpha x_i}}{\sum_{i=1}^{n} e^{\alpha x_i}}$$

Putting it all together

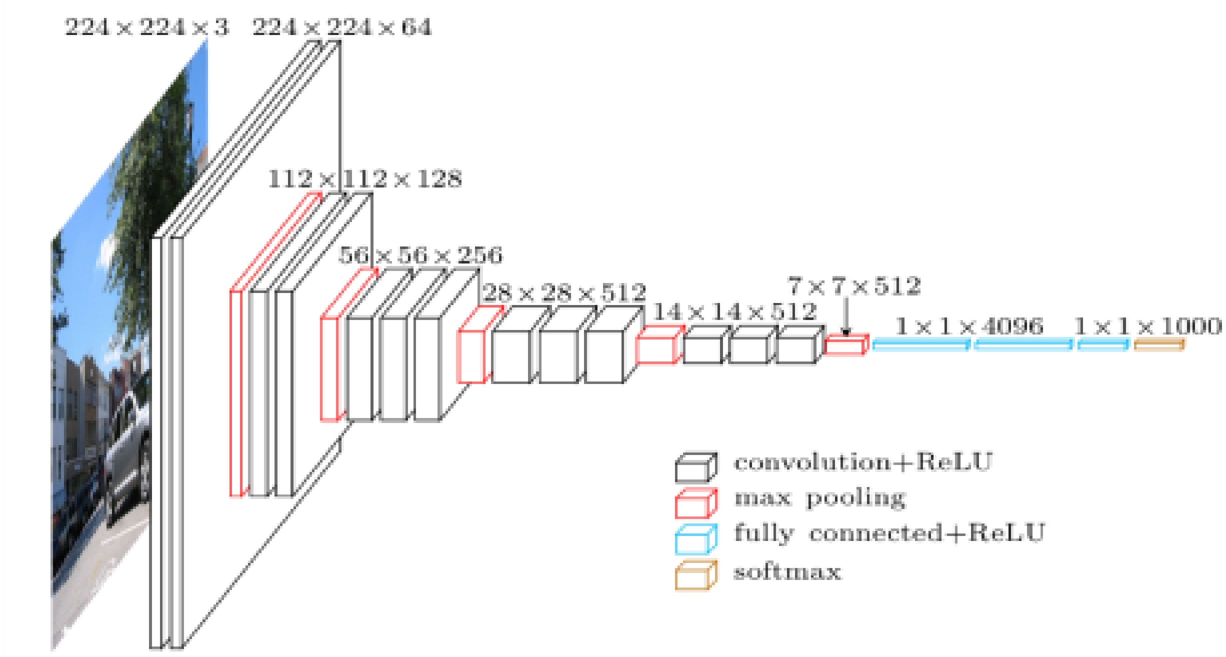
Common architectures

- Start with a convolutional layer follow by non-linear activation and pooling
- Repeat this several times
- Follow with a fully connected (MLP) layer

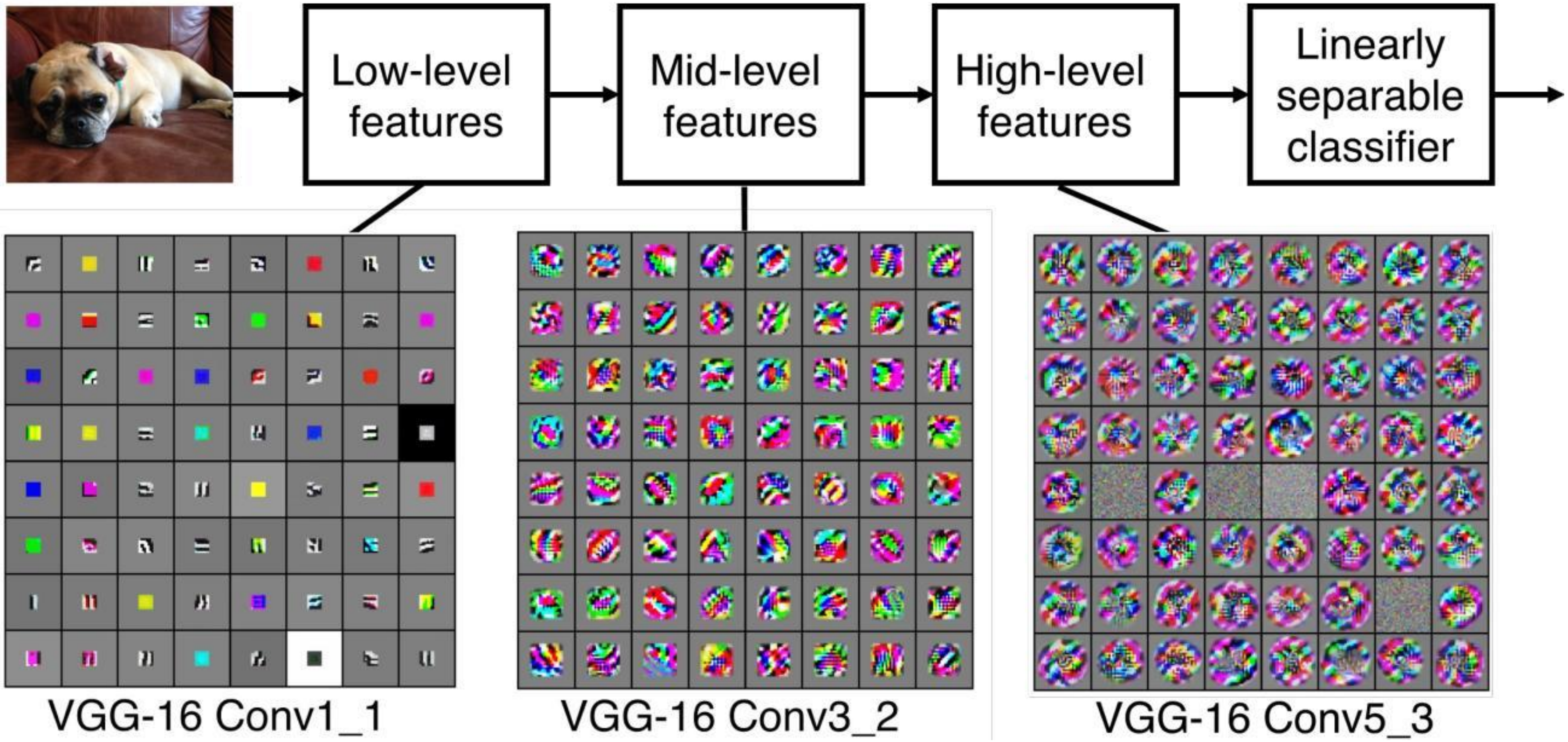


VGGNet model

- Used for object classification task
  - 1000 way classification task – pick one
  - 138 million params

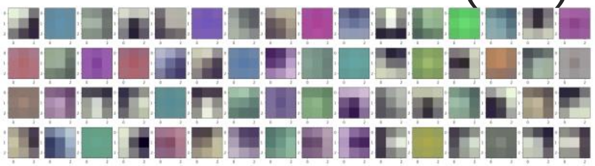


VGGNet Convolution Kernels

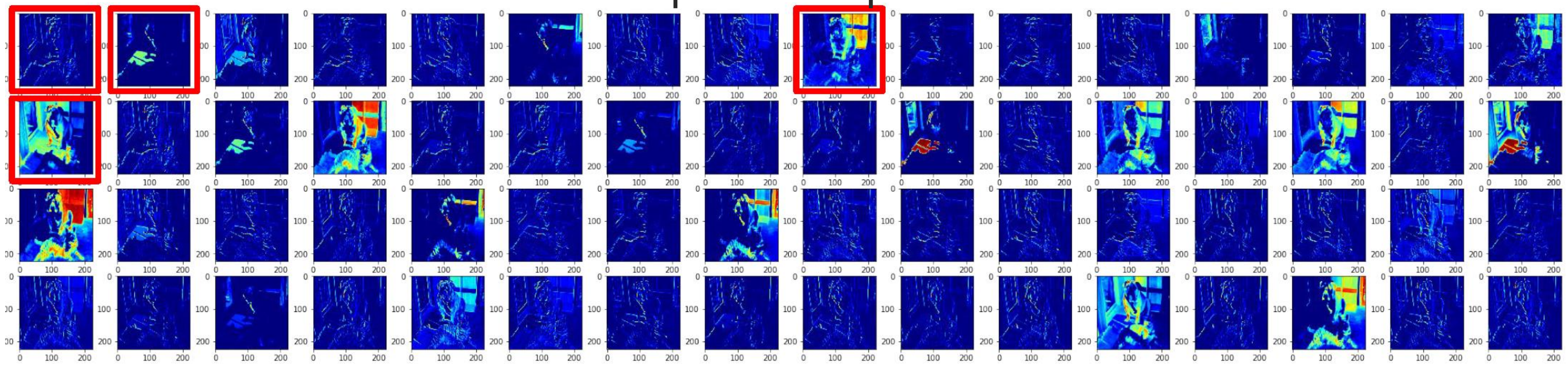


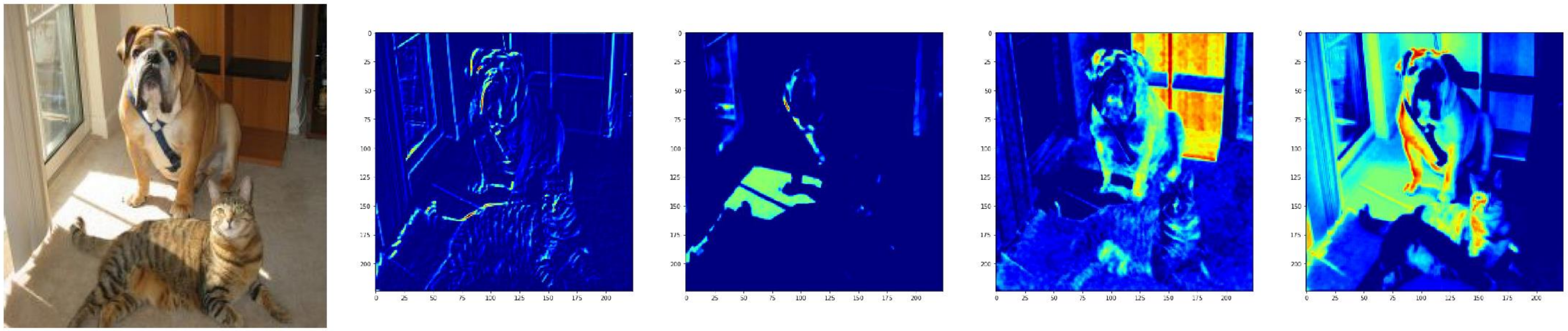
VGGNet Response Maps (aka Activation Maps)

Convolution kernels (3x3)

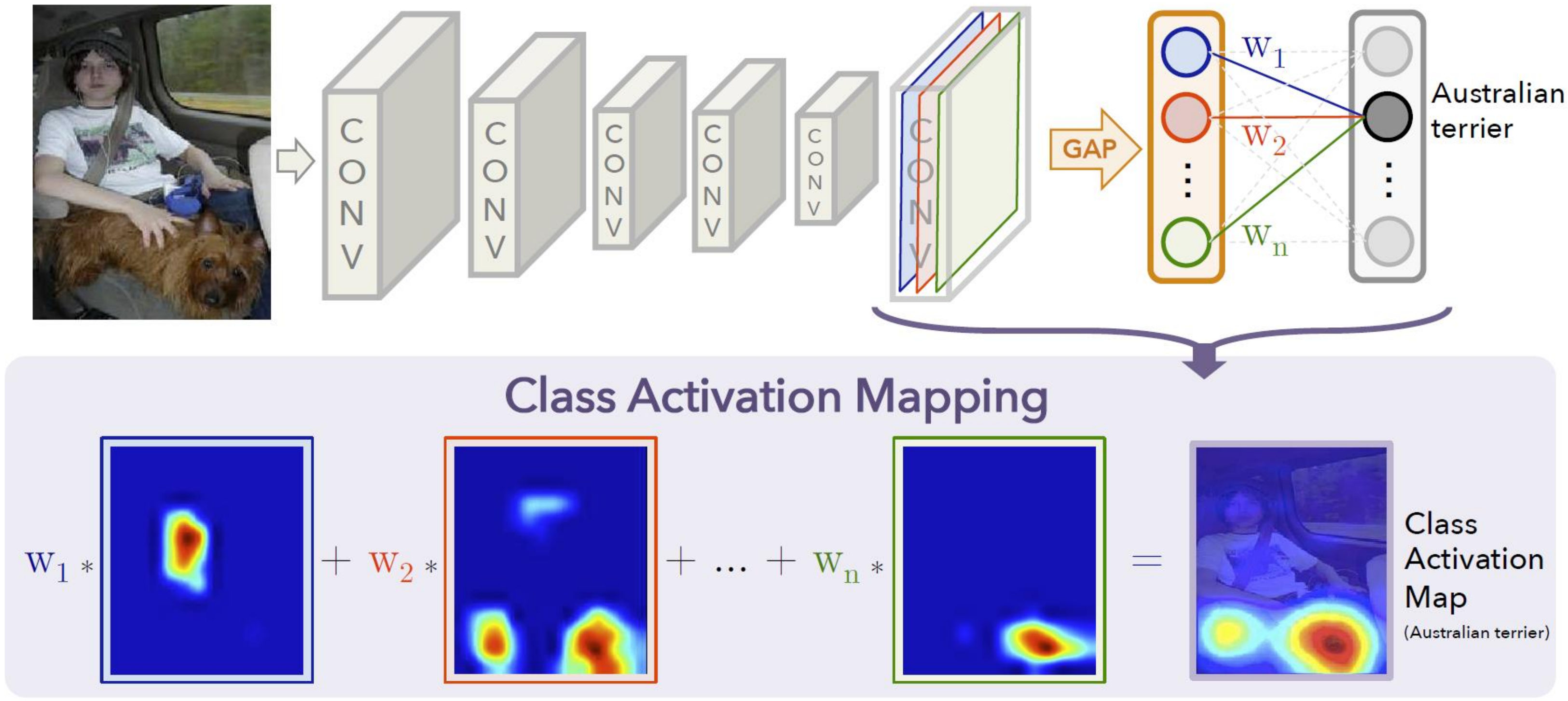


Response Maps



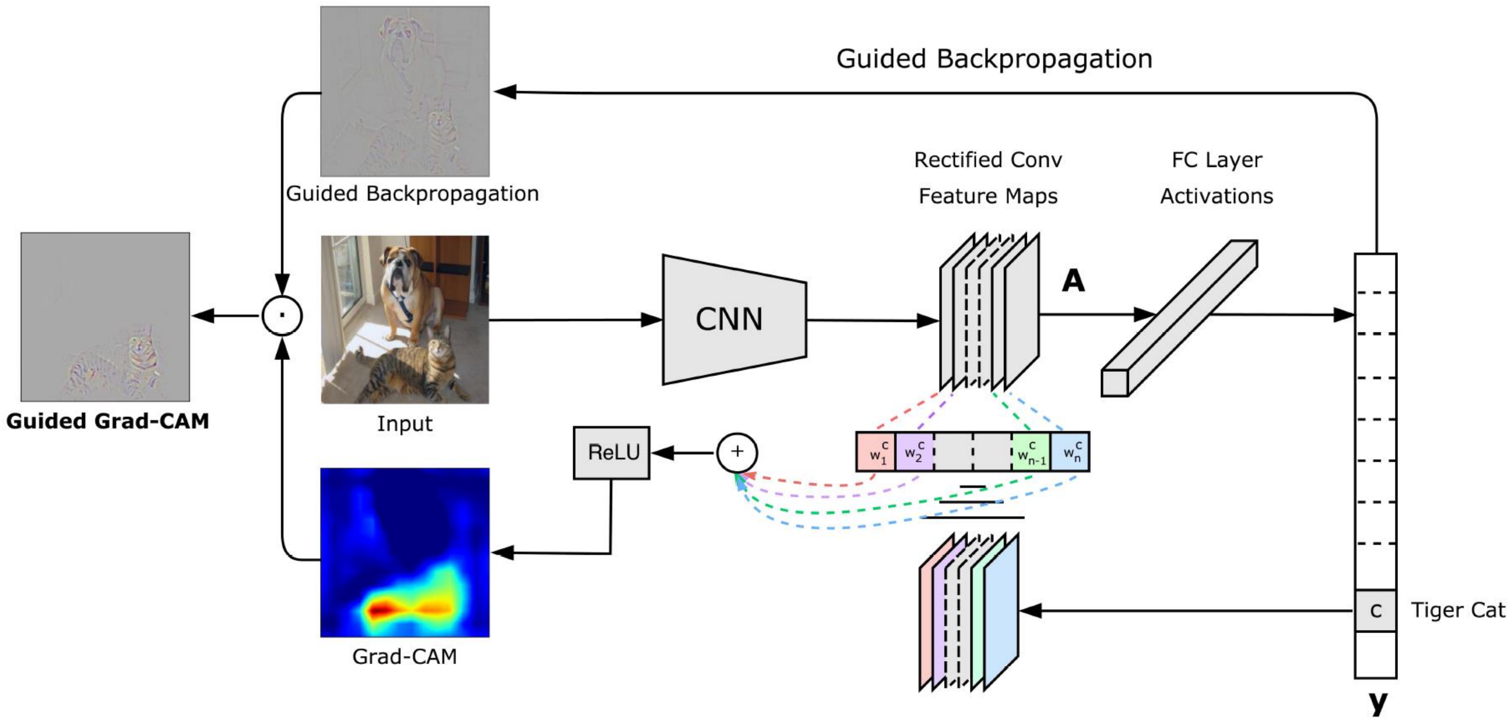


CAM: Class Activation Mapping [CVPR 2016]



$$L^c_{\text{CAM}} = \underbrace{\sum_k w^c_k A^k}_{\text{linear combination}}$$

Grad-CAM



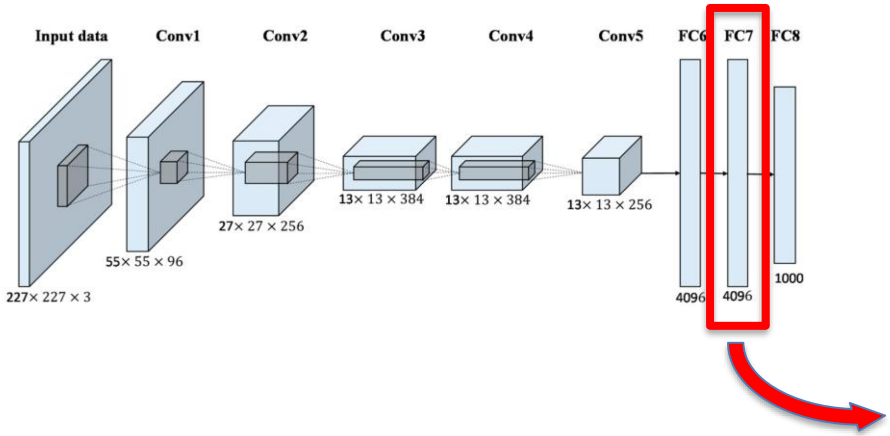
global average pooling

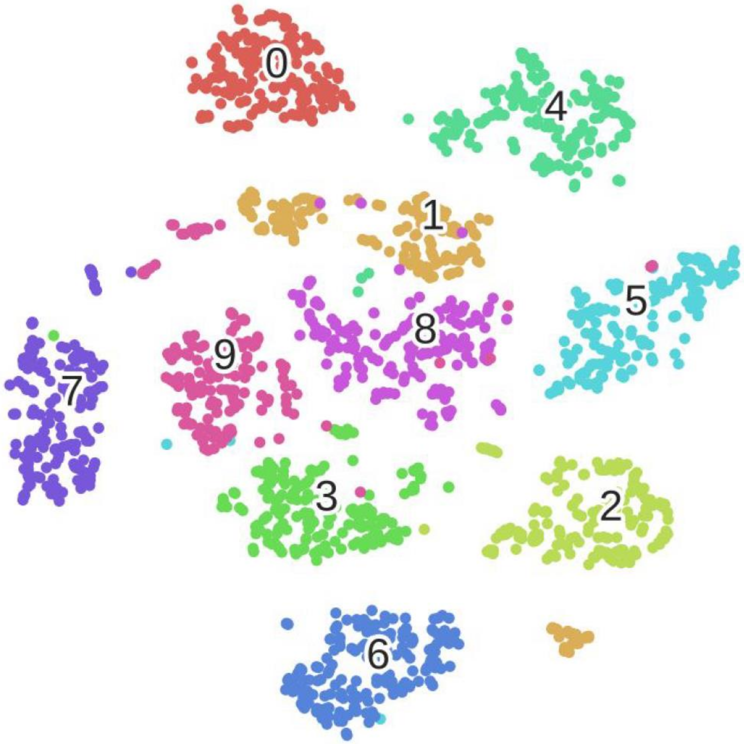
$$\alpha_k^c = \overbrace{\frac{1}{Z}\sum_i \sum_j}^{\text{global average pooling}} \underbrace{\frac{\partial y^c}{\partial A_{ij}^k}}_{\text{gradients via backprop}}$$

$$L_{\text{Grad-CAM}}^c = ReLU \underbrace{\left(\sum_k \alpha_k^c A^k \right)}_{\text{linear combination}}$$

Visualizing the Last CNN Layer: t-sne

Alex Net





Embed high dimensional data points (i.e. feature codes) so that pairwise distances are conserved in local neighborhoods.

Training tricks

- Data augmentation (Create more data)
  - Image scaling
  - Shifting
  - Rotation
  - Mirroring
- Optimization
  - Dropout
  - Regularization
  - Many more tricks/tips that we will discuss in Week 8

Fine tuning for specific tasks

- Often start with an existing architecture and an already trained network (for example AlexNet or VGGNet for object recognition)
- Discard the final layer score function and replace with your own (FC7)
- Perform gradient decent on it
  - Nice thing about neural networks is that we can continue training them with new data

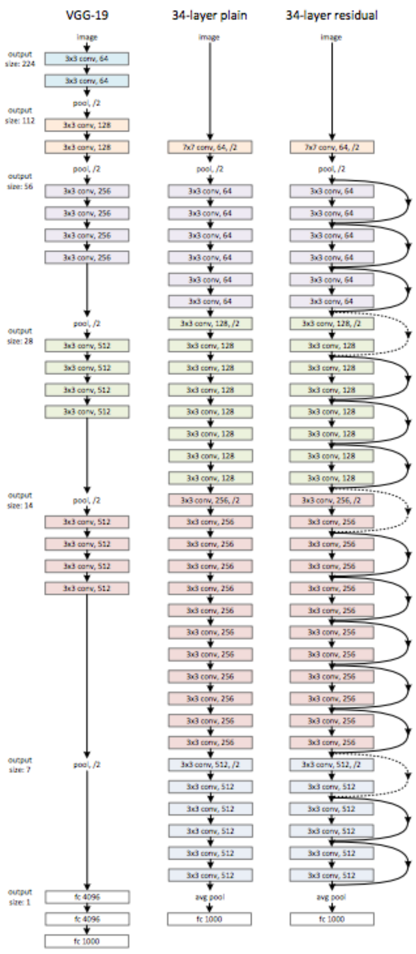
Other popular architectures

- LeNet – an early 5 layer architecture for handwritten digit recognition
- DeepFace – Facebook's face recognition CNN
- AlexNet – Object Recognition

- **Already trained models for object recognition can be found online**

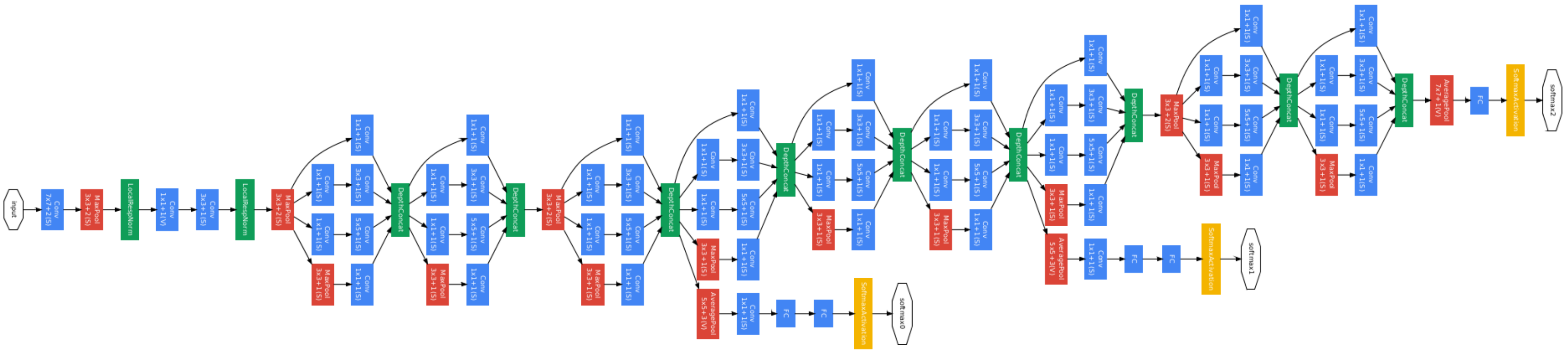
Residual Networks

- Adding residual connections



Googlenet

- Using residual blocks
  - Loss function in different layers of the network



Densely Connected CNN

- Connections between all the layers