Deep Learning I: from shallow to deep

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Agenda

Image classification basics

Searching for human-like image classification methods

Neural networks: from shallow to deep
- Motivation and definitions
- Linear function, loss function, optimization
- Simple Neural Network

Convolutional Neural Networks
- Current Architectures
- Guidelines for training

Image classification example

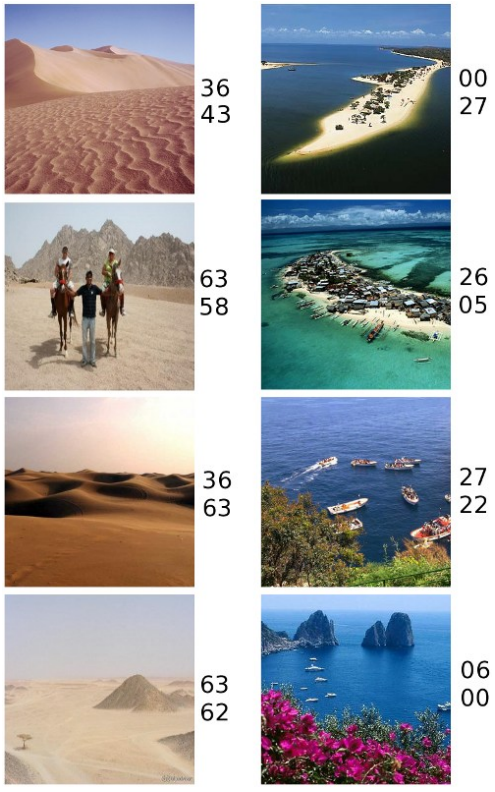
Task: learn how to distinguish two types of images:

- **desert**;
- **beach**.

Objective: given some images, develop a model able to classify unseen images into one of those two classes.

Image classification example

- **Features**: set of values extracted from images that can be used to measure the (dis)similarity between images **Any suggestion?**
  - Use the two most frequent colors as a descriptor!



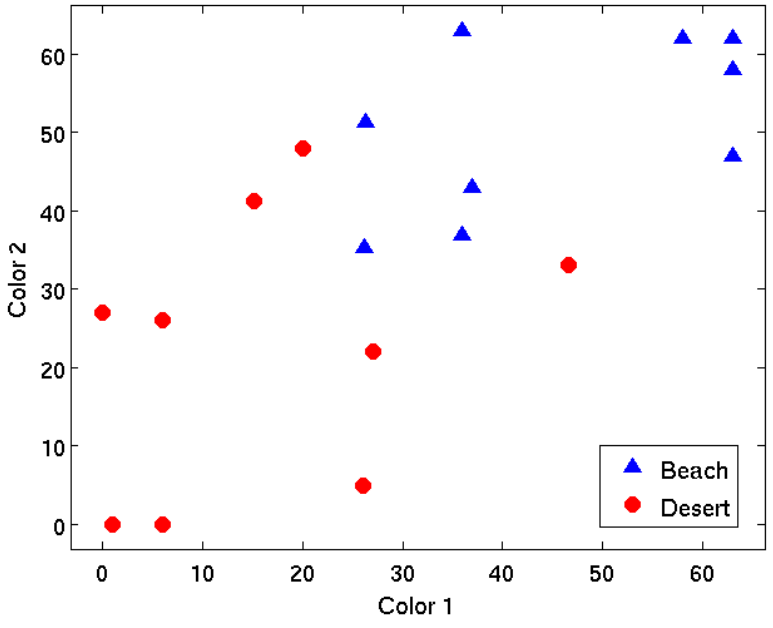


Image classification example

- **Classifier**: a model build using labeled examples (images for which the classes are known). This model must be able to predict the class of a new image. **Any suggestion?**
  - A linear classifier, for instance!

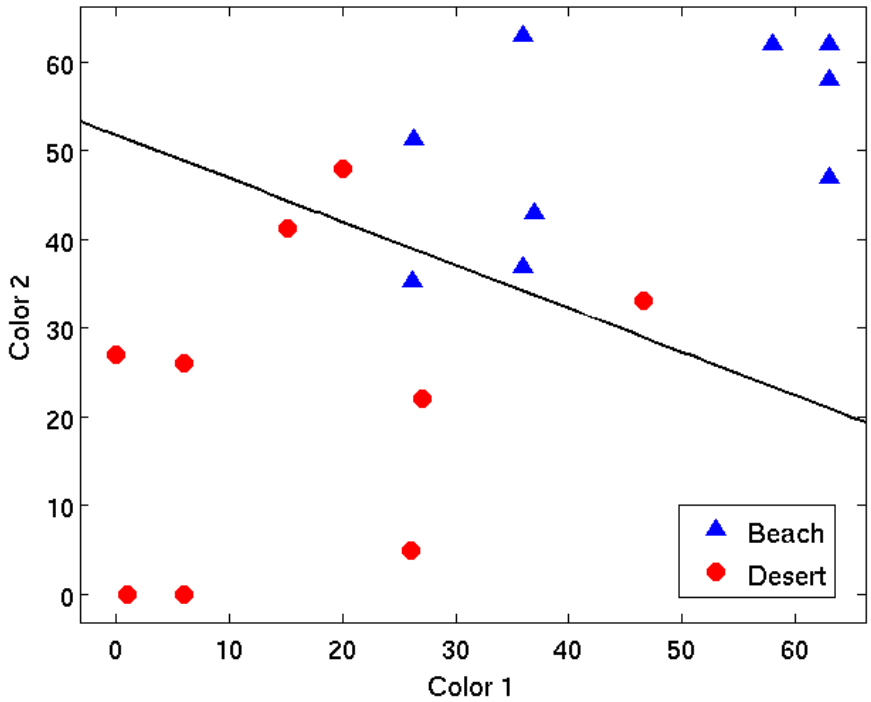


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Image classification example

- Examples used to build the classifier : **training set**.
- Training data is seldom linearly separable
- Therefore there is a **training error**

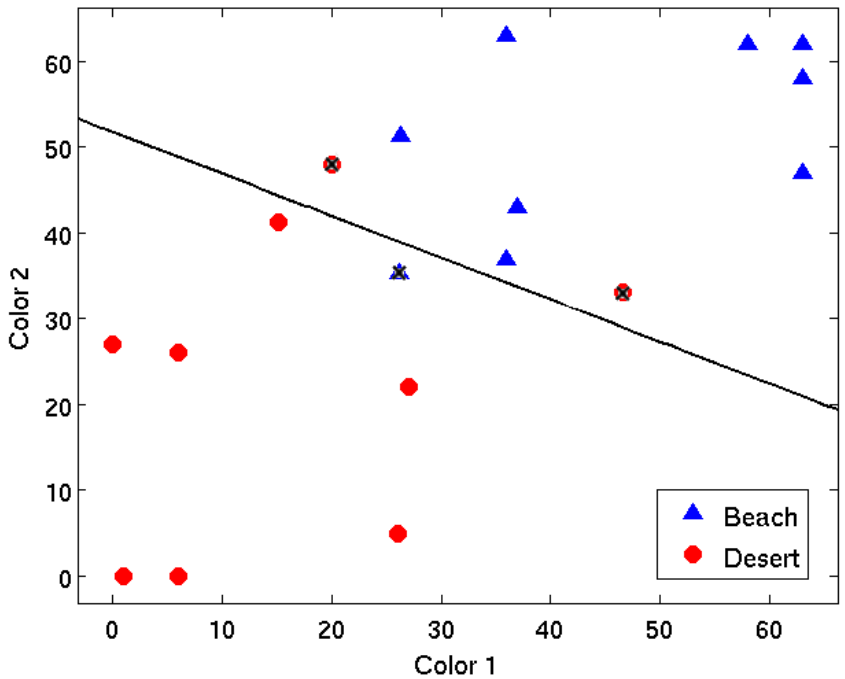


Image classification example

- The model, or **classifier**, can then be used to predict/infer the class of a new **example**.

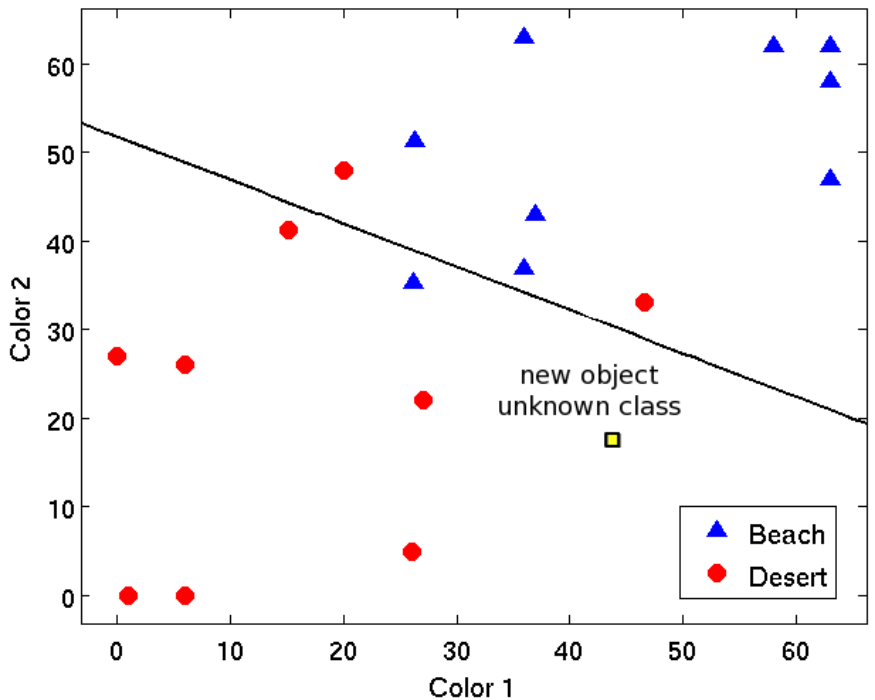
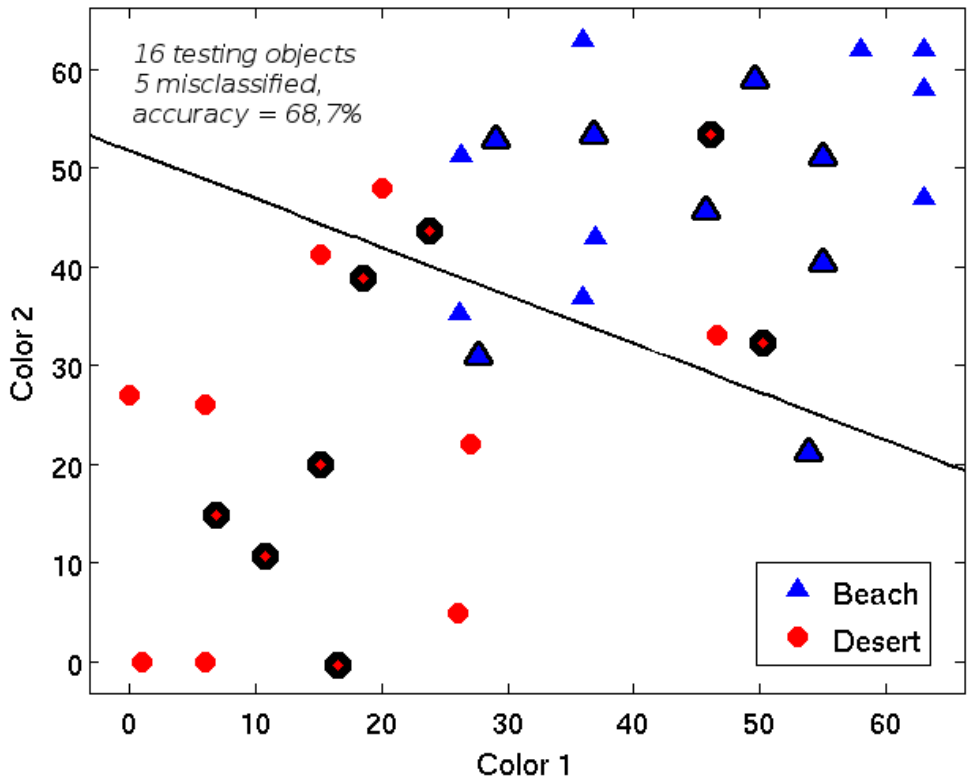


Image classification example

- Now we want to test, for future data (not used in training), the classifier error rate (or alternatively, its accuracy)
- Examples used in this stage compose the **test set**.



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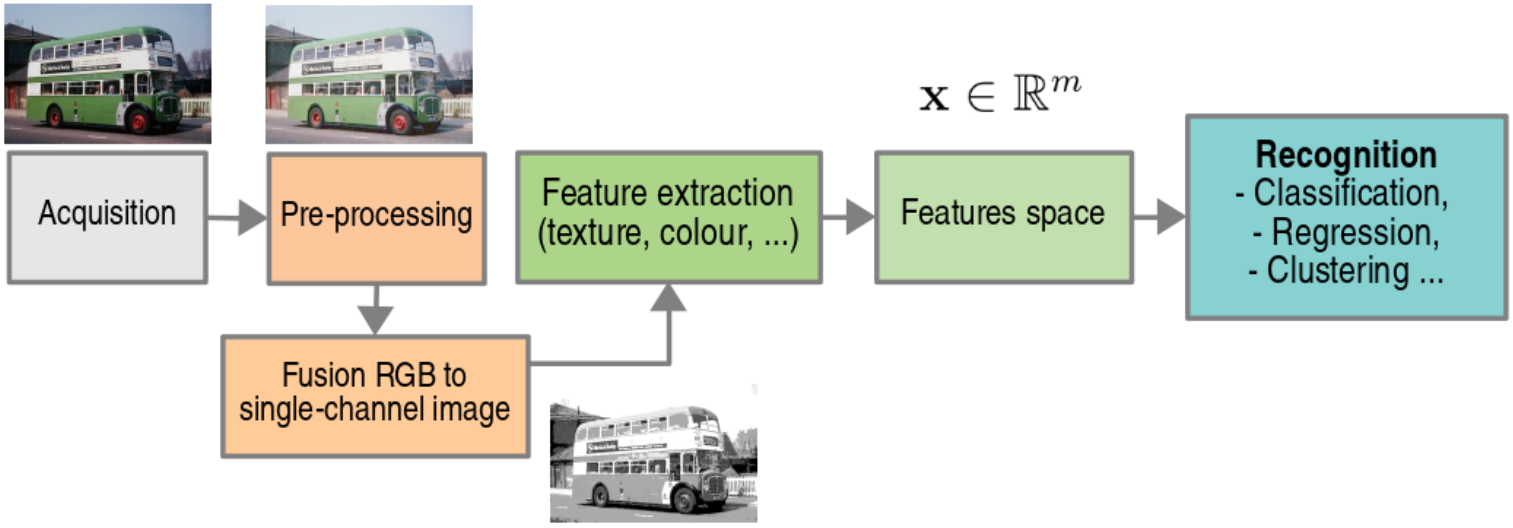
Classic image recognition pipeline



History of methods for computer vision

- Color, shape and texture descriptors (1970-2000)
- SIFT (>1999)
- Histogram of Gradients (>2005)
- Bag of Features (>2004)
- Spatial Pyramid Matching (>2006),

Classic image recognition pipeline

1. Descriptor grid: HoG, LBP, SIFT, SURF
2. Fisher Vectors
3. Spatial Pyramid Matching
4. Classification Algorithm

Not so versatile!

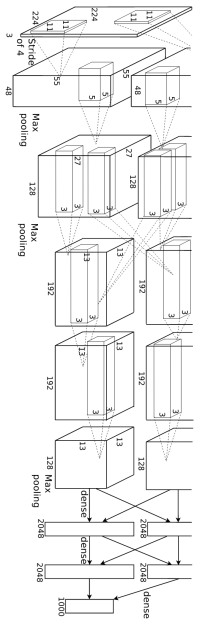
And then, in 2012...

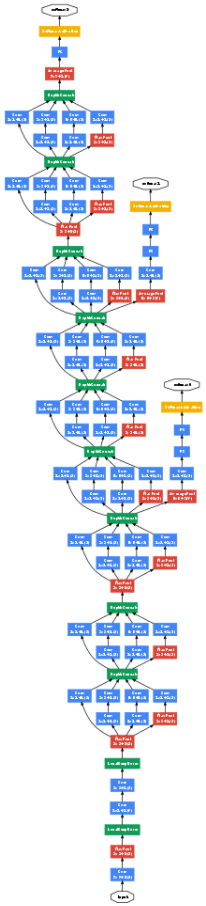
The world didn't end and AlexNet won the ImageNet chalange!

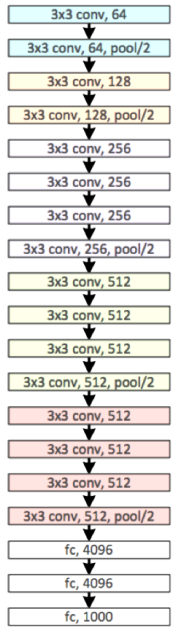
ImageNet Challenge: $\sim$ 1.4 million images, 1000 classes.

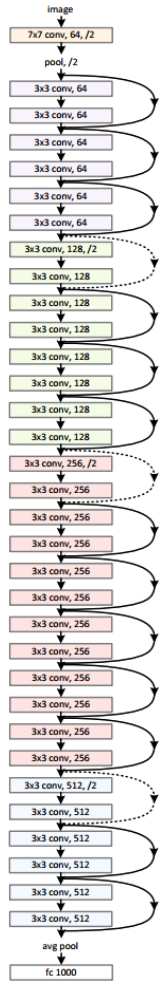
And CNNs continued to dominate image classification

AlexNet (9) GoogLeNet (22) VGG (16/19) ResNet (34+)



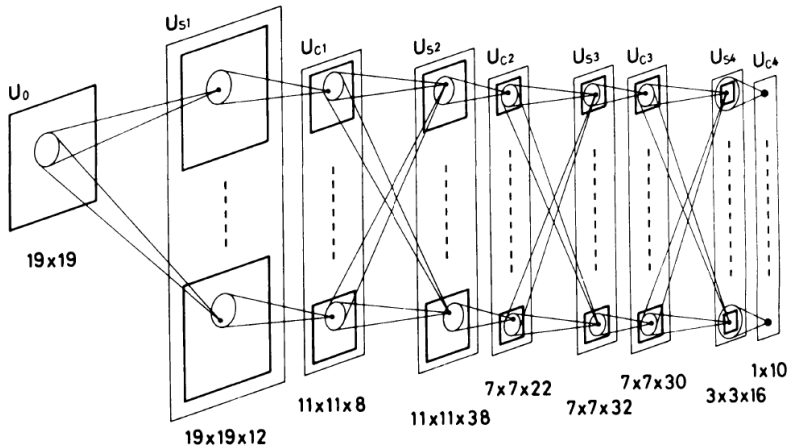




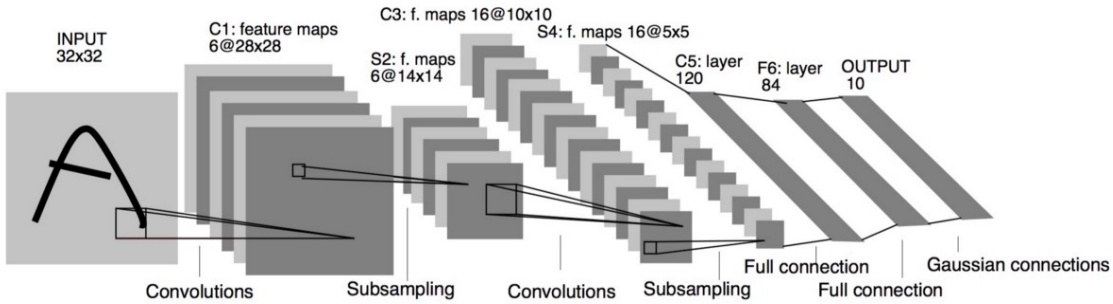


But CNNs were not invented in 2012...

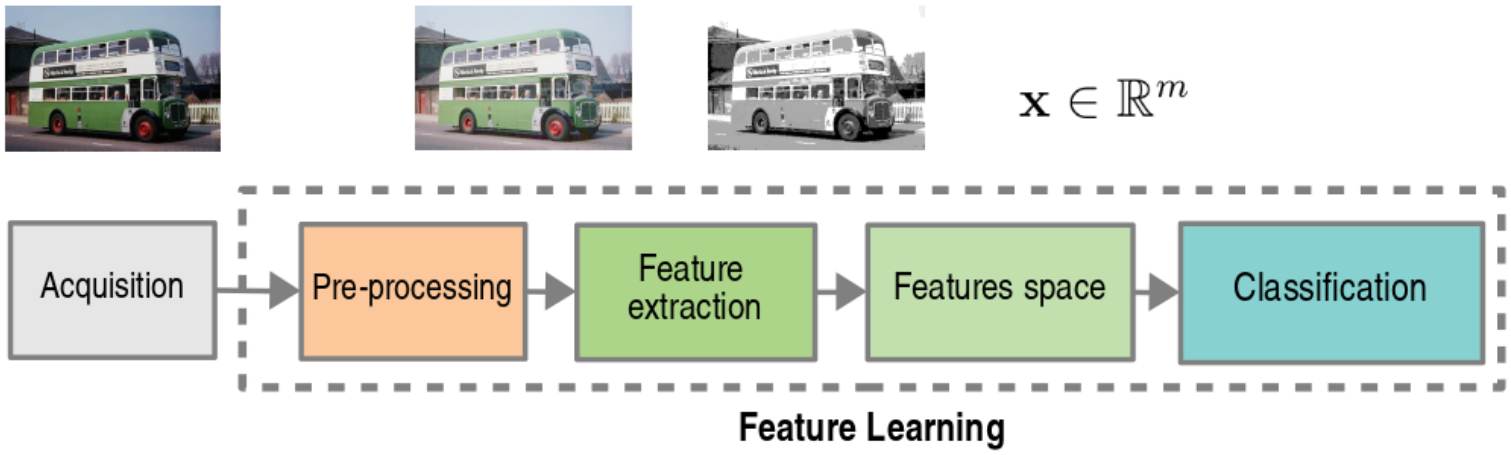
Fukushima's Neocognitron (1989)



LeCun's LeNet (1998)



New image recognition pipeline: feature learning



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Motivation with two problems

We want to find a function in the form $f(\mathbf{x}) = y$ — the meaning of those are dependent on the task!

Image classification: animals

- Data available: pairs (images, labels) from owls, cats and turtles,
- Input: RGB image in the form $\mathbf{x}$,
- Output: predicted label y (e.g. cat) assigned to the input image.

Motivation with two problems

Anomaly detection in Credit Card transactions

- Data available: legitimate transactions from a given client,
- Input: real-valued data including transaction location, currency, value, timestamp, in form of $\mathbf{x}$,
- Output: probability y of observing a fraudulent (anomalous) transaction.

Machine Learning (ML) vs Deep Learning (DL)

Machine Learning

A more broad area that includes DL. Algorithms aims to infer $f()$ from a space of admissible functions given training data.

- "shallow" methods often infer a single function $f(.)$.
- e.g. a linear function $f(x) = w \cdot x + b$,
- Common algorithms: The Perceptron, Support Vector Machines, Logistic Classifier, etc.

Machine Learning (ML) vs Deep Learning (DL)

Deep Learning

Involves learning a sequence of representations via composite functions.
Given an input $\mathbf{x}_1$ several intermediate representations are produced:

$$\mathbf{x}_2 = f_1(\mathbf{x}_1)$$
$$\mathbf{x}_3 = f_2(\mathbf{x}_2)$$
$$\mathbf{x}_4 = f_3(\mathbf{x}_3)$$
$$\dots$$

The output is achieved by several L nested functions in the form:

$$f_L\left(\cdots f_3(f_2(f_1(\mathbf{x}_1, W_1), W_2), W_3) \cdots, W_L\right),$$

W_i are hyperparameters associated with each function i.

A shallow linear classifier

Input  $\rightarrow \mathbf{x}$

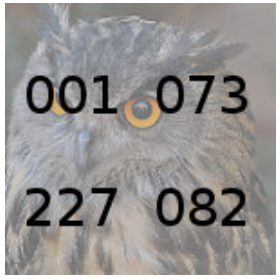
weight matrix — image — bias term

$$f(W, \mathbf{x}) = W \quad \mathbf{x} \quad + \quad \mathbf{b}$$

$$= \text{ scores for possible classes of } \mathbf{x}$$

Linear classifier for image classification

- Input: image (with $N \times M \times 3$ numbers) vectorized into column $\mathbf{x}$
- Classes: cat, turtle, owl
- Output: class scores



$$= \mathbf{x} = [1, 73, 227, 82]$$

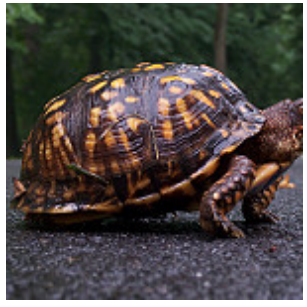
$$f(\mathbf{x}, W) = s \quad \rightarrow \quad \text{3 numbers with class scores}$$

$$W\mathbf{x} + \mathbf{b}$$

$$\begin{bmatrix} 0.1 & -0.25 & 0.1 & 2.5 \\ 0 & 0.5 & 0.2 & -0.6 \\ 2 & 0.8 & 1.8 & -0.1 \end{bmatrix} \times \begin{bmatrix} 1 \\ 73 \\ 227 \\ 82 \end{bmatrix} + \begin{bmatrix} -2.0 \\ 1.7 \\ -0.5 \end{bmatrix} = \begin{bmatrix} -337.3 \\ -38.6 \\ 460.30 \end{bmatrix}$$

Linear classifier for image classification





cat	-337.3	**380.3**	8.6
owl	**460.3**	160.3	**26.3**
turtle	38.6	17.6	21.8

We need:

- a **loss function** that quantifies undesired scenarios in the training set
- an **optimization algorithm** to find W so that the loss function is minimized!

Linear classifier for image classification

- We want to optimize some function to produce the best classifier
- This function is often called **loss function**,

Let (x_i, y_i) be a training example: x_i are the features, y is the label, and $f(.)$ a classifier that maps any x_i into a class using parameters W.
A loss for a single example is some function in the form:

$$\ell\left(f(W, \mathbf{x}_i), y_i\right) \tag{1}$$

Linear classifier for image classification

In practice, we measure the loss $\mathcal{L}$, over a set X, Y of N examples. Common functions are:

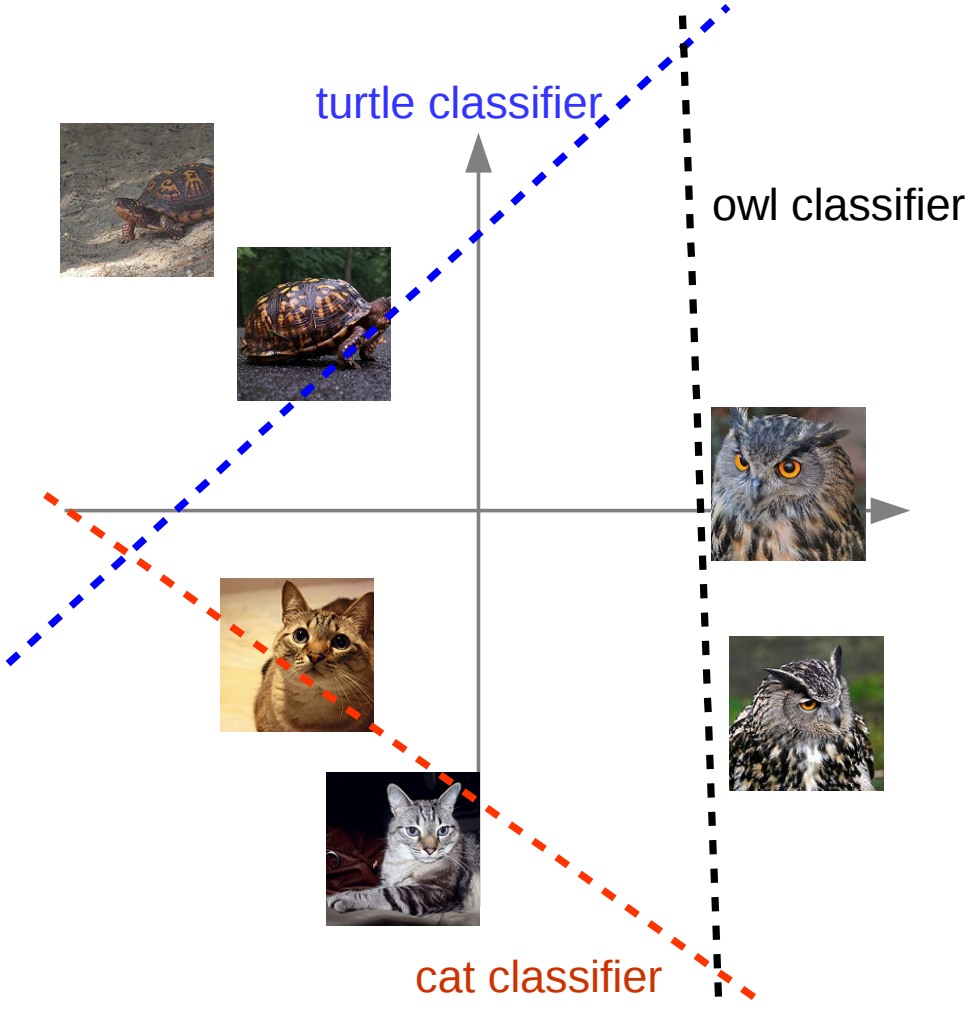
Mean squared error (continuous values)

$$\mathcal{L}\left(f(W,X,Y)\right) = \mathcal{L}\left(\hat{Y},Y\right) = \frac{1}{N}\sum_{i=1}^{N}(\underbrace{\hat{y}_i}_{\text{predicted label}} - \underbrace{y_i}_{\text{true label}})^2$$

Cross entropy (bits or probability vectors)

$$\mathcal{L}\left(\hat{Y},Y\right) = \frac{1}{N}\sum_{i=1}^{N} y_i \log \hat{y}_i + (1-\hat{y}_i)\log(1-\hat{y}_i)$$

A linear classifier we would like



Minimizing the loss function

Use the slope of the loss function over the space of parameters! For each dimension j:

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

$$\frac{d\ell\left(f(w_j, \mathbf{x}_i)\right)}{dw_j} = \lim_{\delta \to 0} \frac{f(w_j+\delta, \mathbf{x}_i) - f(w_j, \mathbf{x}_i)}{\delta}$$

We have multiple dimensions, therefore a gradient (vector of derivatives).

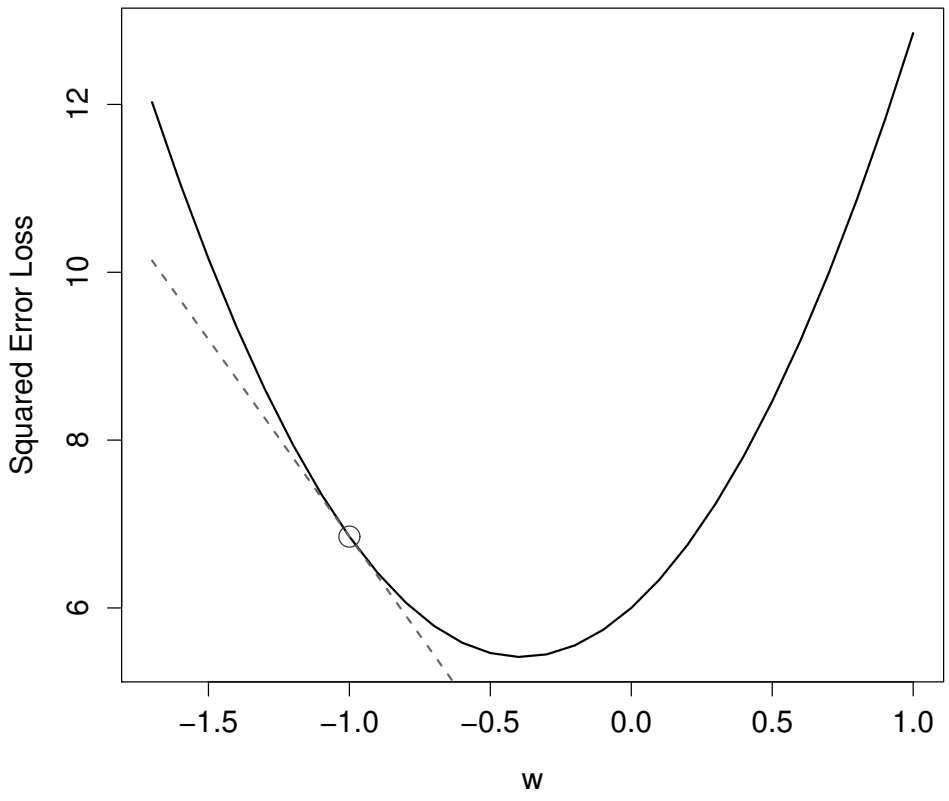
We may use:

1. Numerical gradient: approximate
2. Analytic gradient: exact

Gradient descent — search for the valley of the function, moving in the direction of the negative gradient.

Gradient descent

Changes in a parameter affects the loss (ideal example)



Gradient descent

W

$$\begin{bmatrix} 0.1, \\ -0.25, \\ 0.1, \\ 2.5, \\ 0, \\ ..., \\ -0.1 \end{bmatrix}$$

$\ell(f(W)) = 2.31298$

$w_i + \delta$

$$\begin{bmatrix} 0.1 + \mathbf{0.001}, \\ -0.25, \\ 0.1, \\ 2.5, \\ 0, \\ ..., \\ -0.1 \end{bmatrix}$$

$\ell(f(W')) = 2.31\mathbf{201}$

dw_i

$$\begin{bmatrix} ?, \\ , \\ , \\ , \\ , \\ ..., \\ \end{bmatrix}$$

$(f(w_i+\delta)-f(w_i))/\delta$

Gradient descent

W

$$\begin{bmatrix} 0.1, \\ -0.25, \\ 0.1, \\ 2.5, \\ 0, \\ ..., \\ -0.1 \end{bmatrix}$$

$\ell(f(W)) = 2.31298$

$w_i + \delta$

$$\begin{bmatrix} 0.1 + \mathbf{0.001}, \\ -0.25, \\ 0.1, \\ 2.5, \\ 0, \\ ..., \\ -0.1 \end{bmatrix}$$

$\ell(f(W')) = 2.31\mathbf{201}$

dw_i

$$\begin{bmatrix} -0.97, \\ , \\ , \\ , \\ , \\ ..., \end{bmatrix}$$

$(f(w_i+\delta)-f(w_i))/\delta$

Gradient descent

W

$$\begin{bmatrix} 0.1, \\ -0.25, \\ 0.1, \\ 2.5, \\ 0, \\ ..., \\ -0.1 \end{bmatrix}$$

$\ell(f(W)) = 2.31298$

$w_i + \delta$

$$\begin{bmatrix} 0.1, \\ -0.25 + \mathbf{0.001}, \\ 0.1, \\ 2.5, \\ 0, \\ ..., \\ -0.1 \end{bmatrix}$$

$\ell(f(W')) = 2.31298$

dw_i

$$\begin{bmatrix} -0.97, \\ 0.0, \\ , \\ , \\ , \\ ..., \end{bmatrix}$$

$(f(w_i+\delta)-f(w_i))/\delta$

Gradient descent

W

$$\begin{bmatrix} 0.1, \\ -0.25, \\ 0.1, \\ 2.5, \\ 0, \\ ..., \\ -0.1 \end{bmatrix}$$

$\ell(f(W)) = 2.31298$

$w_i + \delta$

$$\begin{bmatrix} 0.1, \\ -0.25, \\ 0.1 + \mathbf{0.001}, \\ 2.5, \\ 0, \\ ..., \\ -0.1 \end{bmatrix}$$

$\ell(f(W1)) = 2.31\mathbf{459}$

dw_i

$$\begin{bmatrix} -0.97, \\ 0.0, \\ +1.61, \\ -, \\ -, \\ ..., \\ - \end{bmatrix}$$

$(f(w_i+\delta)-f(w_i))/\delta$

Gradient descent

W

$$\begin{bmatrix} 0.1, \\ -0.25, \\ 0.1, \\ 2.5, \\ 0, \\ ..., \\ -0.1 \end{bmatrix}$$

$\ell(f(W)) = 2.31298$

$w_i + \delta$

$$\begin{bmatrix} 0.1, \\ -0.25, \\ 0.1, \\ 2.5, \\ 0, \\ ..., \\ -0.1 \end{bmatrix}$$

$\ell(f(W')) =$
$\mathbf{2.08720}$

dw_i

$$\begin{bmatrix} -0.93, \\ 0.0, \\ -1.61, \\ +0.02, \\ +0.5, \\ ..., \\ -3.7 \end{bmatrix}$$

$(f(w_i+\delta)-f(w_i))/\delta$

Stochastic Gradient Descent (SGD)

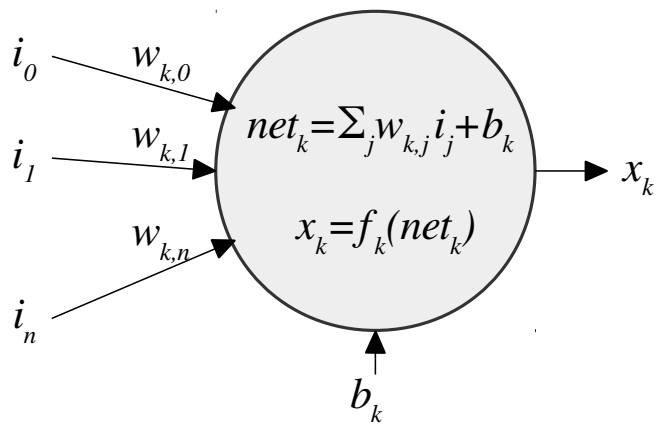
It is hard to compute the gradient, when N is large.

SGD:
Approximate the sum using a **minibatch** (random sample) of instances: something between 32 and 512.
Because it uses only a fraction of the data:

- fast
- often gives bad estimates on each iteration, needing more iterations

Neuron

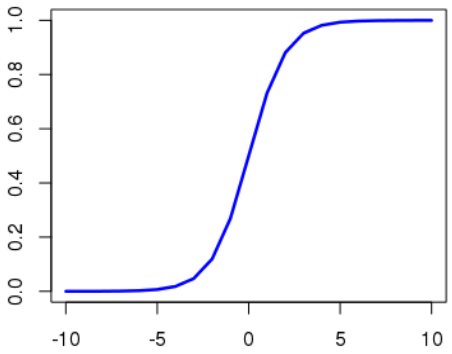
- input: several values (e.g. organized in a vector)
- output: a single value x.
- each input is associated with a weight w (connection strength)
- often there is a bias value b (intercept)
- to learn is to adapt the parameters: weights w and b
- function $f(.)$ is called activation function (transforms output)



Some activation functions

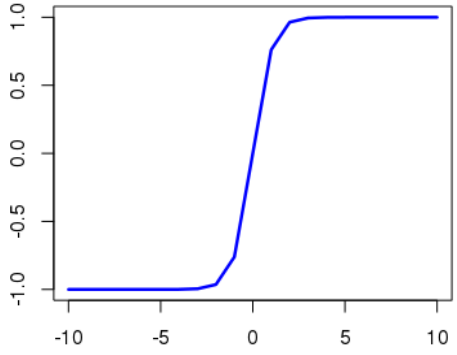
Sigmoid

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



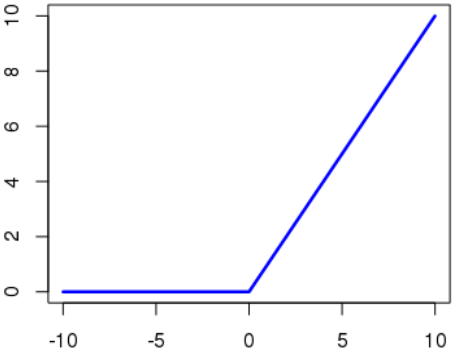
Hiperbolic Tangent

$$f(x) = \tanh(x)$$



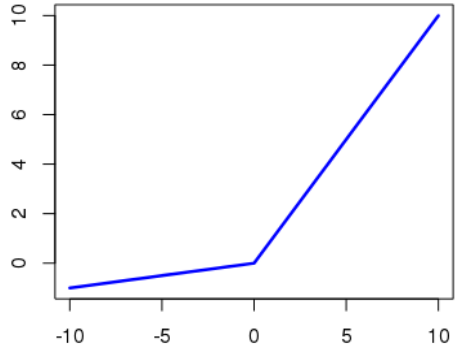
ReLU

$$f(x) = \max(0, x)$$



Leaky ReLU

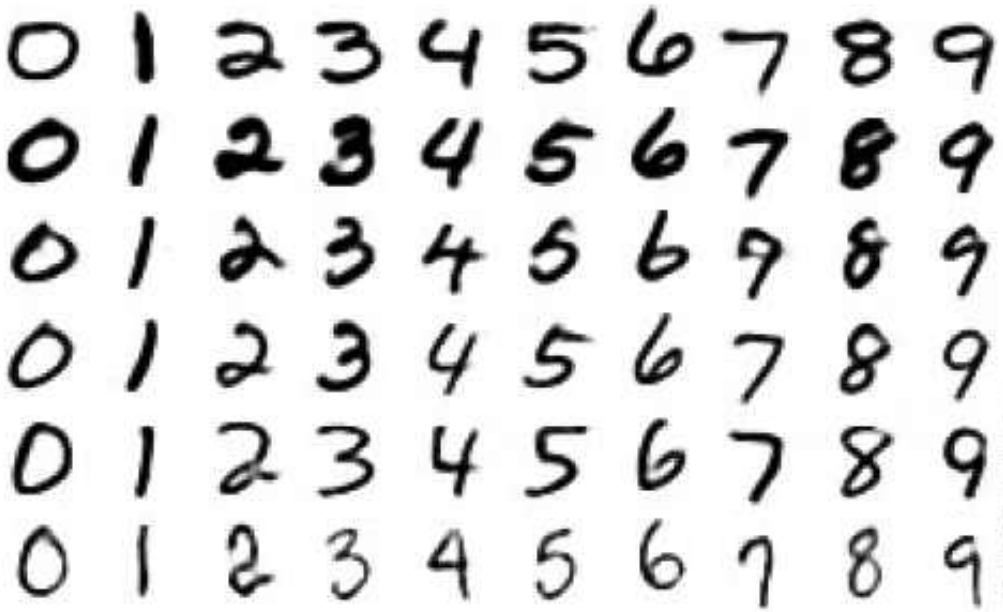
$$f(x) = \max(0.1x, x)$$



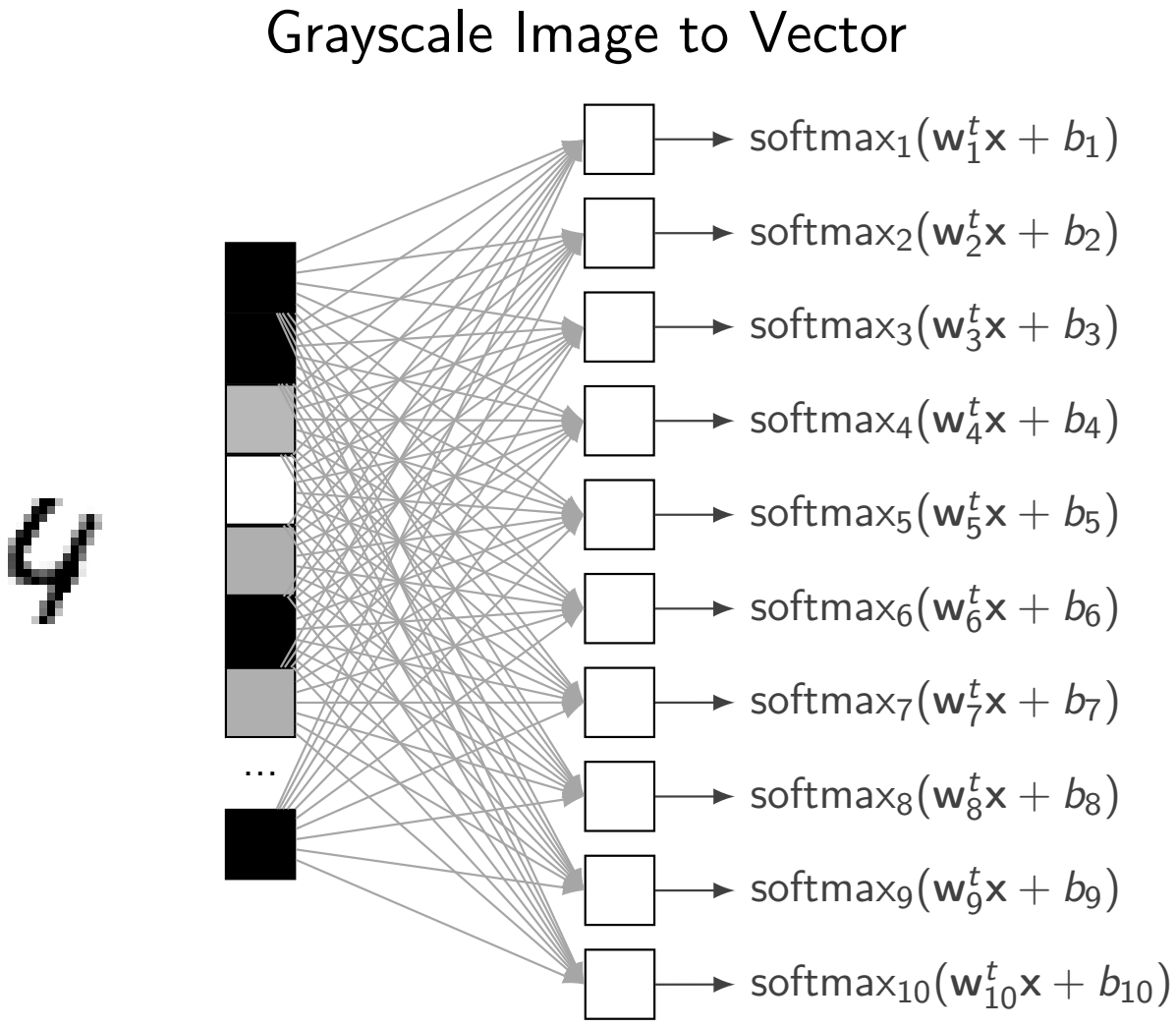
Backpropagation

- Algorithm that recursively apply chain rule to compute weight adaptation for all parameters.
- **Forward**: compute the loss function for some training input over all neurons,
- **Backward**: apply chain rule to compute the gradient of the loss function, propagating through all layers of the network, in a graph structure

A simple problem: digit classification



Neural Network with Single Layer



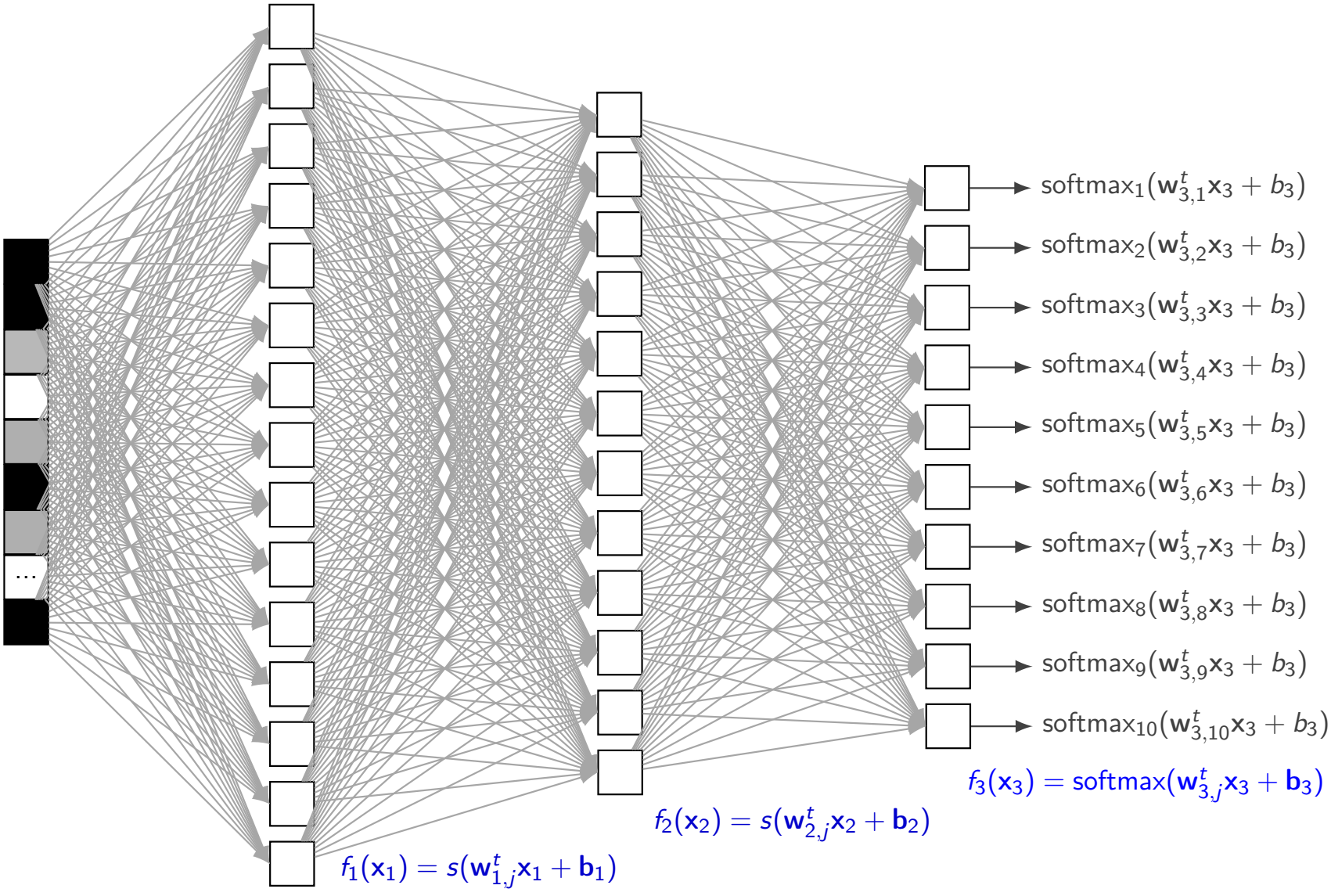
A simple problem: digit classification

$$\begin{bmatrix} x_{0,0} & x_{0,1} & x_{0,2} & \cdots & x_{0,783} \\ x_{1,0} & x_{0,1} & x_{1,2} & \cdots & x_{0,783} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_{63,0} & x_{63,1} & x_{63,2} & \cdots & x_{63,783} \end{bmatrix} \cdot \begin{bmatrix} w_{0,0} & w_{0,1} & \cdots & w_{0,9} \\ w_{1,0} & w_{1,1} & \cdots & w_{1,9} \\ w_{2,0} & w_{2,1} & \cdots & w_{2,9} \\ \vdots & \vdots & \ddots & \vdots \\ w_{783,0} & w_{783,1} & \cdots & w_{783,9} \end{bmatrix} + \begin{bmatrix} b_0 & b_1 & b_2 & \ldots & b_9 \end{bmatrix}$$

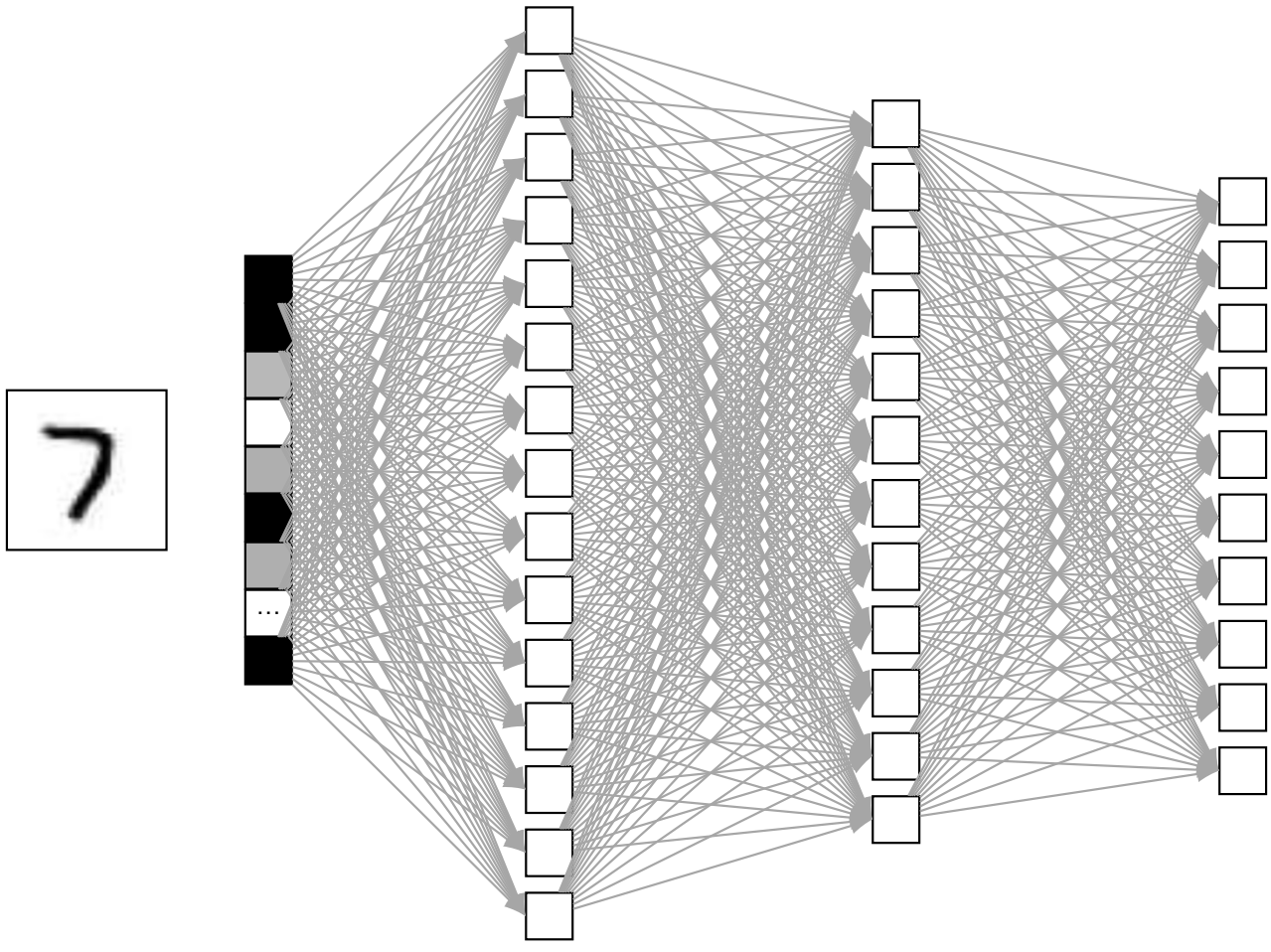
$$\mathbf{Y} = \text{softmax}(\mathbf{X} \cdot \mathbf{W} + \mathbf{b})$$

$$\mathbf{Y} = \begin{bmatrix} y_{0,0} & y_{0,1} & y_{0,2} & \cdots & y_{0,9} \\ y_{1,0} & y_{1,1} & y_{1,2} & \cdots & y_{1,9} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ y_{63,0} & y_{63,1} & y_{63,2} & \cdots & y_{63,9} \end{bmatrix}$$

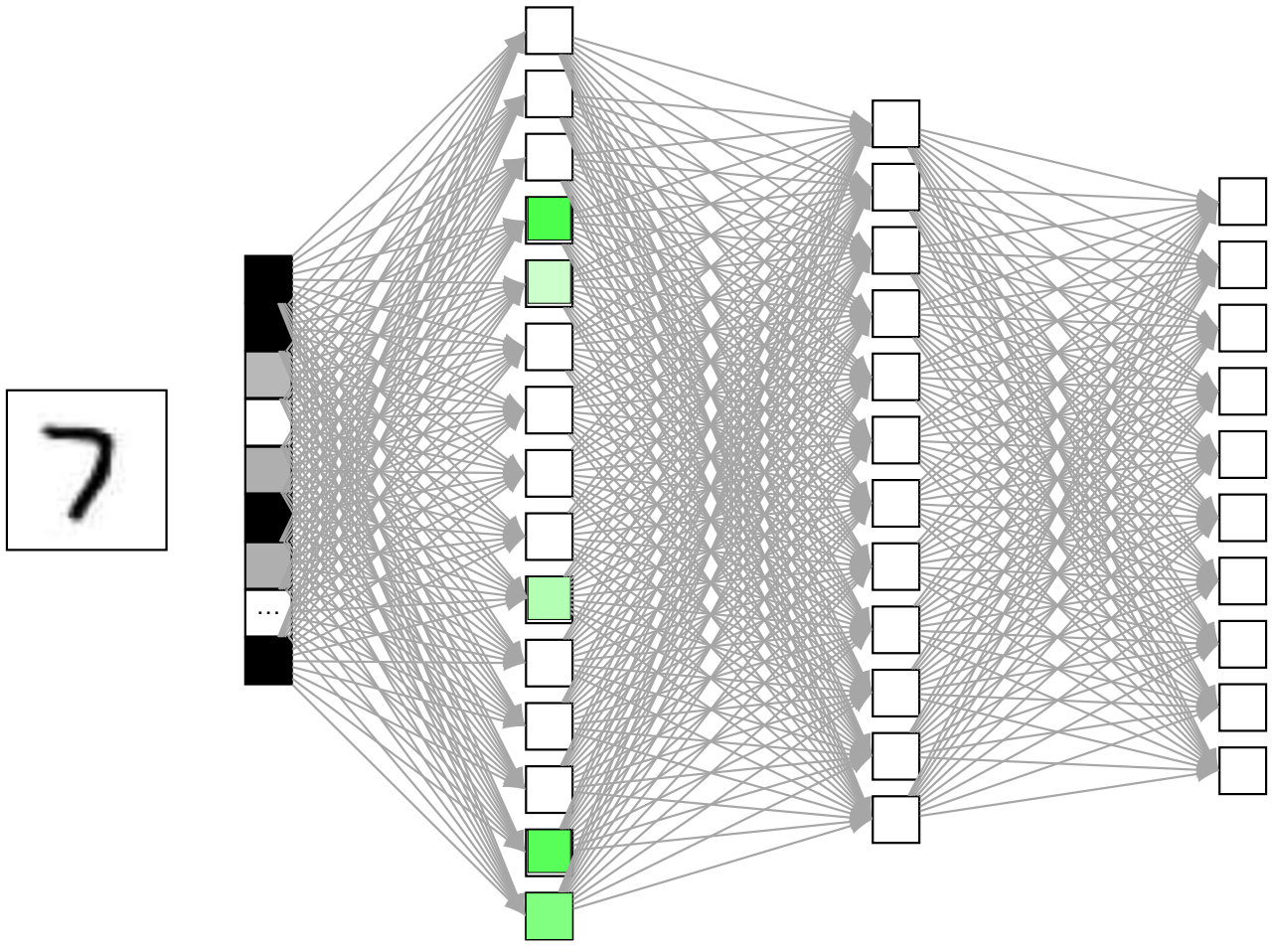
"Deep" NN with two hidden layers



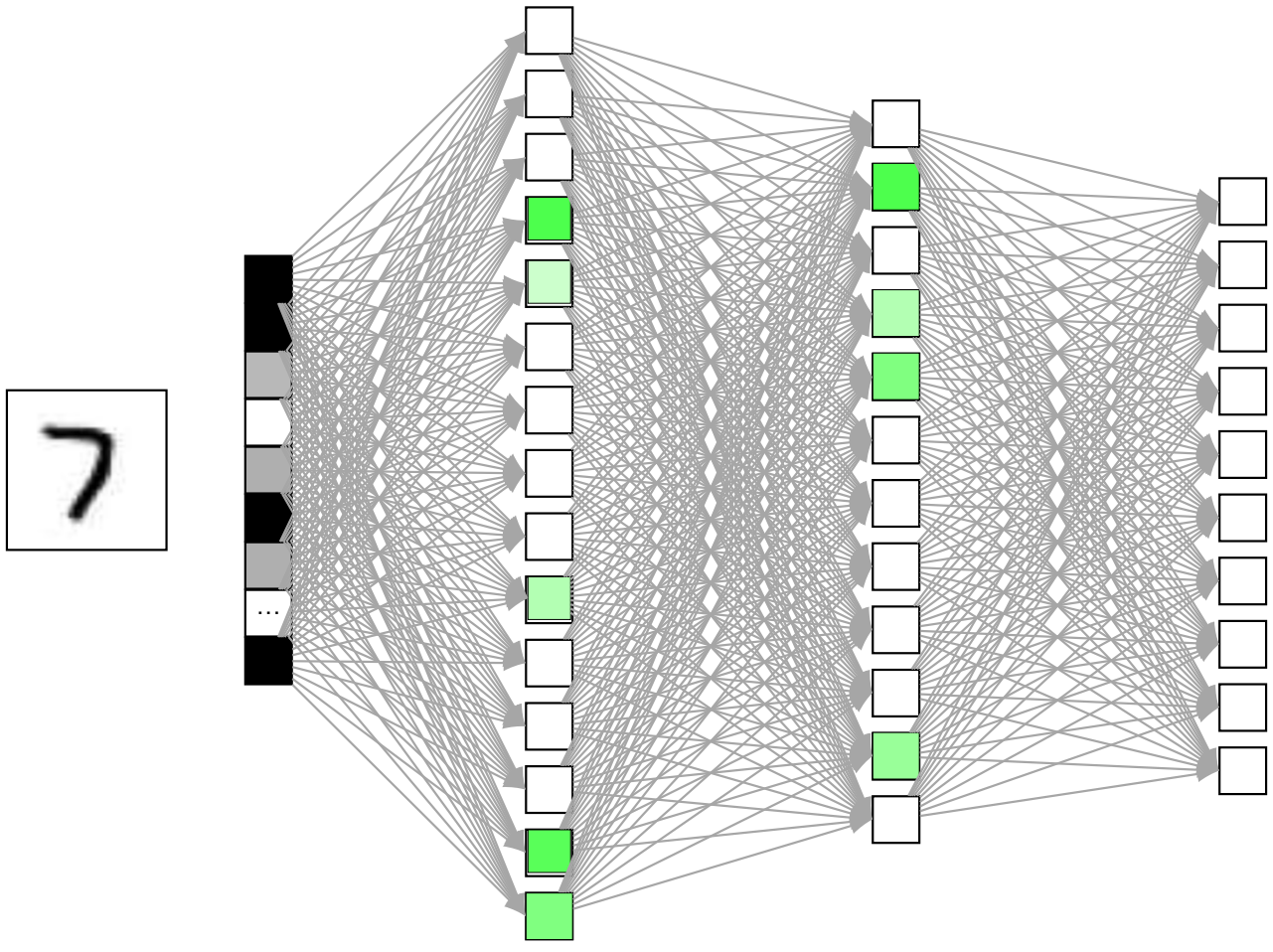
"Deep" NN with two hidden layers : Input



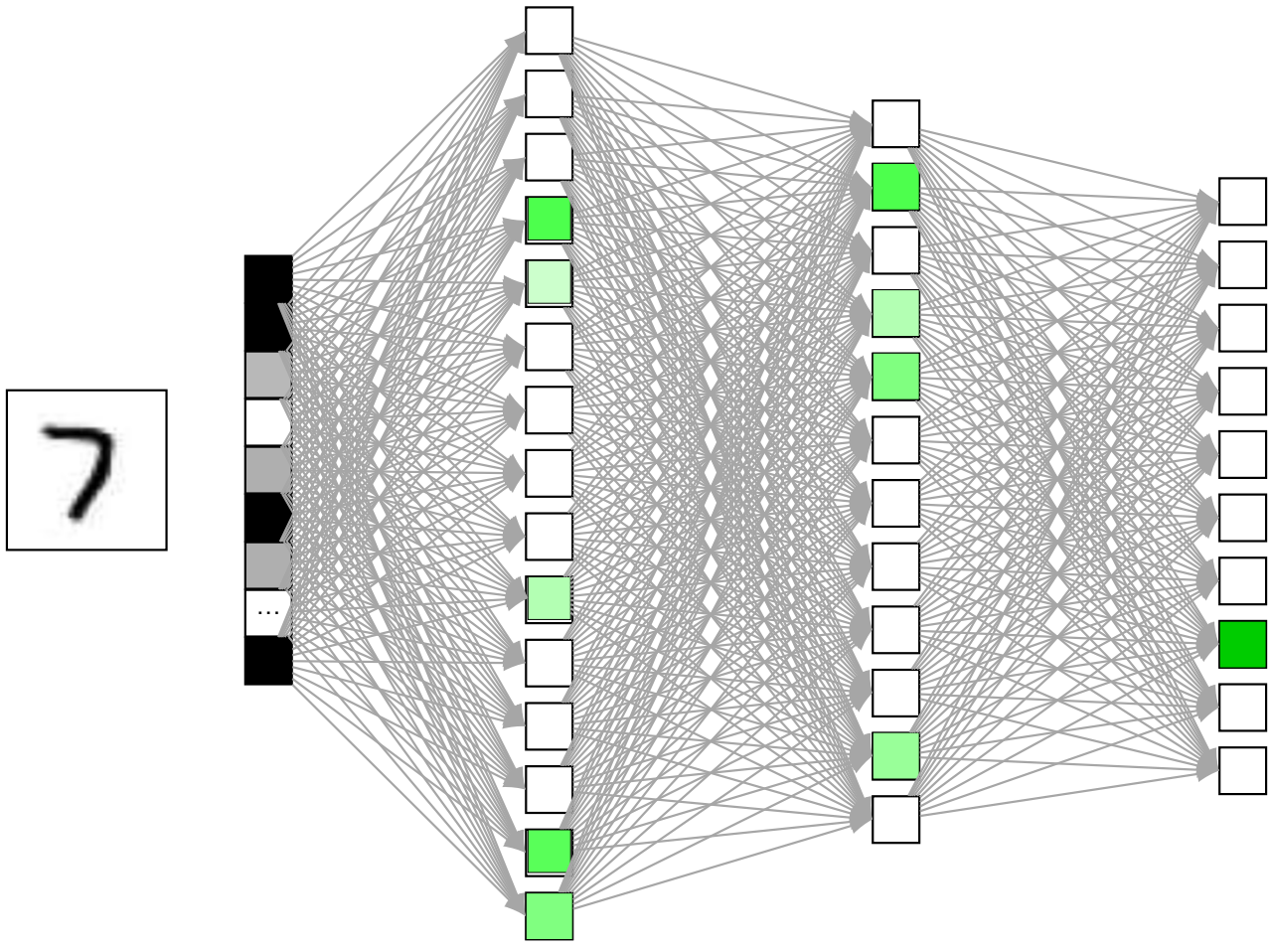
"Deep" NN with two hidden layers : Hidden layer 1



"Deep" NN with two hidden layers : Hidden layer 2



"Deep" NN with two hidden layers : output



Agenda

Image classification basics

Searching for human-like image classification methods

Neural networks: from shallow to deep
- Motivation and definitions
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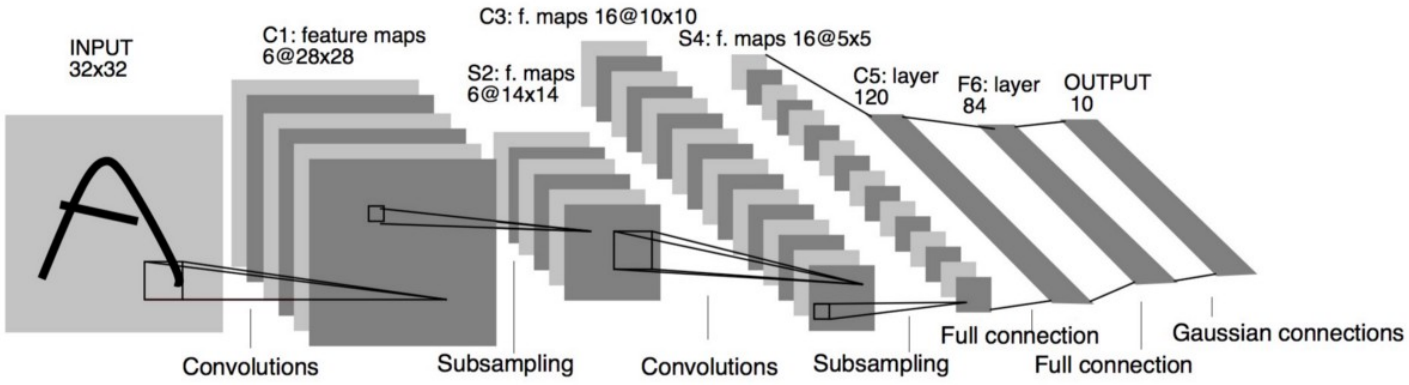
- Simple Neural Network

Convolutional Neural Networks
- Current Architectures
- Guidelines for training

Architecture LeNet



New terminology:

- Convolutional layer
- Pooling
- Feature (or Activation) maps
- Fully connected (or Dense) layer

Convolutional layer

Input $(N \times M \times L)$  e.g. $32 \times 32 \times 3$

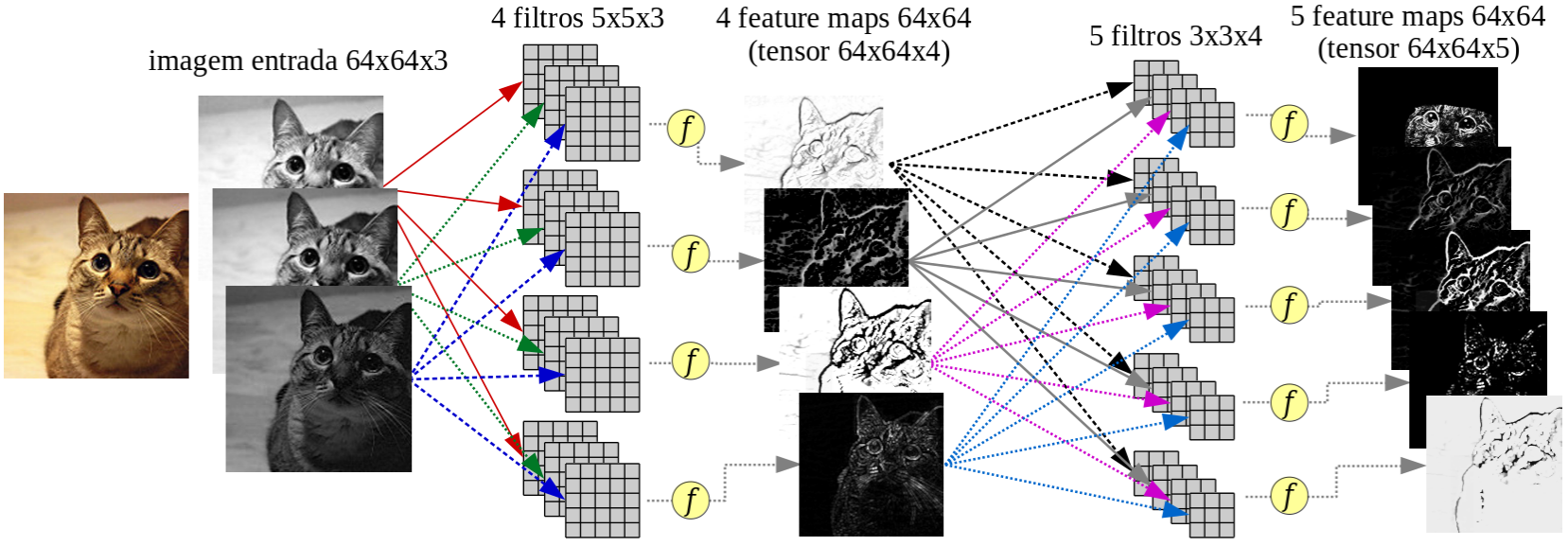
Filter (neuron) w with $P \times Q \times D$, e.g. $5 \times 5 \times 3$ (keeps depth)

- Each neuron/filter performs a convolution with the input image

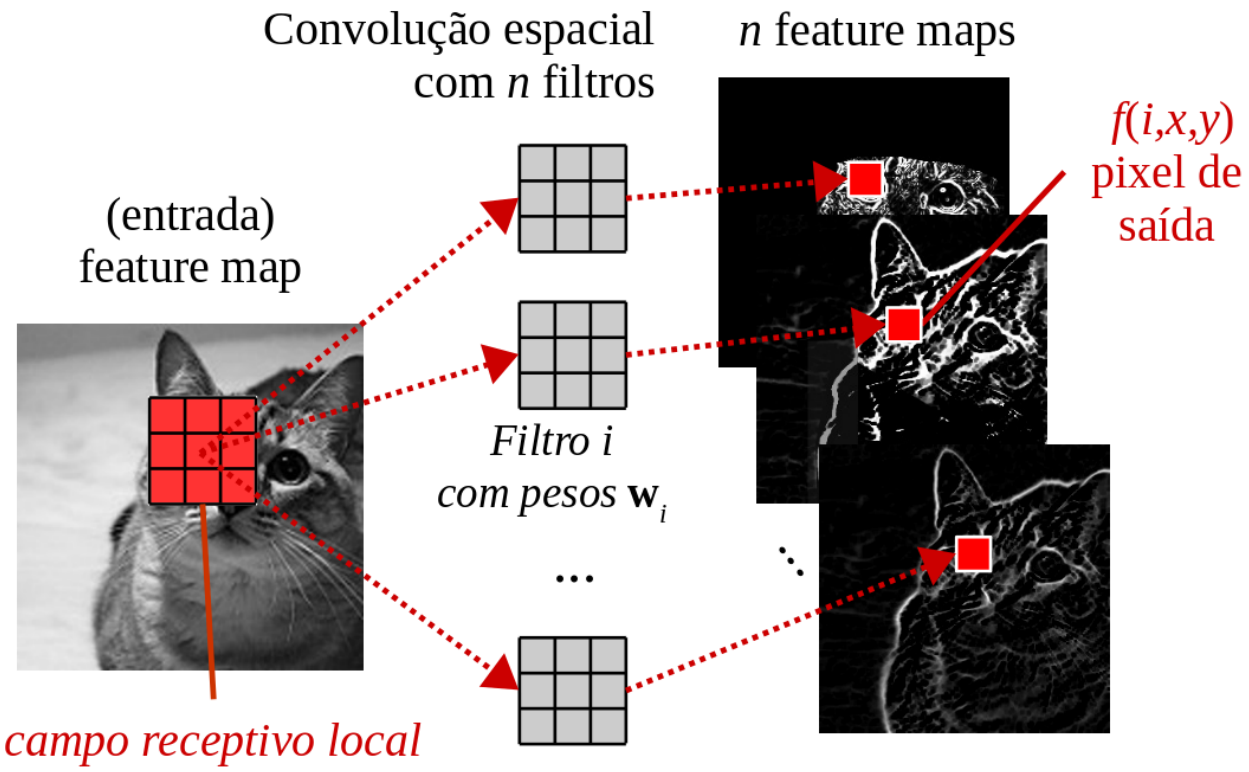
Centred at a specific pixel, we have, mathematically

$$w^T x + b$$

Convolutional layer: feature maps



Convolutional layer: local receptive field



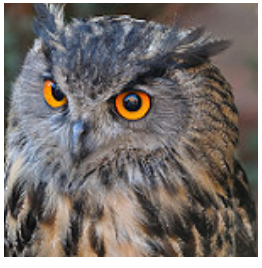
Convolutional layer: input x filter x stride

The convolutional layer must take into account

- input size
- filter size
- convolution stride

Convolutional layer

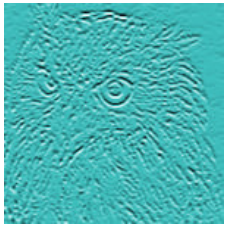
- Feature maps after convolution with filters followed by an activation function (e.g. ReLU) are stacked, forming a tensor.



$(32 \times 32 \times 3)$

convolution layer
10 filters of $5 \times 5 \times 3$

$\rightarrow$



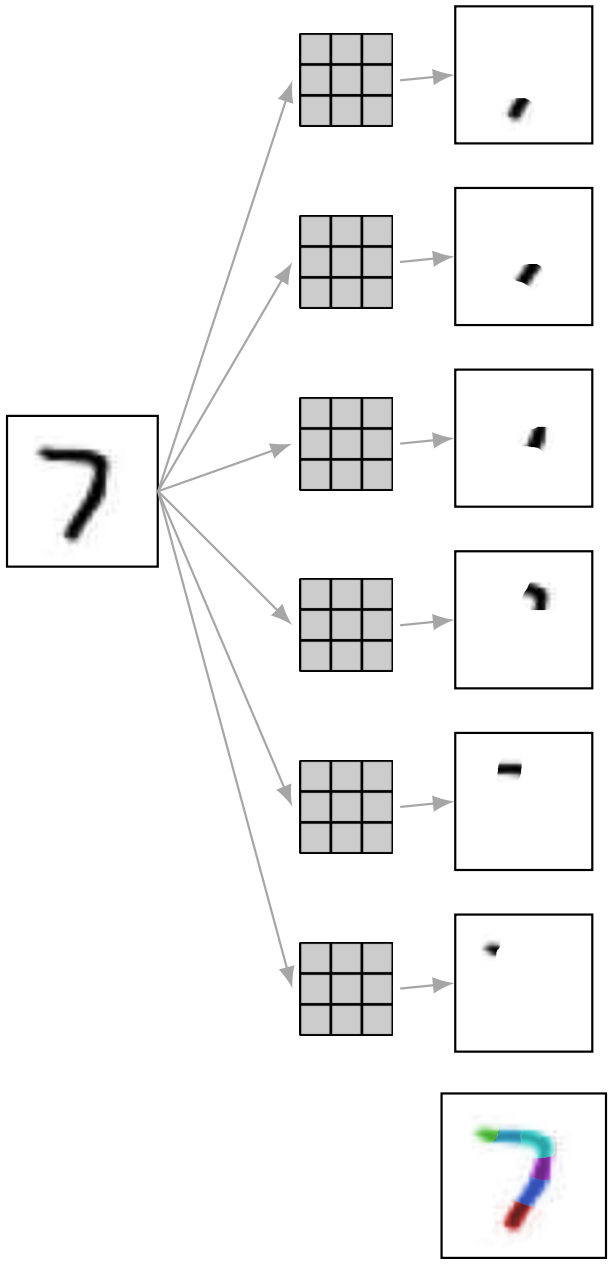
01

02

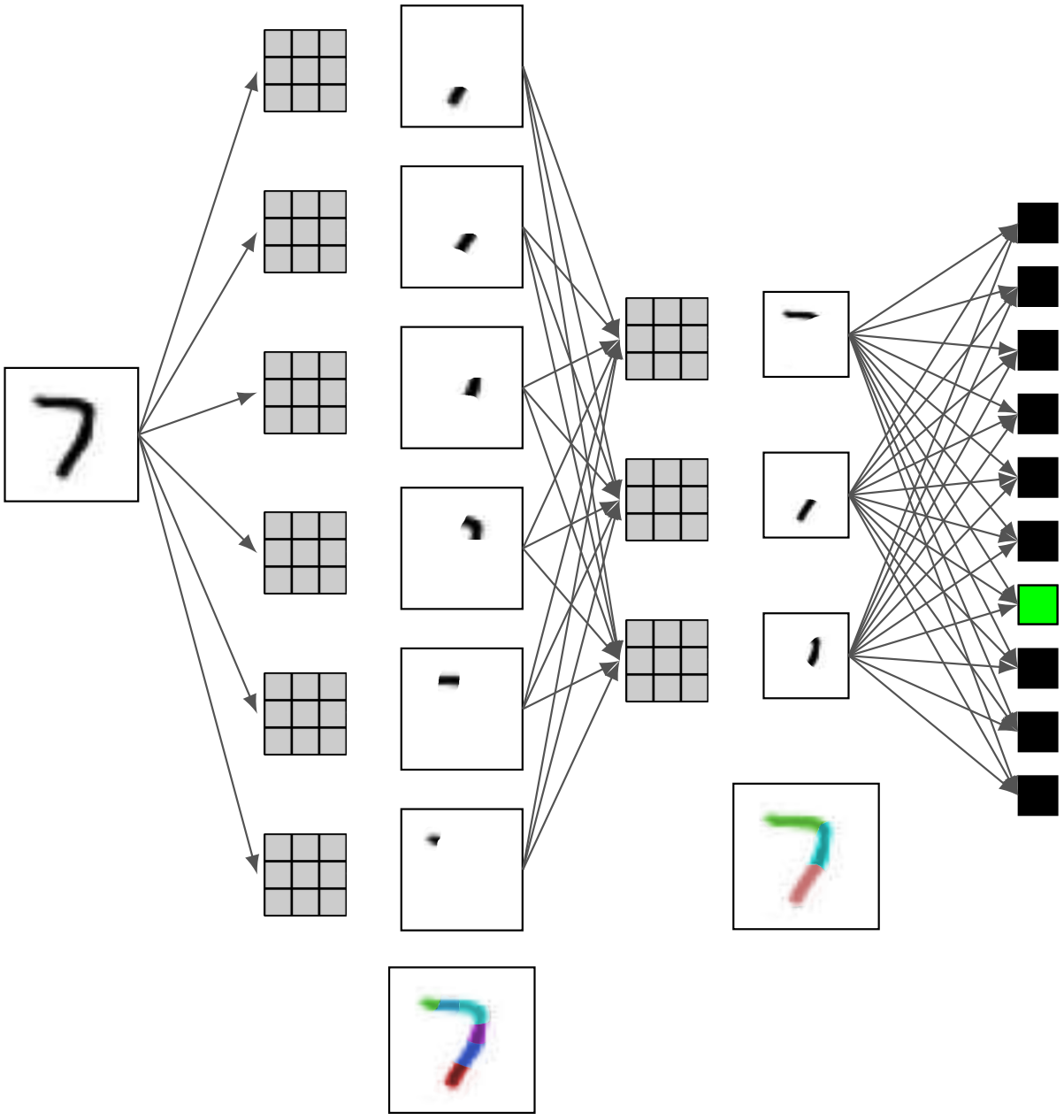
...

10

The MNIST example: now hidden layers are conv layers



The MNIST example: now hidden layers are conv layers



Convolutional layer: zero padding

In practice, zero padding is used to avoid losing borders. Example:

- input size: 10×10
- filter size: 5×5
- convolution stride: 1
- zero padding: 2
- output: 10×10

General rule: zero padding size to preserve image size: $(P-1)/2$

Example: $32 \times 32 \times 3$ input with $P = 5$, $s = 1$ and zero padding $z = 2$

Output size: $(N_I + (2 \cdot z) - P)/s + 1 = (32 + (2 \cdot 2) - 5)/1 + 1 = 32$

Convolutional layer: number of parameters

Parameters in a convolutional layer is $[(P \times P \times d) + 1] \times K$:

- filter weights: $P \times P \times d$, d *is given by input depth*
- number of filters(neurons): K *(each processes input in a different way)*
- $+1$ is the bias term

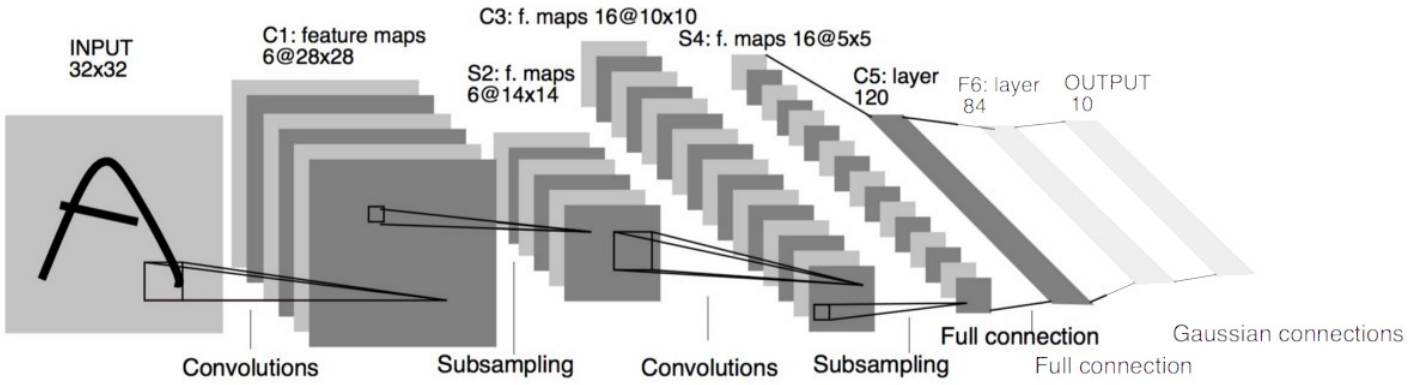
Example, with an image input $32 \times 32 \times 3$:

- Conv Layer 1: $P = 5$, $K = 8$
- Conv Layer 2: $P = 5$, $K = 16$
- Conv Layer 3: $P = 1$, $K = 32$
- # parameters Conv layer 1: $[(5 \times 5 \times 3) + 1] \times 8 = 608$
- # parameters Conv layer 2: $[(5 \times 5 \times 8) + 1] \times 16 = 3216$
- # parameters Conv layer 3: $[(1 \times 1 \times 16) + 1] \times 32 = 544$

Convolutional layer: pooling

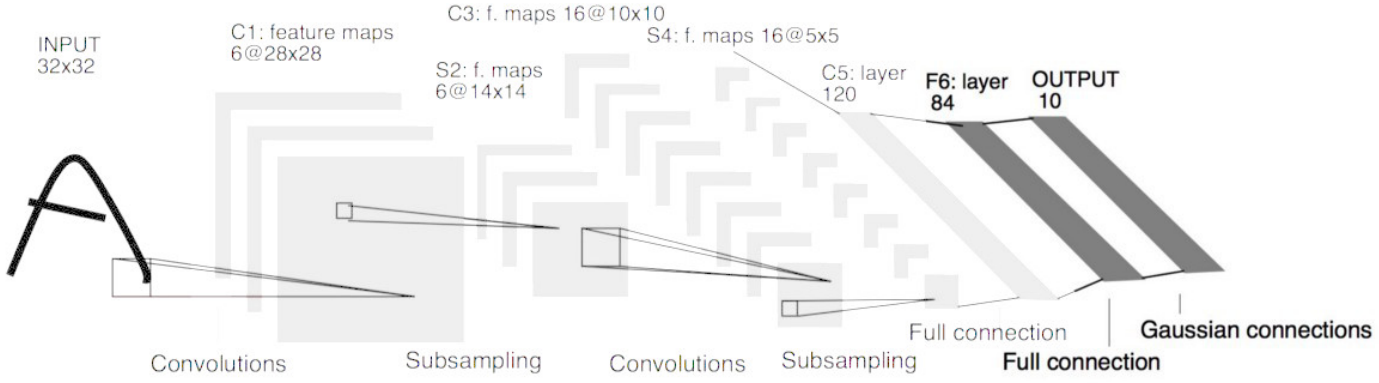
Operates over each feature map, to make the data smaller
Example: max pooling with downsampling factor 2 and stride 2.

Convolutional layer: convolution + activation + pooling



- Convolution: as seen before
- Activation: ReLU
- Pooling: maxpooling

Fully connected layer + Output layer



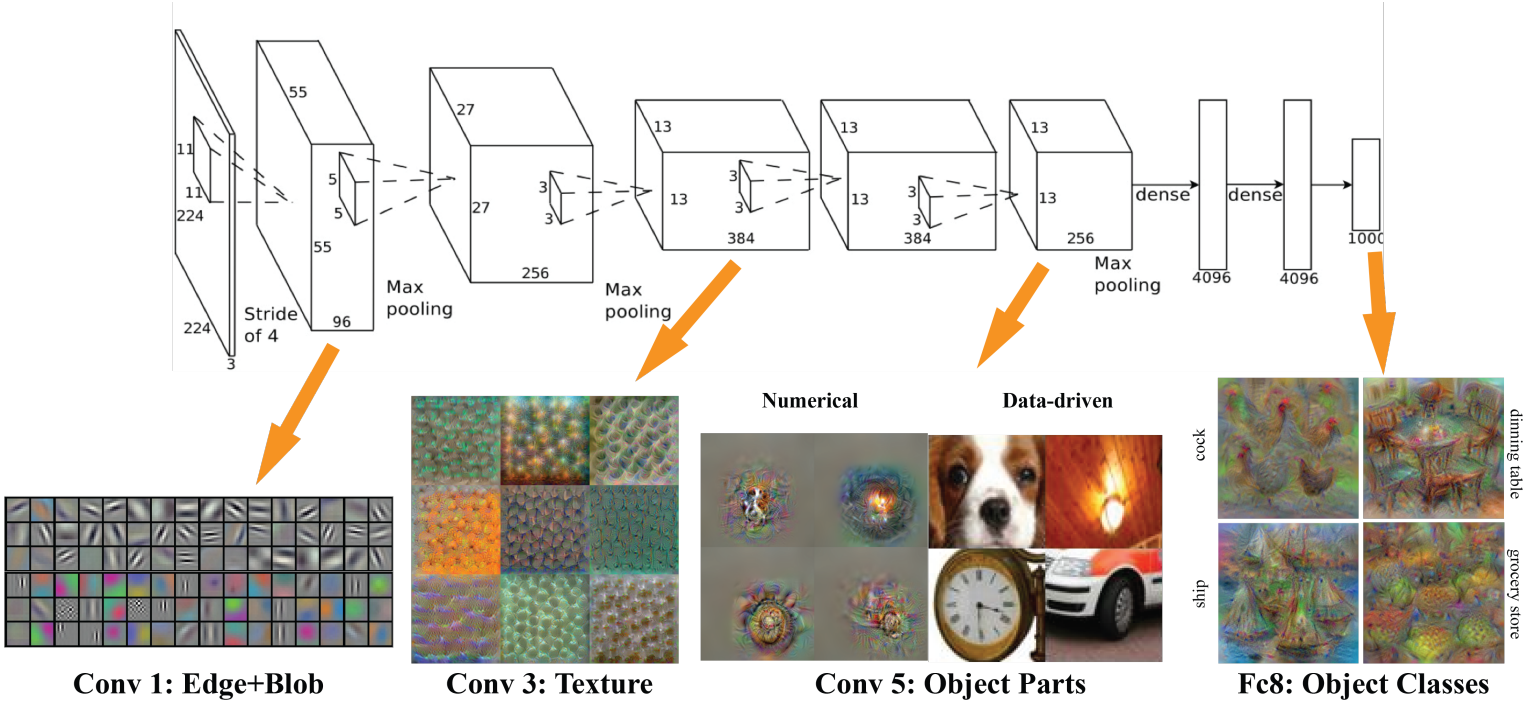
Fully connected (FC) layer:

- FC layers work as in a regular Multilayer Perceptron
- A given neuron operates over all values of previous layer

Output layer:

- each neuron represents a class of the problem

Visualization



Donglai et al. Understanding Intra-Class Knowledge Inside CNN, 2015, Tech Report

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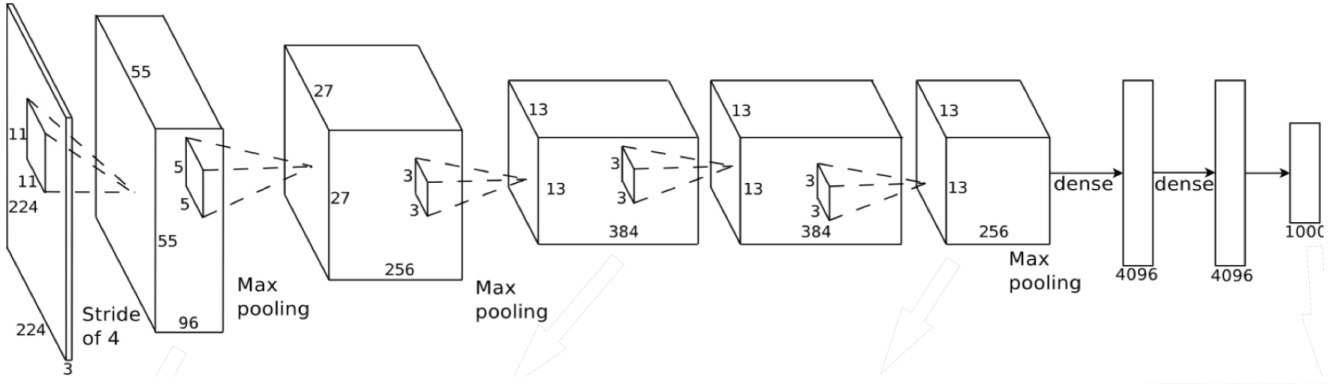
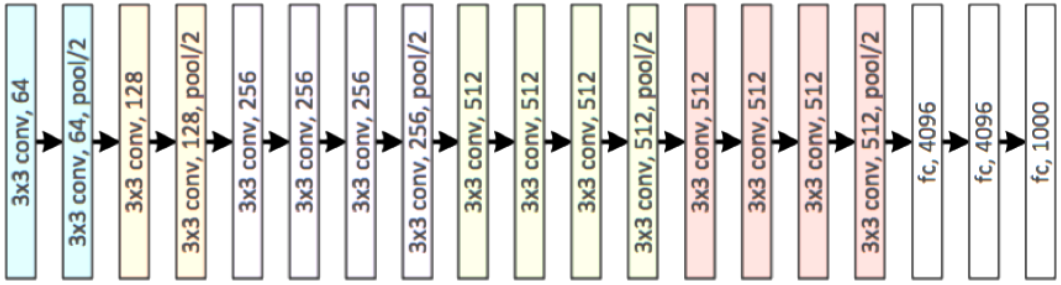
AlexNet (Krizhevsky, 2012)

- 60 million parameters.
- input 224×224
- conv1: $K = 96$ filters with $11 \times 11 \times 3$, stride 4,
- conv2: $K = 256$ filters with $5 \times 5 \times 48$,
- conv3: $K = 384$ filters with $3 \times 3 \times 256$,
- conv4: $K = 384$ filters with $3 \times 3 \times 192$,
- conv5: $K = 256$ filters with $3 \times 3 \times 192$,
- fc1, fc2: $K = 4096$.



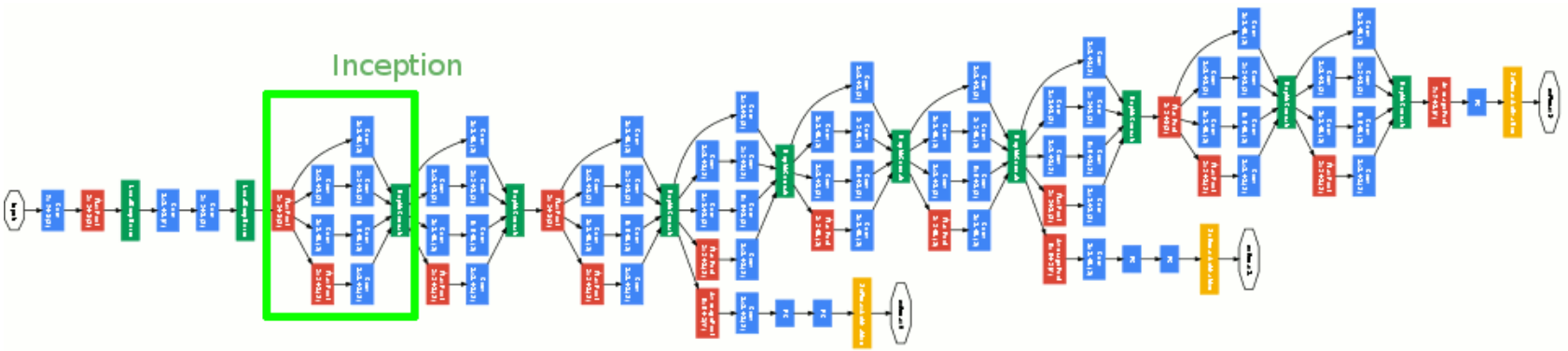
VGG 19 (Simonyan, 2014)

- +layers, −filter size = less parameters
- input 224×224,
- filters: all 3×3,
- conv 1-2: $K = 64$ + maxpool
- conv 3-4: $K = 128$ + maxpool
- conv 5-6-7-8: $K = 256$ + maxpool
- conv 9-10-11-12: $K = 512$ + maxpool
- conv 13-14-15-16: $K = 512$ + maxpool
- fc1, fc2: $K = 4096$

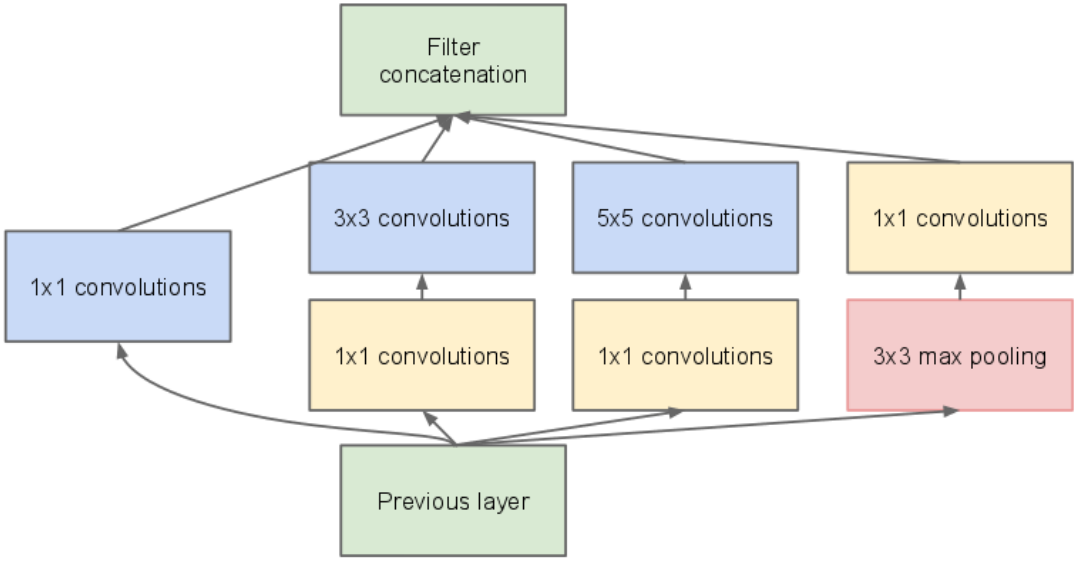


GoogLeNet (Szegedy, 2014)

- 22 layers
- Starts with two convolutional layers
- *Inception layer* ("filter bank"):
  - filters 1×1, 3×3, 5×5 + max pooling 3×3;
  - reduce dimensionality using 1×1 filters.
  - 3 classifiers in different parts
- Blue = convolution,
- Red = pooling,
- Yellow = Softmax loss fully connected layers
- Green = normalization or concatenation



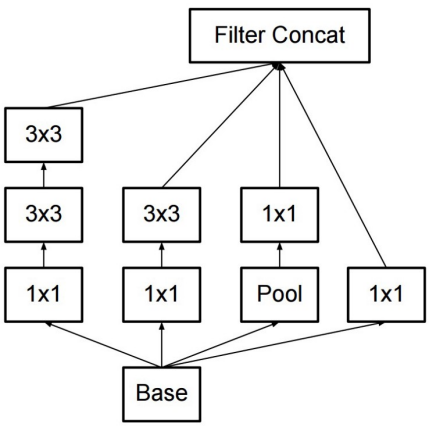
GoogLeNet: inception module



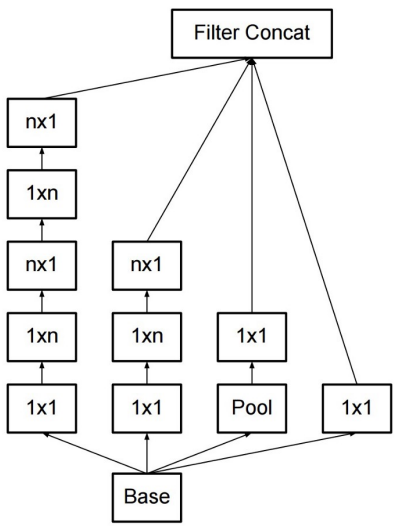
- 1×1 convolution reduces the depth of previous layers by half
- this is needed to reduce complexity (e.g. from 256 to 128 d)
- concatenates 3 filters plus an extra max pooling filter (because).

Inception modules (V2 and V3)

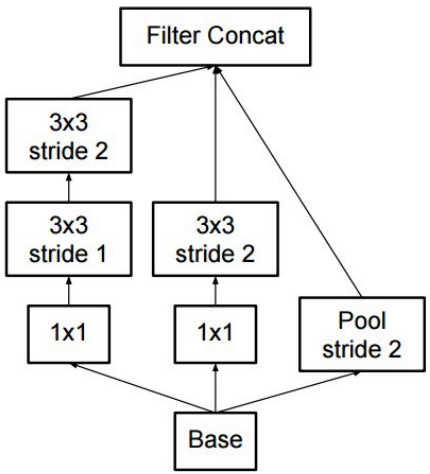
multiple 3×3 convs.



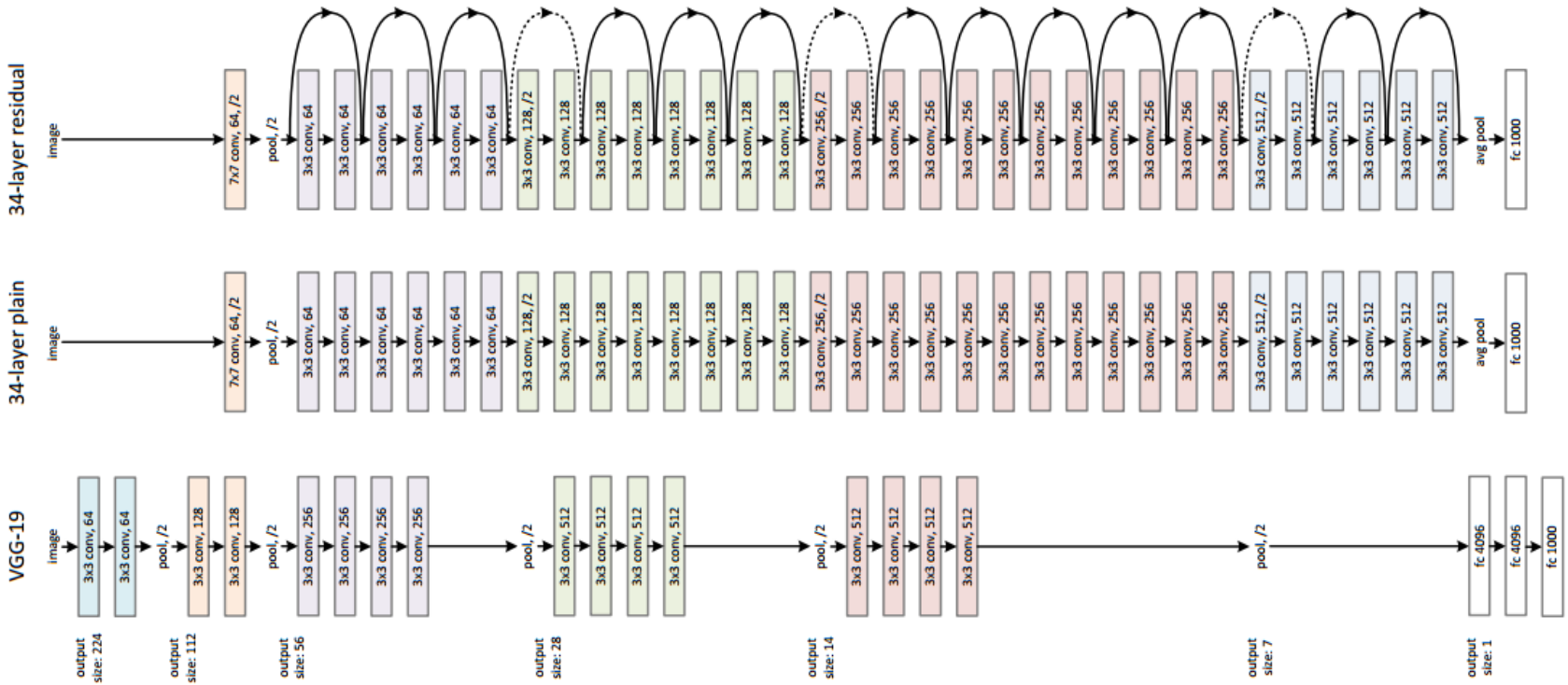
flattened conv.



decrease size

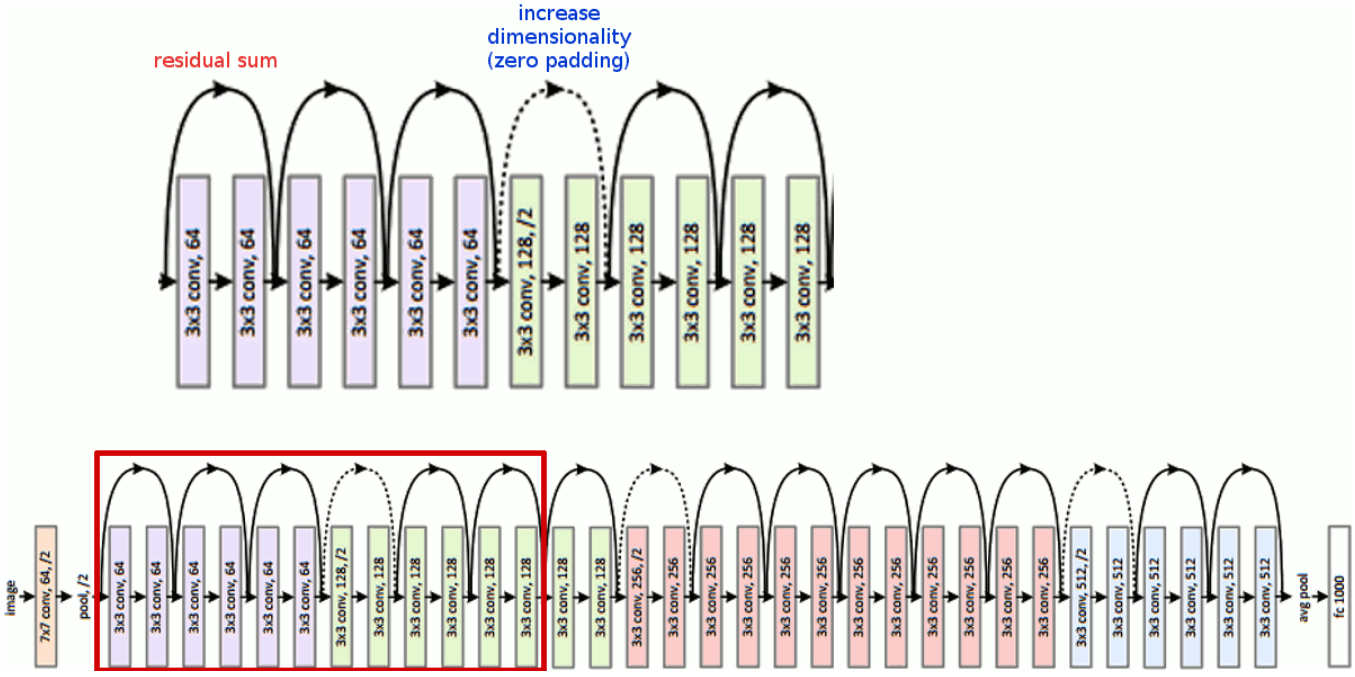


VGG19 vs "VGG34" vs ResNet34

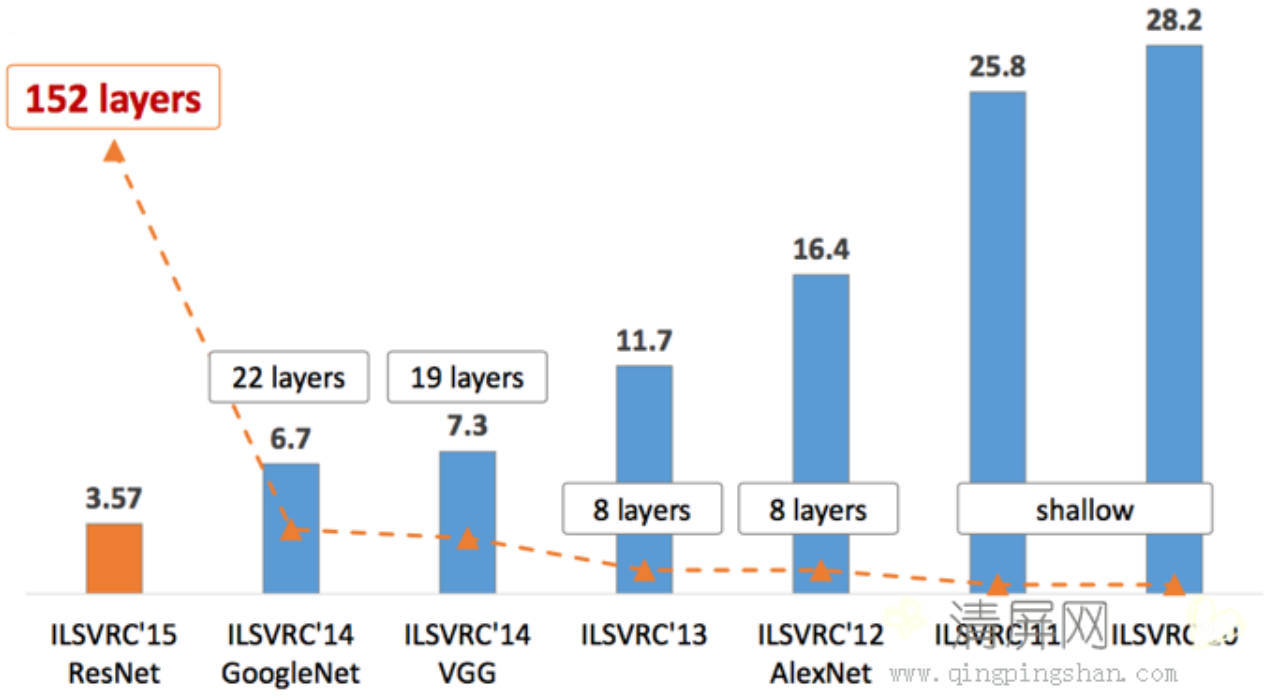


Residual Network — ResNet (He et al, 2015)

Reduces number of filters, increases number of layers (34-1000).
Residual architecture: add identity before activation of next layer.



Comparison



Thanks to Qingping Shan `www.qingpingshan.com`

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How to Train

Batch Stochastic Gradient Descent

- **Mini-batch size**: default is 16 or 32, but more might be used to speed-up.
- **Learning rate**: adjust learning rate with decay.
- **Optimizers**: try RMSProp, which employ the concept of momentum, or others (Adam, Adadelta, ...).

Convergence and training set

- **Clean data**: cleaniness of the data is very important,
- **Data augmentation**: generate new examples by perturbation of existing ones (e.g. noise, affine),
- **Loss, validation and training error**: plot values for each epoch.

Regularization: on loss functions

$$\ell(W) = \frac{1}{N}\sum_{i=1}^{N} \ell_i(x_i, y+i, W) + \underbrace{\lambda R(W)}_{\text{regularization}}$$

$$\nabla_W \ell(W) = \frac{1}{N}\sum_{i=1}^{N} \nabla_W \ell_i(x_i, y+i, W) + \lambda \nabla_W R(W)$$

Regularization will help the model to keep it simple. Possible methods

- $L2: R(W) = \sum_i \sum_j W_{i,j}^2$
- $L1: R(W) = \sum_i \sum_j |W_{i,j}|$

Alternative methods that help convergence and prevent overfitting

- **Dropout**: randomly turn off a percentage of the neurons during training.
  - That means the activation function of that neuron sets the output to zero.
  - It is a way to "bootstrap" the training.
- **Batch normalization**: z-score normalization over all data
  - subtract the mean, divide by the standard deviation of all batch examples,
  - performed before/after layer processing.
  - for deep nets, it is employed before every block (e.g. residual block, inception block, etc.),

Guidelines for new data

Classification (finetuning)

- Data similar to ImageNet: freeze all Conv Layers, train output (or other) dense layers from scratch

- Data not similar to ImageNet: freeze lower Conv Layers, train output (or other) layers from scratch

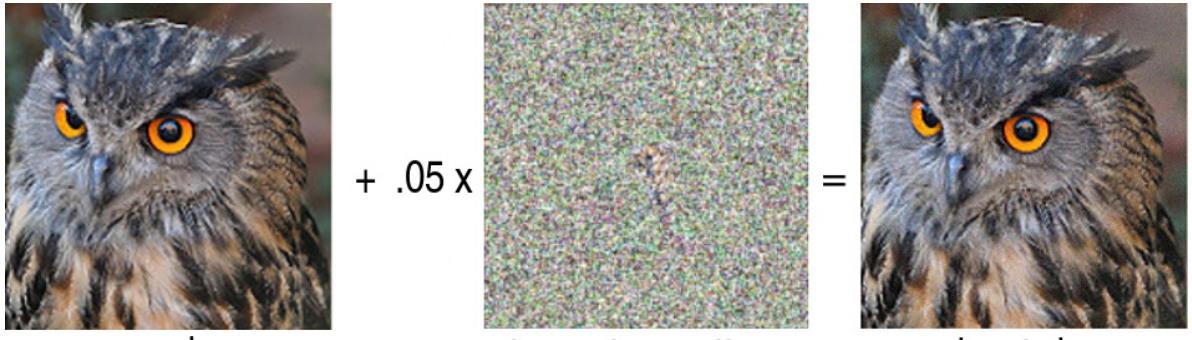
Guidelines for new data

Feature extraction for image classification and retrieval

- Perform forward, get activation values of higher Conv and/or dense layers
- Apply some dimensionality reduction: e.g. PCA, Product Quantization, etc. after extraction
- Use external classifier: e.g. SVM, Random Forest, etc.

Limitations

CNNs are easily fooled



owl
(73% confidence)

cheetah gradient
features

cheetah
(99% confidence)

Concluding remarks

- Deep Learning is not a panacea;
- There are important concerns about generalization of Deep Networks;
- However those methods can be really useful for finding representations;
- Many challenges and research frontiers for more complex tasks.

Bibliography

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