Lecture 09:

Convolutional Neural Networks (CNN) – Part I

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Machine Learning Algorithms

MSSE 277B, 3 Units

Course Map

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classic ML tools & algorithms

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Lecture 3: Dimensionality Reduction: Principal Component Analysis

Lecture 4: Linear and Non-linear Regression and Classification

Lecture 5: Unsupervised Learning: K-Means, GMM, Trees

Lecture 6: Adaptive Learning and Gradient Descent Optimization Algorithms

ANNs/AI/Deep Learning

Lecture 7: Introduction to Artificial Neural Networks - The Perceptron

Lecture 8: Introduction to Artificial Neural Networks - Building Multiple Dense Layers

Lecture 9: Convolutional Neural Networks (CNNs) - Part I

Lecture 10: CNNs - Part II

Lecture 11: Recurrent Neural Networks (RNNs) and Long Short-Term Memory (LSTMs)

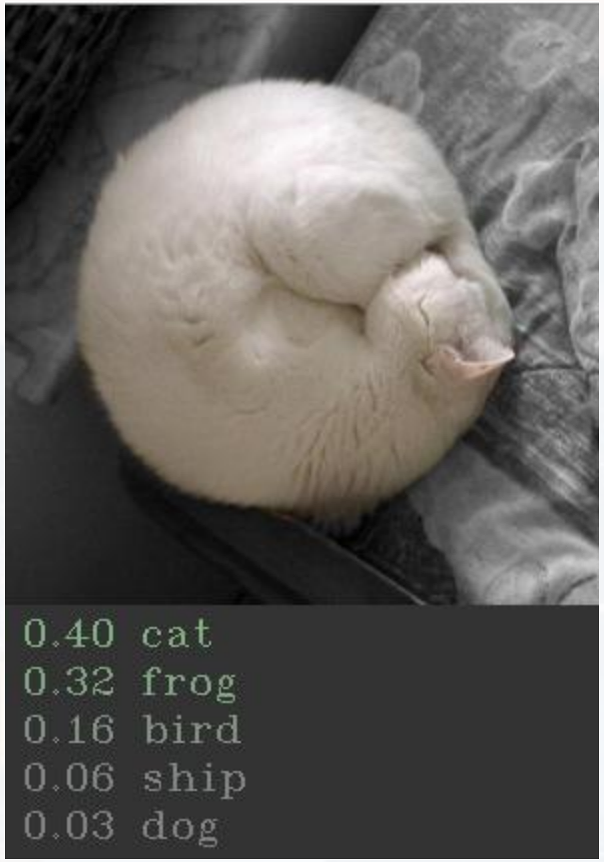
Lecture 12: Combining LSTMs and CNNs

Lecture 13: Running Models on GPUs and Parallel Processing

Lecture 14: Project Presentations

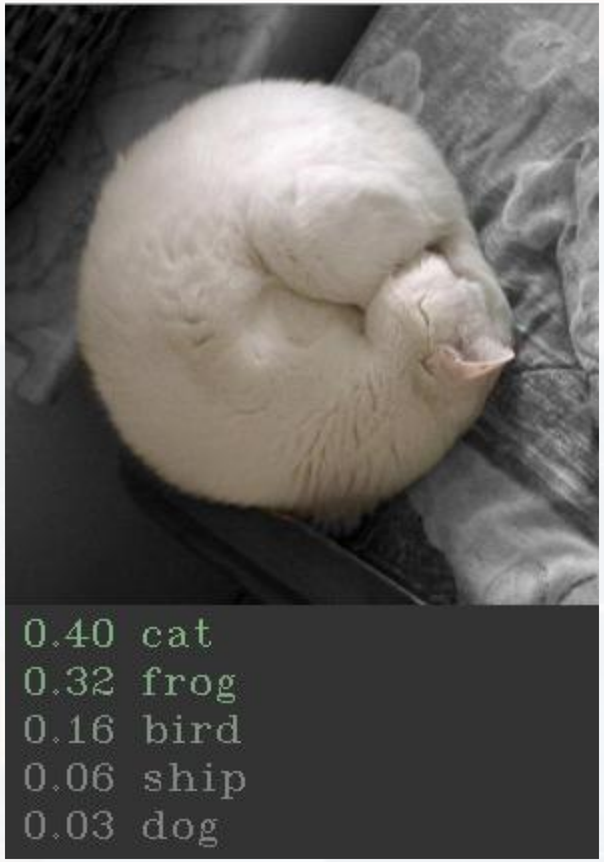
Lecture 15: Transformer

Lecture 16: GNN



Outline

- The Problem
- What is Convolution
- The CNN Architectures
- Data Preparation & Training
- A Simple Example



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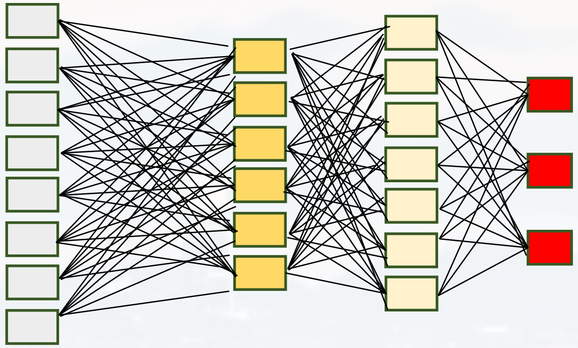
Convolutional Neural Networks: The Problem

so far:

data features →

data points ↓

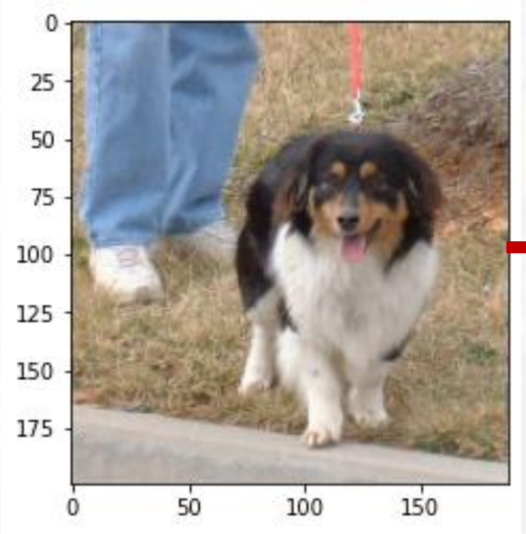
```
[[5.1 3.5 1.4 0.2]
 [4.9 3.  1.4 0.2]
 [4.7 3.2 1.3 0.2]
 [4.6 3.1 1.5 0.2]
 [5.  3.6 1.4 0.2]
 [5.4 3.9 1.7 0.4]
 [4.6 3.4 1.4 0.3]
 [5.  3.4 1.5 0.2]
```



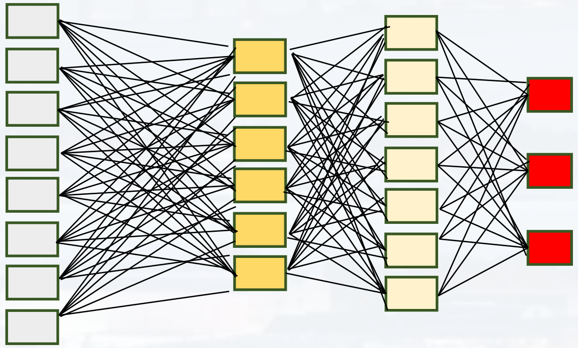
data points are **not related**, no spatial information

row = data point

now:



?



data points are **related**, **lots** of spatial information

Convolutional Neural Networks: The Problem

so far:

data features

data points

```
[[5.1 3.5 1.4 0.2]
 [4.9 3.  1.4 0.2]
 [4.7 3.2 1.3 0.2]
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```
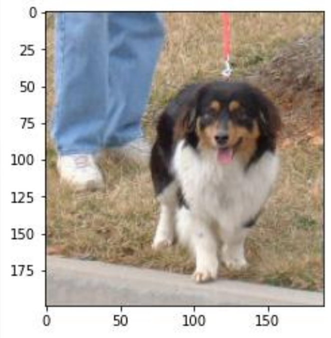
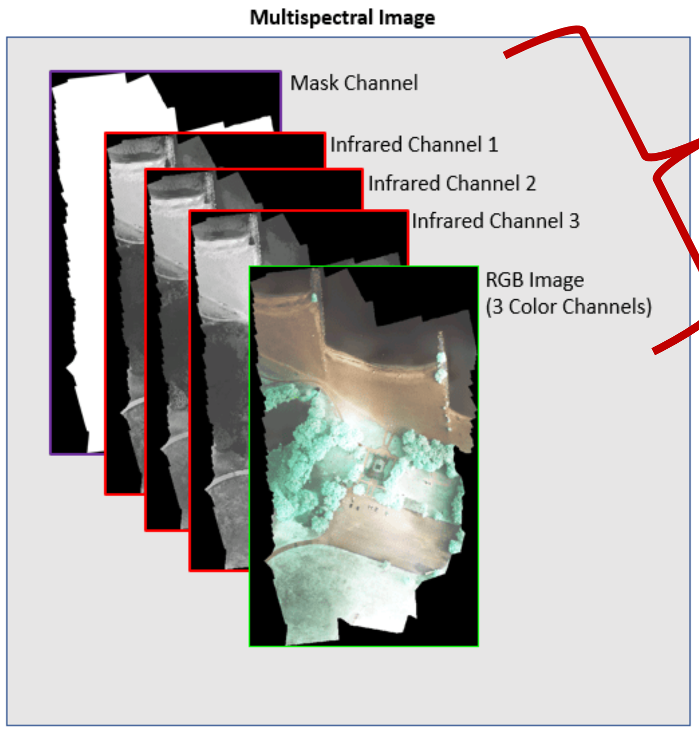

row = data point

now:



matrix = data point



matrices can have n color channels

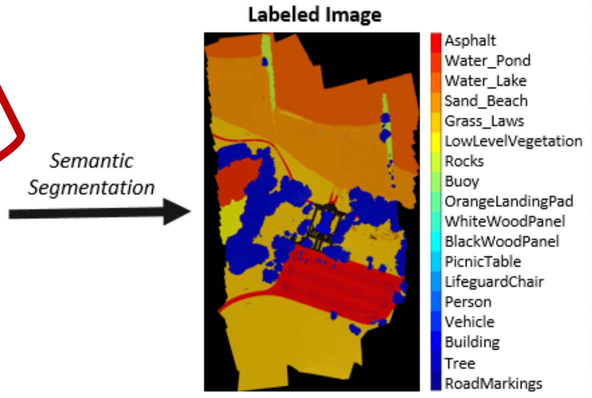
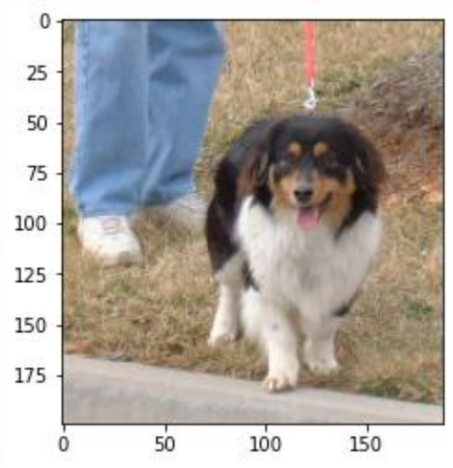


image curtesy: Mathworks

Convolutional Neural Networks: The Problem

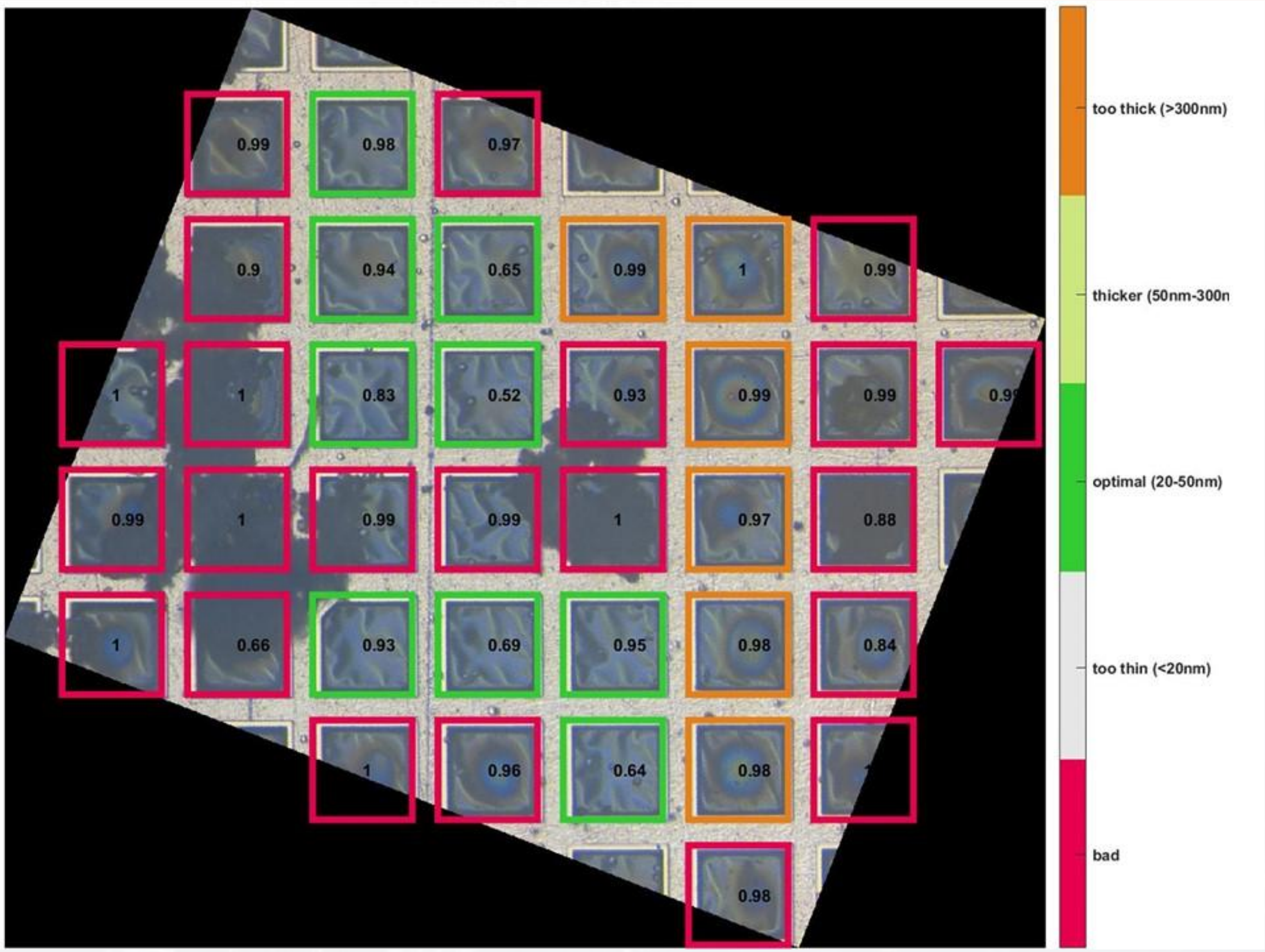
classification: between different images



different pixel within images aka **segmentation**

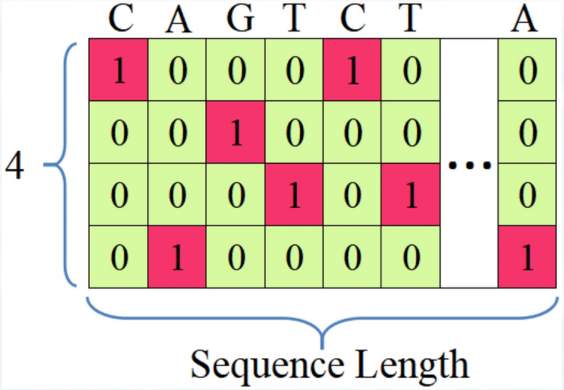
Convolutional Neural Networks:

segmentation *for* classification

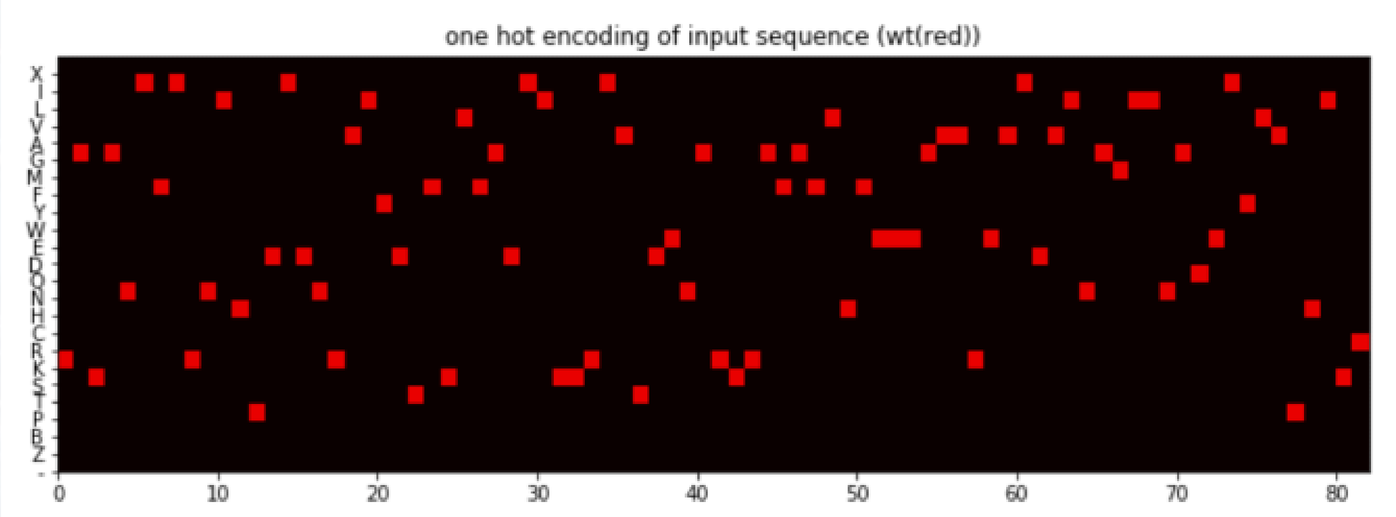


Convolutional Neural Networks:

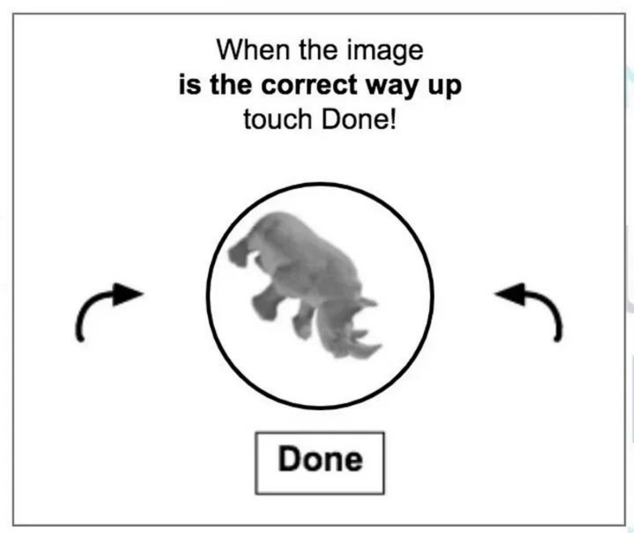
motif finding / sequence analysis



one – hot encoded NT or AA sequences can be interpreted as b/w images!

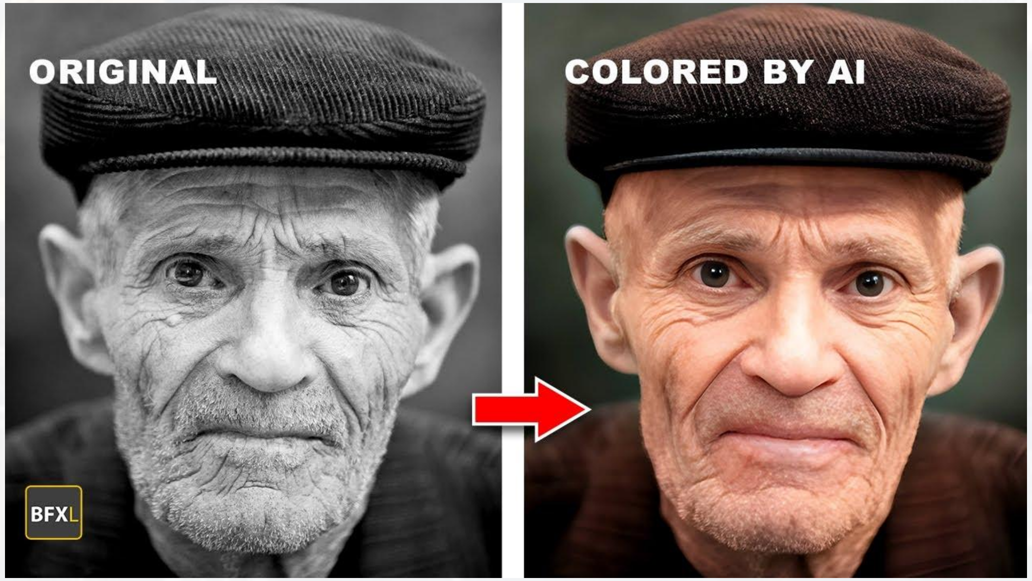


regression:

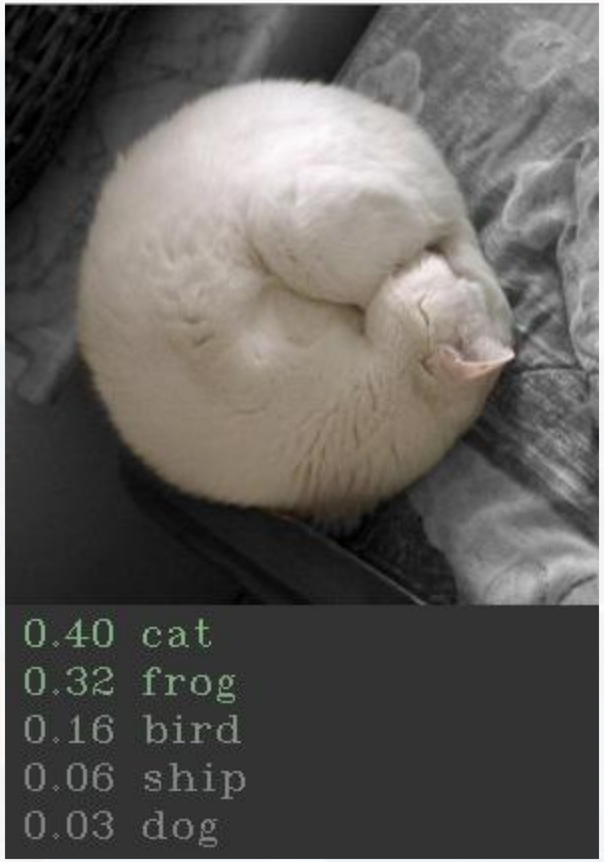


turning images the right way

part of GenAI:



source: TopviewAI



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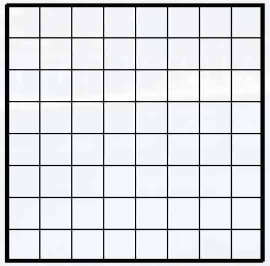
<u>goal:</u> - maintaining the spatial information → convolution
- learning which features are important → training the convolution filter

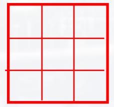
<u>What is convolution?</u>

$$(f * g)(x) := \int_{\mathbb{R}^n} f(\zeta)\boldsymbol{g}(\boldsymbol{x}-\boldsymbol{\zeta})d\zeta$$

image ***f*** and filter ***g***



image

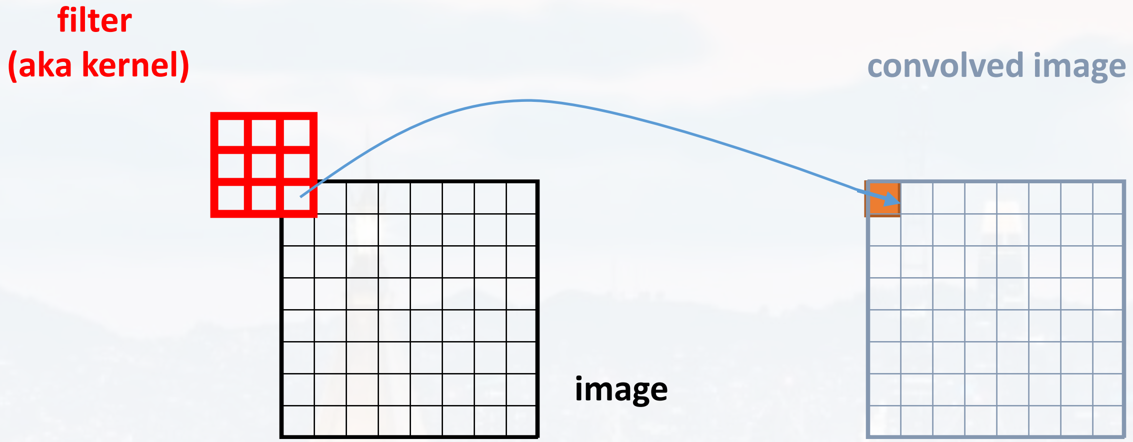


filter
(aka kernel)

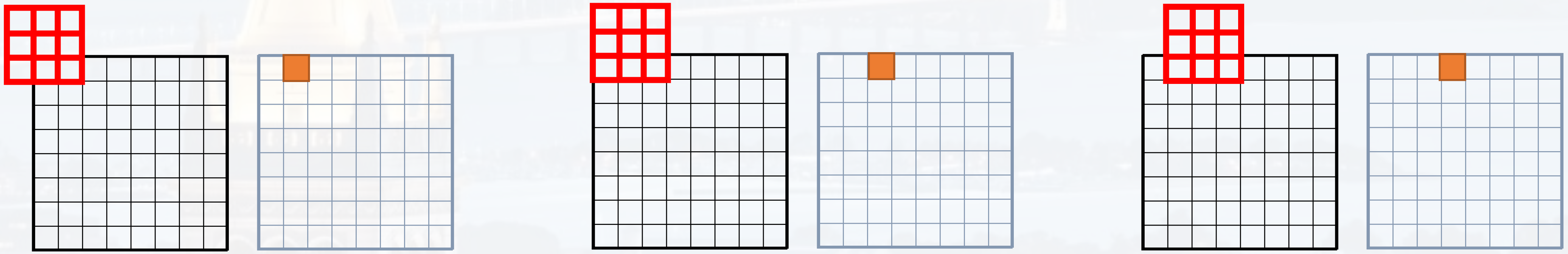
Convolutional Neural Networks: Convolution

What is convolution?

image ***f*** and filter ***g***



1) multiplying matrix values pixelwise
2) summing up products
3) → value for new matrix

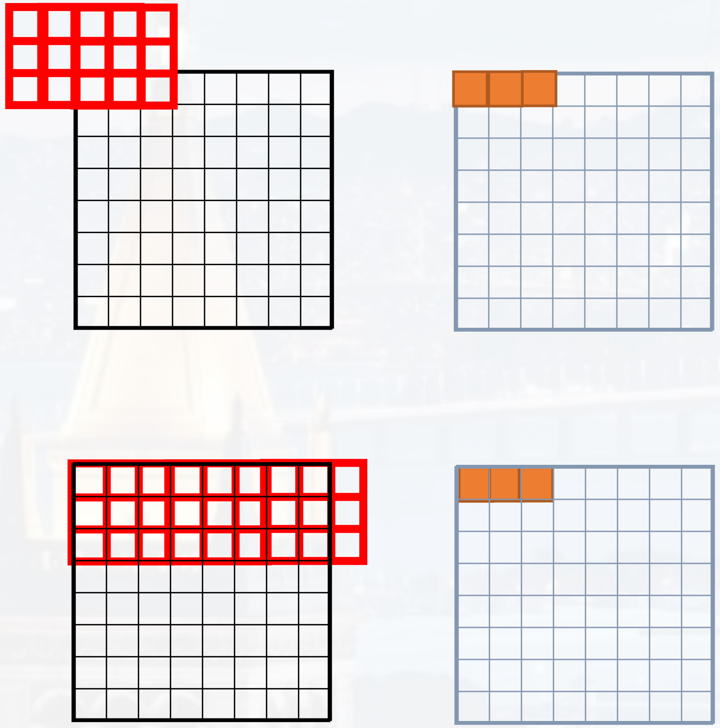


What is convolution?

image ***f*** and filter ***g***

different techniques:

1) multiplying matrix values pixelwise
2) summing up products
3) → value for new matrix



padding = 2; stride length = 1

padding = 0; stride length = 3

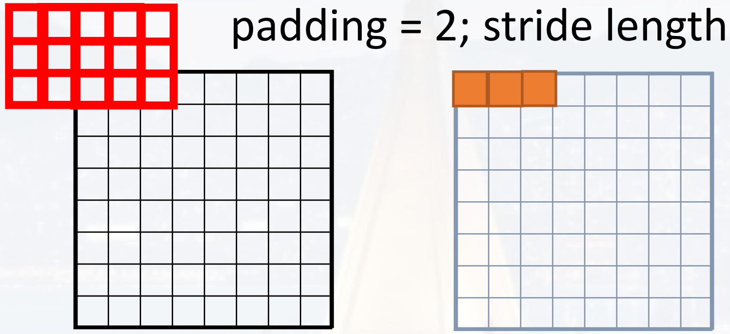
What is convolution?

image ***f*** and filter ***g***

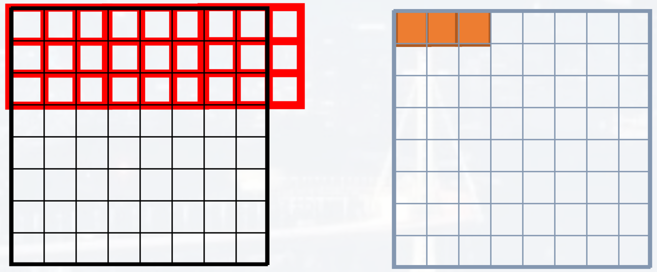
different techniques:

1) multiplying matrix values pixelwise
2) summing up products
3) → value for new matrix

padding = 2; stride length = 1



padding = 0; stride length = 3



the resulting image has the following size (N is the number of rows/columns):

$$N_{out} = \frac{(N_{in} - N_{filt} + 2 * padding)}{stride\ length} + 1$$

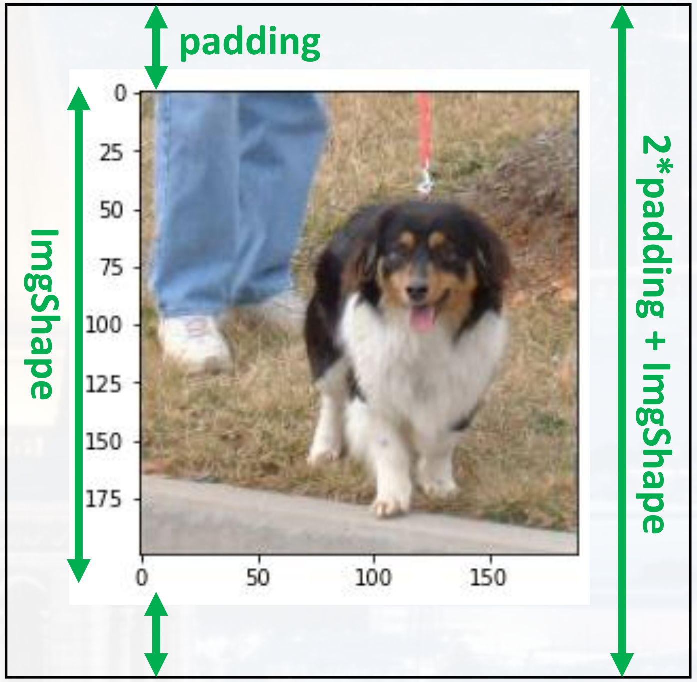
Convolutional Neural Networks:

What is convolution?

image ***f*** and filter ***g***

the resulting image has the following size (N is the number of rows/columns):

$$N_{out} = \frac{(N_{in} - N_{filt} + 2 * padding)}{stride\ length} + 1$$

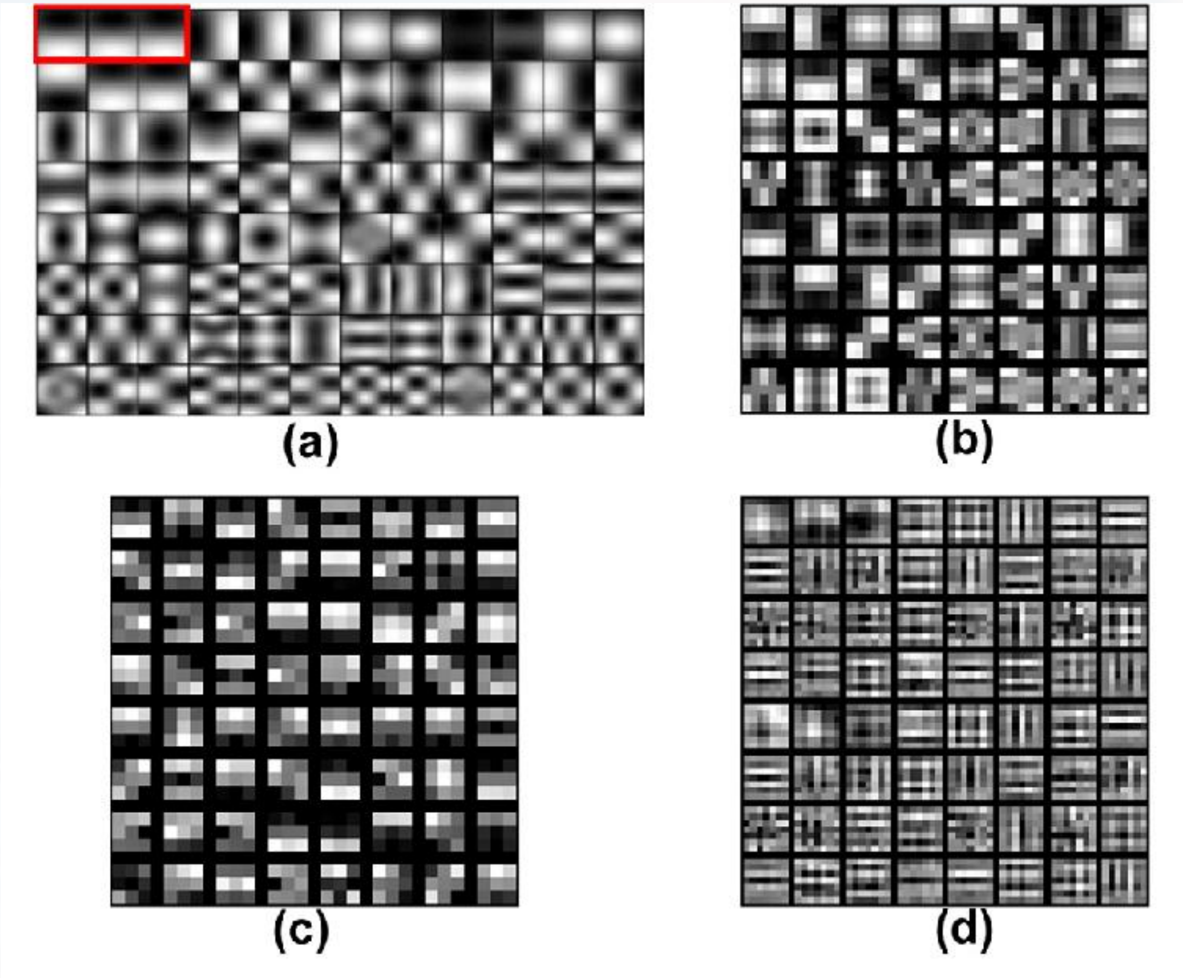


Convolutional Neural Networks: Convolution

What is convolution?

image ***f*** and filter ***g***

filters:



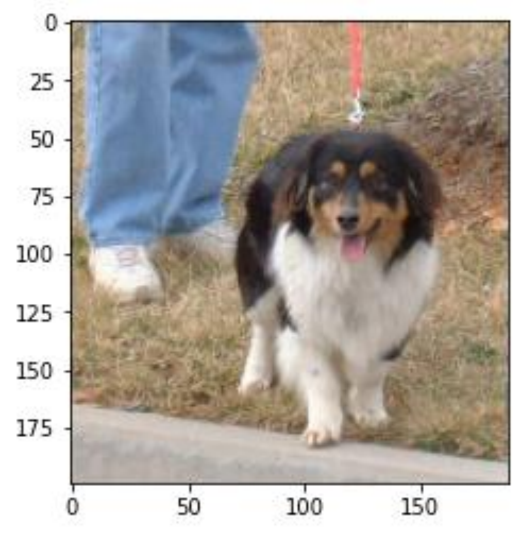
1) multiplying matrix values pixelwise
2) summing up products
3) → value for new matrix

DOI:10.1016/j.actbio.2017.09.025

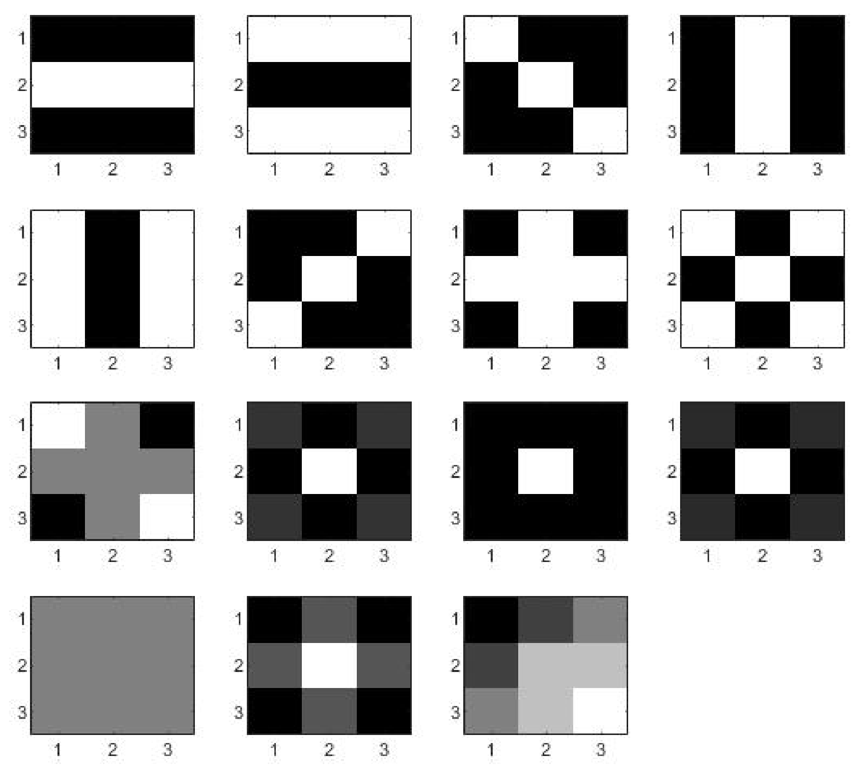
Convolutional Neural Networks: Convolution

see `Convolution.ipynb` for visualizing the impact of different convolution filter on the image

image

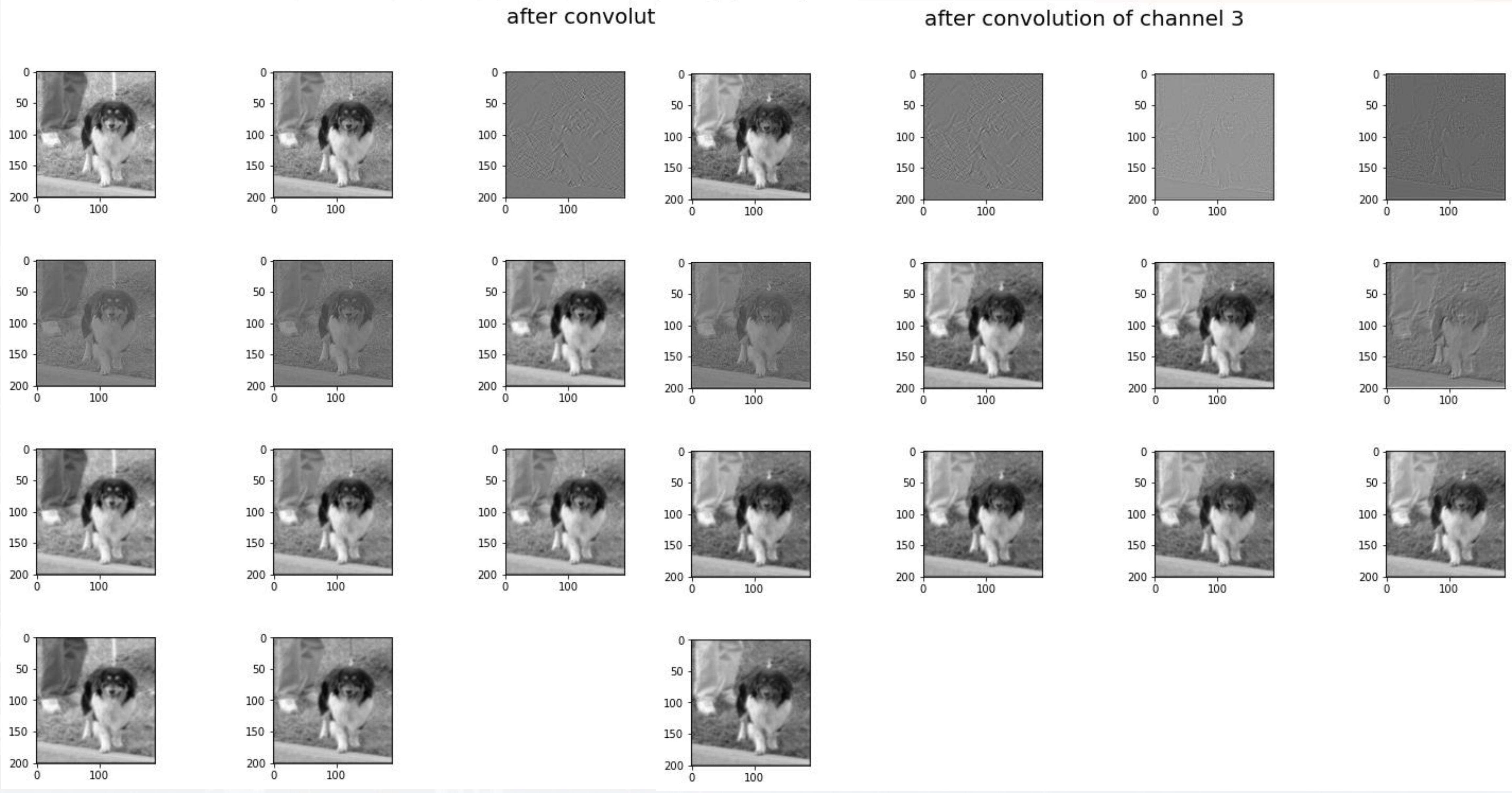


filter



Convolutional Neural Networks: Convolution

see `Convolution.ipynb` for the impact of different convolution filter on the image



Convolutional Neural Networks: Convolution

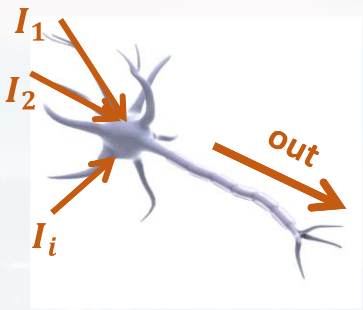
CNN:

- kernel act like **neurons with weights**
- start with random values for all kernels

→ the ANN **learns the filter values**

→ that's how the ANN learns which features are important

$$(f * g)(x) := \int_{\mathbb{R}^n} f(\zeta)\,\boldsymbol{g(x-\zeta)}\,d\zeta$$



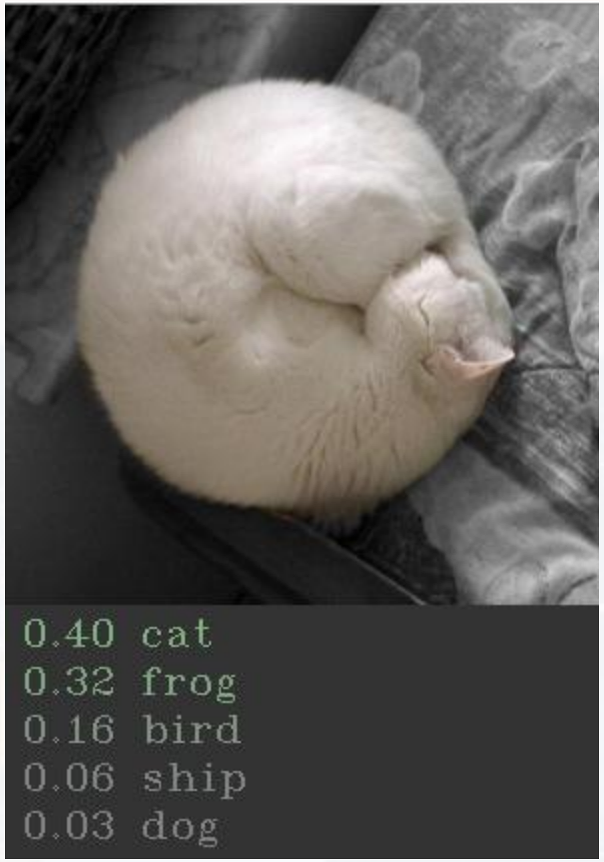
$$\boxed{net = \sum_i I_i \cdot w_i + b}$$

inputs are pixel values

kernel weights

$$\sum_i I_i\, \boldsymbol{w_i} + \boldsymbol{b}$$

can be interpreted as a neuron!



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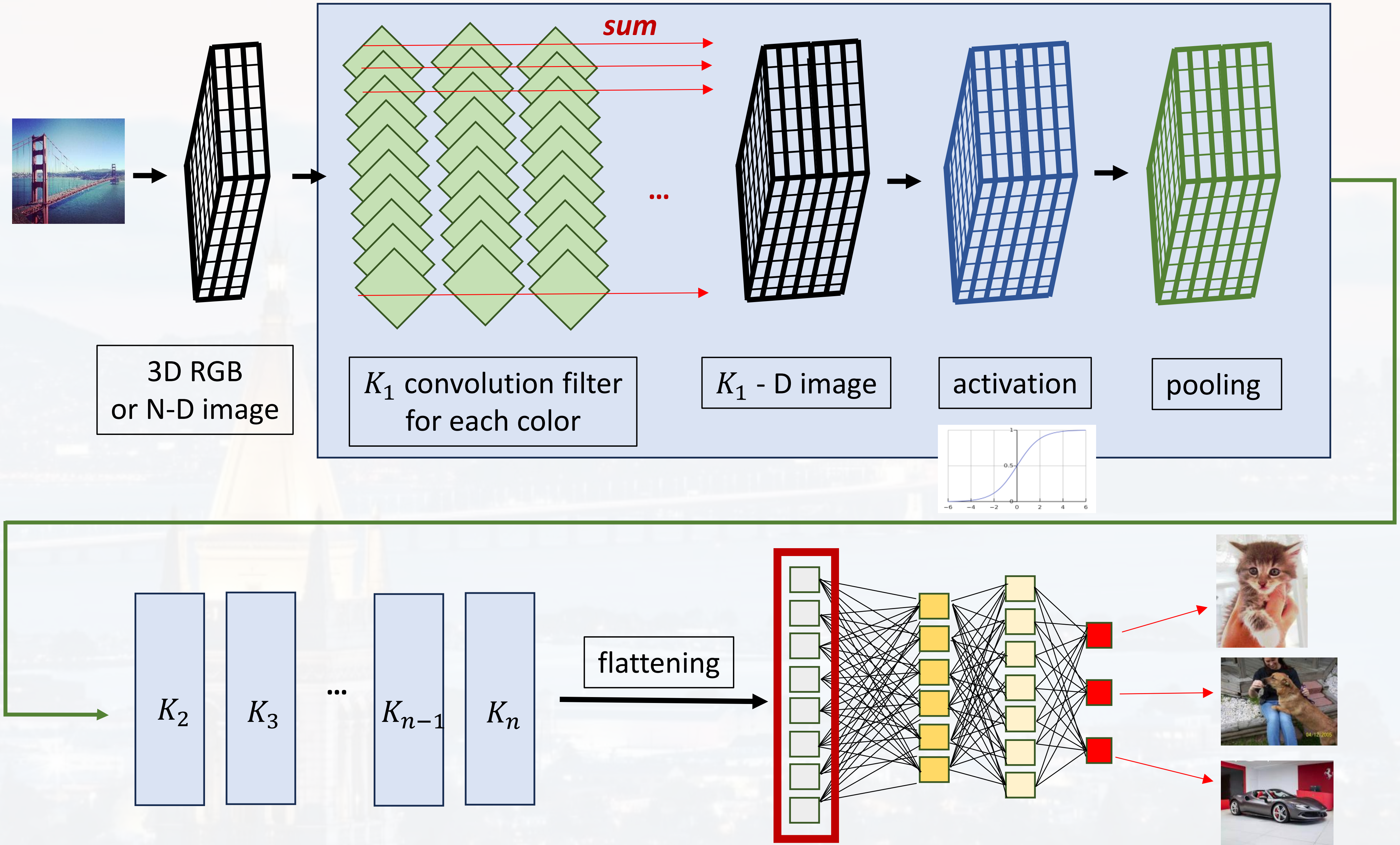
Convolutional Neural Networks: Architectures

classification



Convolutional Neural Networks: Architectures

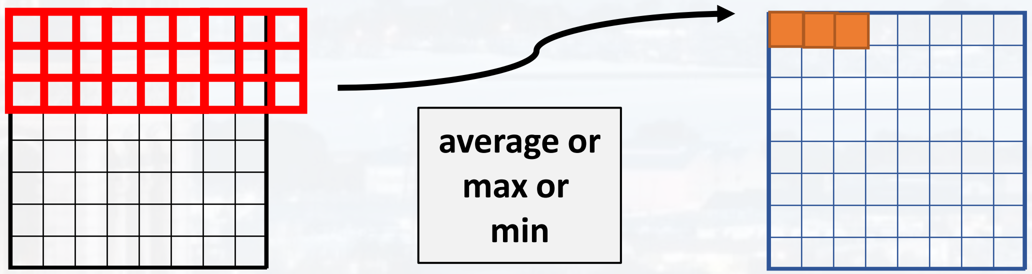
pooling:

there are three different main pooling methods

→ **average pool:** **blurs the image**, reduces edges (not what we want here)

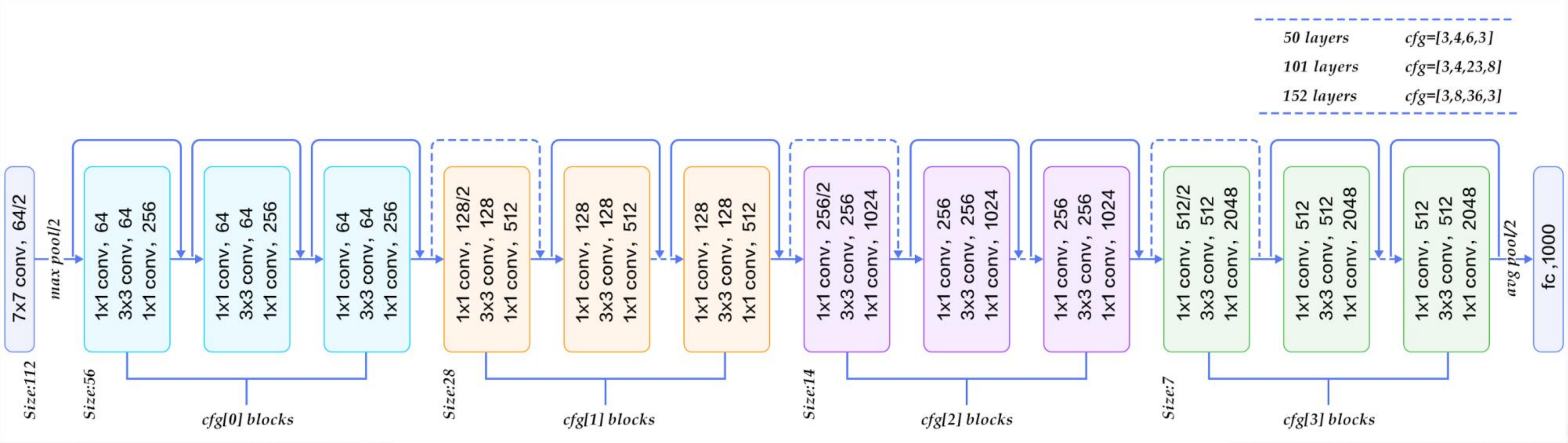
→ **max pool:** **reduces dark background** (those pixel values are usually low) and **enhances brighter foreground objects** (exactly what we need here)

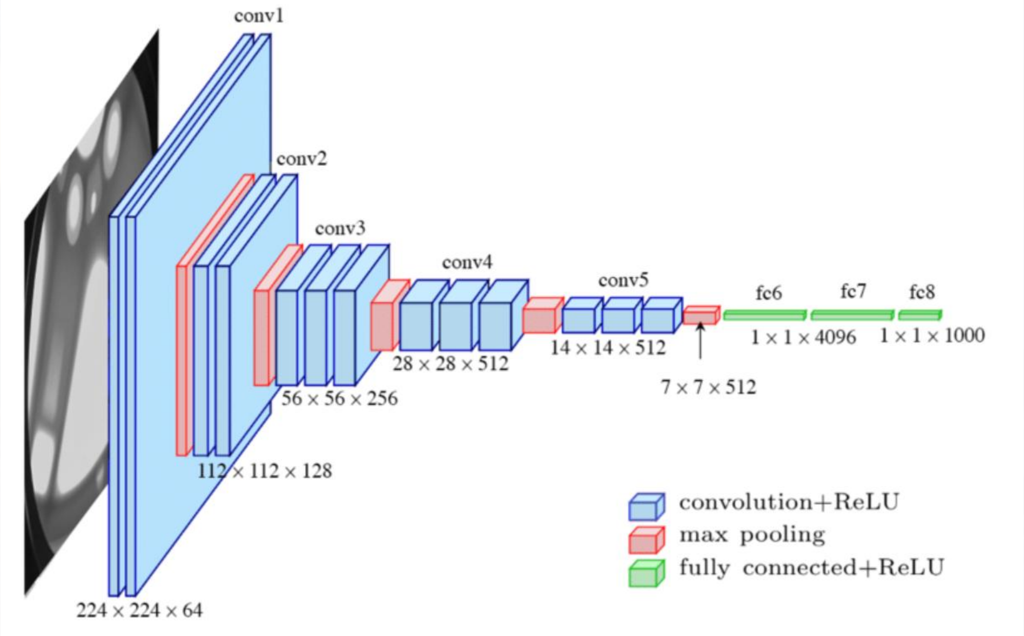
→ **min pool:** does the opposite of max pool



Convolutional Neural Networks: Architectures

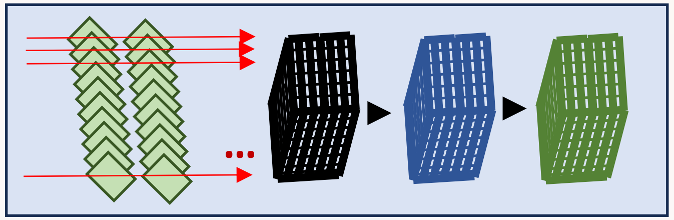
classification



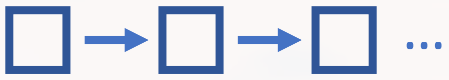


Convolutional Neural Networks: Architectures

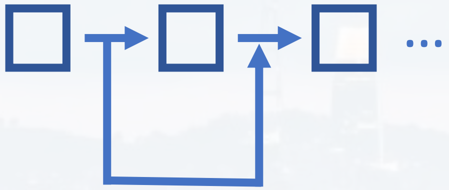
classification



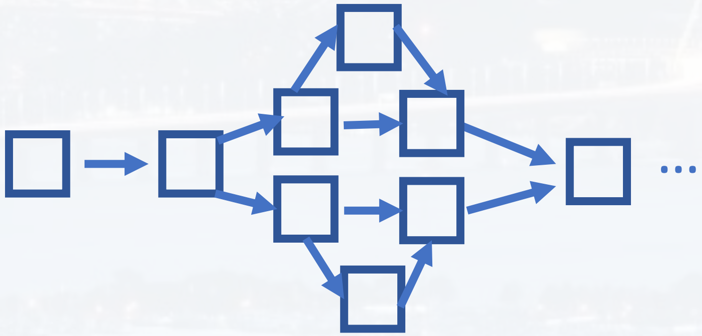
sequential CNNs



Residual**Net**



Inception Net



many others…

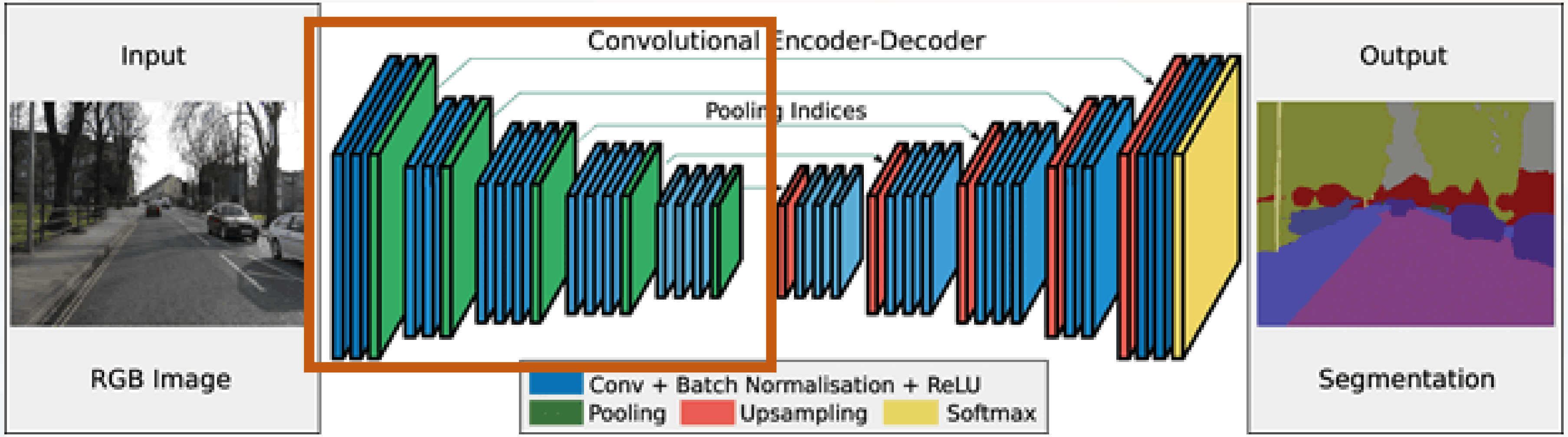
Convolutional Neural Networks: Architectures

classification

common pretrained classification CNNs

Network	Depth	Size	Parameters (Millions)	rel computation time	Image Input Size
nasnetlarge	*	360 MB	88,9	45	331-by-331
darknet19	19	72.5 MB	21	5,5	256-by-256
densenet201	201	77 MB	20	22	224-by-224
resnet50	50	96 MB	25,6	3,5	224-by-224
resnet101	101	167 MB	44,6	5	224-by-224
inceptionv3	48	89 MB	23,9	8	299-by-299
resnet18	18	44 MB	11,7	1,8	224-by-224
xception	71	85 MB	22,9	12	299-by-299
darknet53	53	145 MB	41	10	256-by-256
inceptionresnetv2	164	209 MB	55,9	14	299-by-299
shufflenet	50	6.3 MB	1,4	1,5	224-by-224
googlenet	22	27 MB	7	2	224-by-224
mobilenetv2	53	13 MB	3,5	4	224-by-224
alexnet	8	227 MB	61	1,2	227-by-227
nasnetmobile	*	20 MB	5,3	5	224-by-224
squeezenet	18	4.6 MB	1,24	1	227-by-227
vgg16	16	515 MB	138	6,5	224-by-224
vgg19	19	535 MB	144	8,5	224-by-224

segmentation

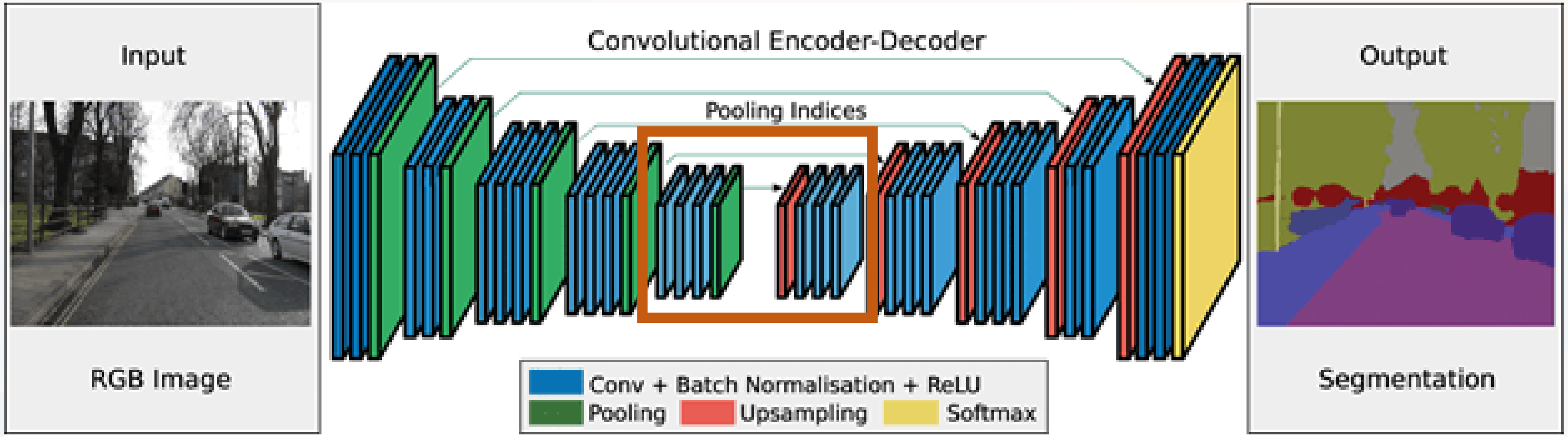


Vijay Badrinarayanan et. al 2017 "SegNet: A Deep Convolutional Encoder-Decoder Architecture for Image Segmentation"

1) down-sampling as before (= **encoder**)

Convolutional Neural Networks: Architectures

segmentation



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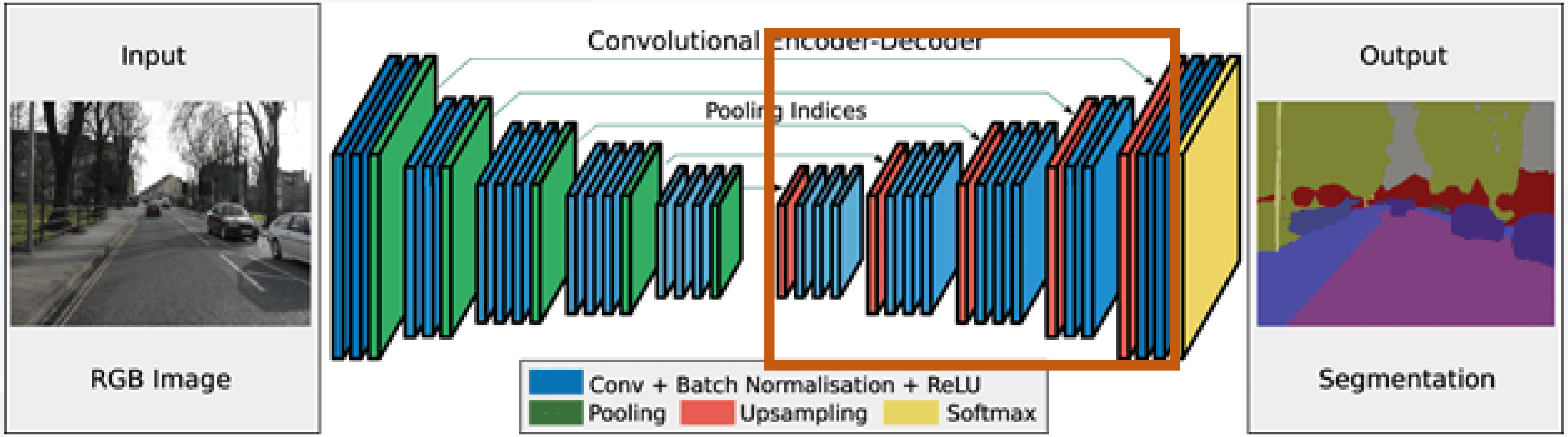
1) down-sampling as before (= **encoder**)

2) down to bottle neck

Convolutional Neural Networks: Architectures

segmentation



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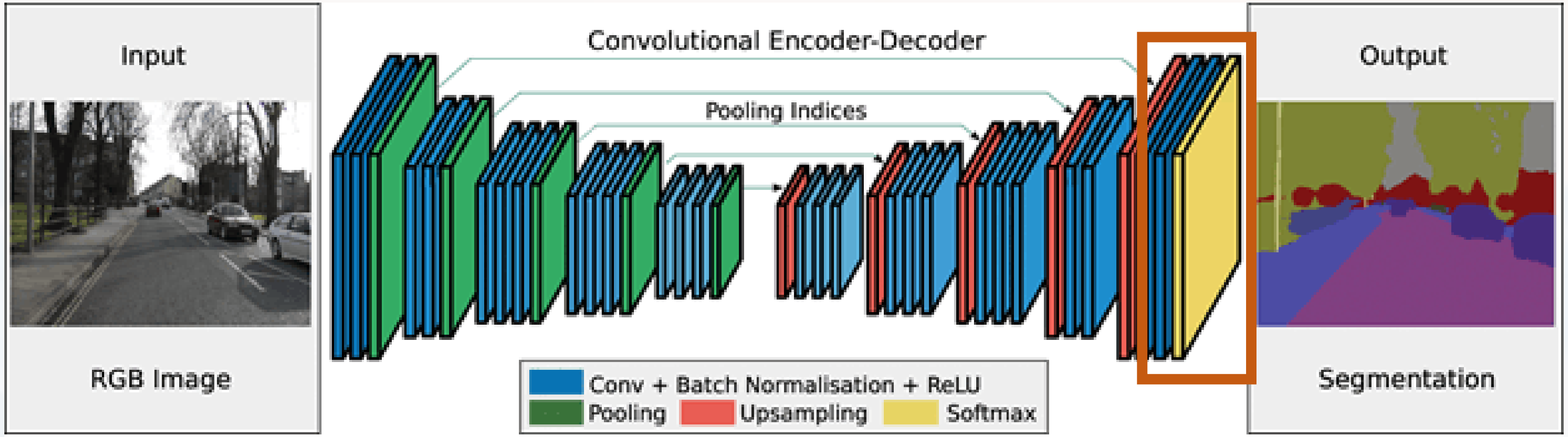
2) down to bottle neck

3) up-sampling (= **decoder**; how: see later) in order to generate output image of the same size as input image, where number of channels = number of pixel classes

Convolutional Neural Networks: Architectures

segmentation



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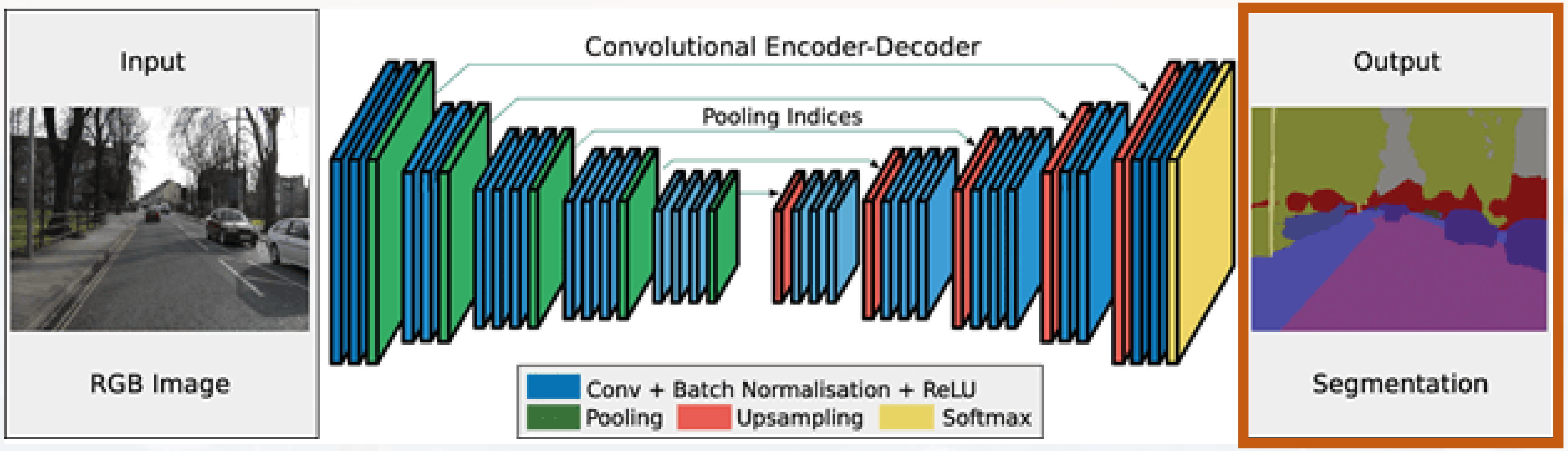
4) softmax, in order to turn output of last layer into probabilities

Convolutional Neural Networks:

segmentation



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1) down-sampling as before (= encoder)

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3) up-sampling (= **decoder;** how: see later) in order to generate output image of the same size as input image, where number of channels = number of pixel classes

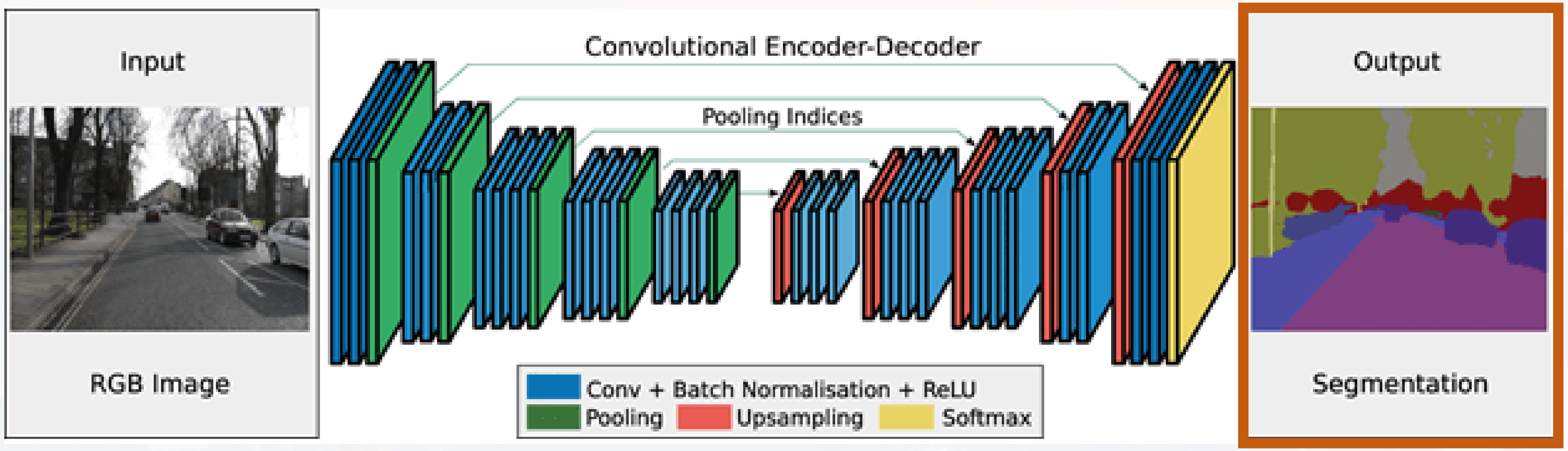
4) softmax, in order to turn output of last layer into probabilities

5) generates segmentation mask from highest probabilities

= (arbitrary) colors are class labels and correspond to pixel class

Convolutional Neural Networks: Architectures

segmentation



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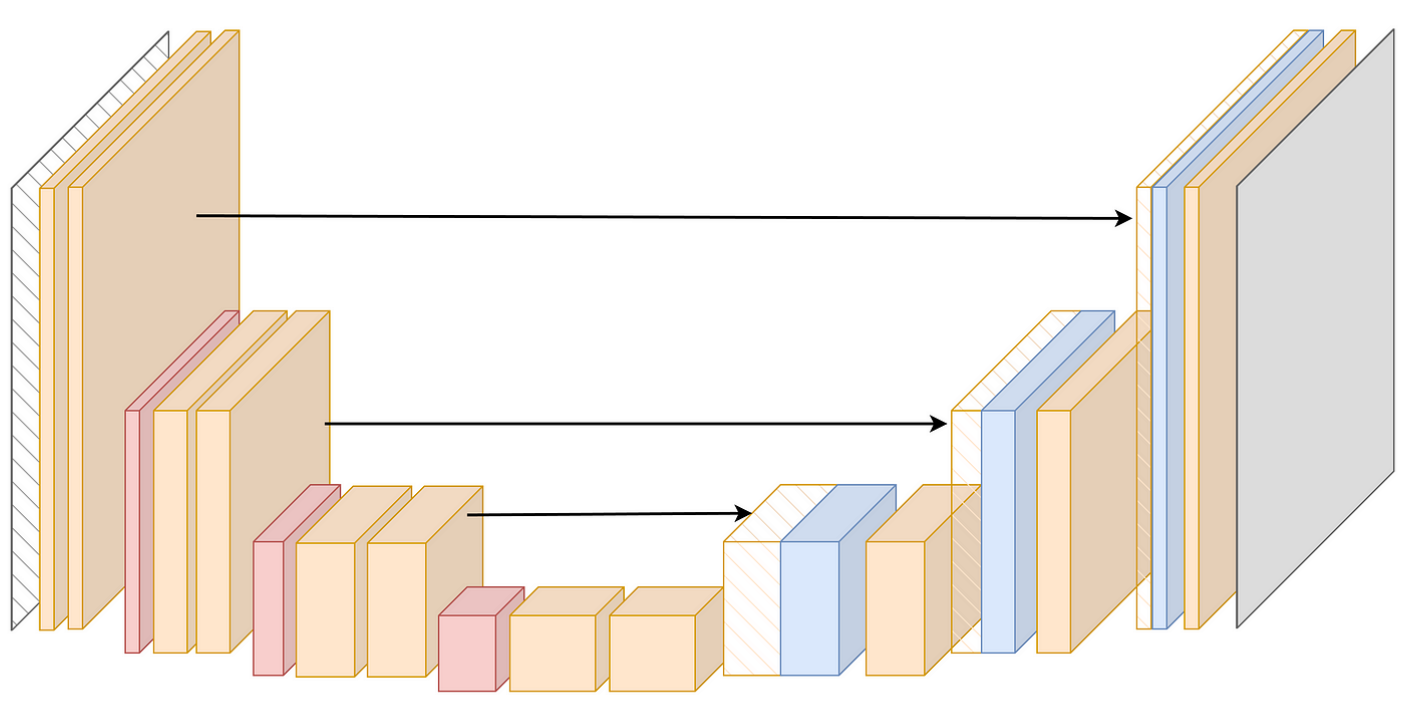
depending on the architecture, the decoder has **different learning mechanisms**

- standard: up-sampling = inverse convolution: weights and biases are learnables
- U-Net: skips connections and concatenates decoder layer with corresponding encoder layer information
- transformer encoder: use attention (see later)

segmentation

U-net segmentation CNN



https://towardsdatascience.com/u-net-explained-understanding-its-image-segmentation-architecture-56e4842e313a

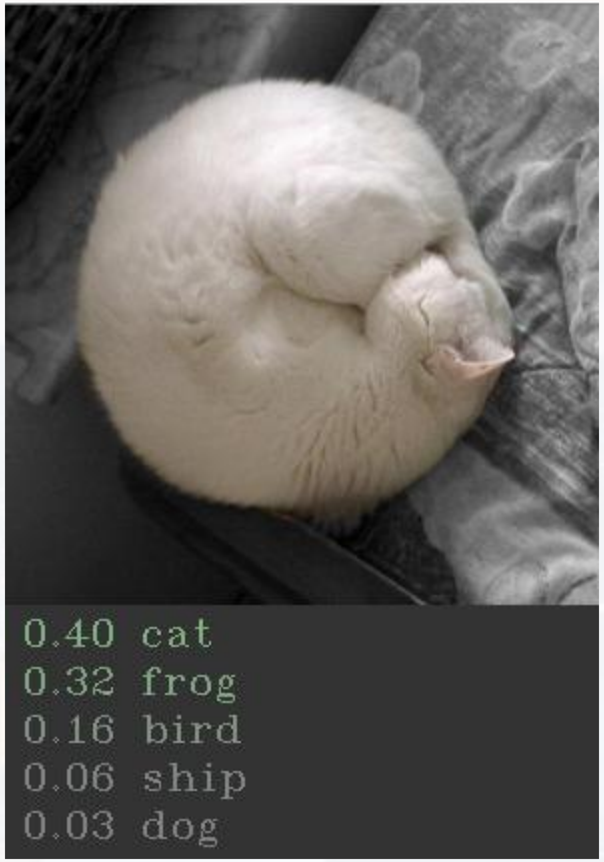
Convolutional Neural Networks: Architectures

segmentation

common pretrained segmentation CNNs

note: the input size is usually 5 – 10 times larger than compared to a classification CNN!

Type	Names
VGG	`'vgg16'` `'vgg19'`
ResNet	`'resnet18'` `'resnet34'` `'resnet50'` `'resnet101'` `'resnet152'`
SE-ResNet	`'seresnet18'` `'seresnet34'` `'seresnet50'` `'seresnet101'` `'seresnet152'`
ResNeXt	`'resnext50'` `'resnext101'`
SE-ResNeXt	`'seresnext50'` `'seresnext101'`
SENet154	`'senet154'`
DenseNet	`'densenet121'` `'densenet169'` `'densenet201'`
Inception	`'inceptionv3'` `'inceptionresnetv2'`
MobileNet	`'mobilenet'` `'mobilenetv2'`
EfficientNet	`'efficientnetb0'` `'efficientnetb1'` `'efficientnetb2'` `'efficientnetb3'` `'efficientnetb4'` `'efficientnetb5' efficientnetb6' efficientnetb7'`



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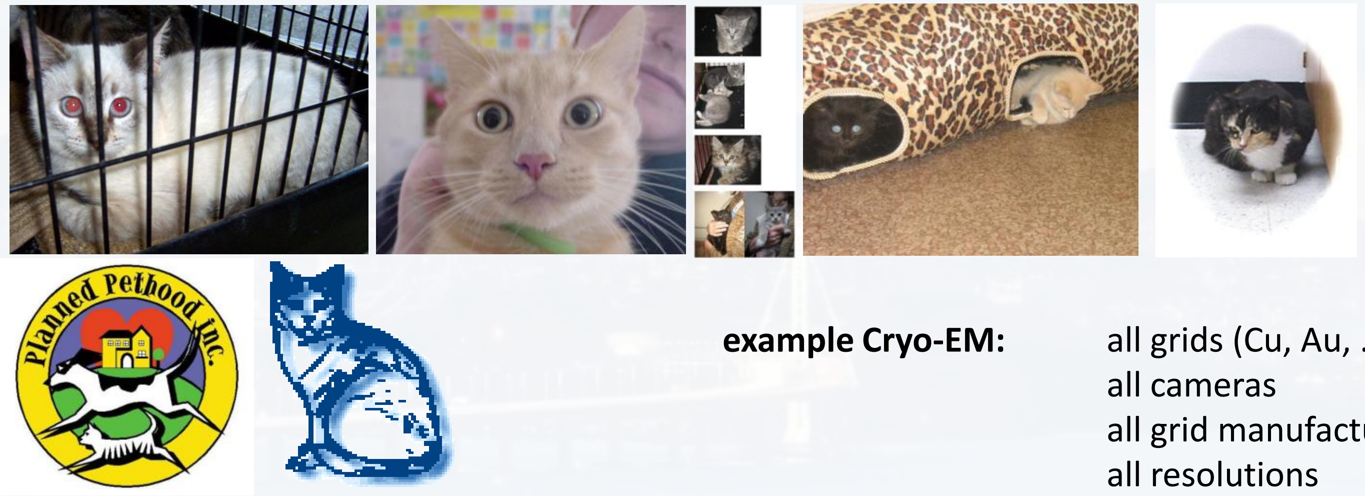
Convolutional Neural Networks:

data acquisition

1) classes should be **well balanced**

2) dataset should be **diverse**



example Cryo-EM:

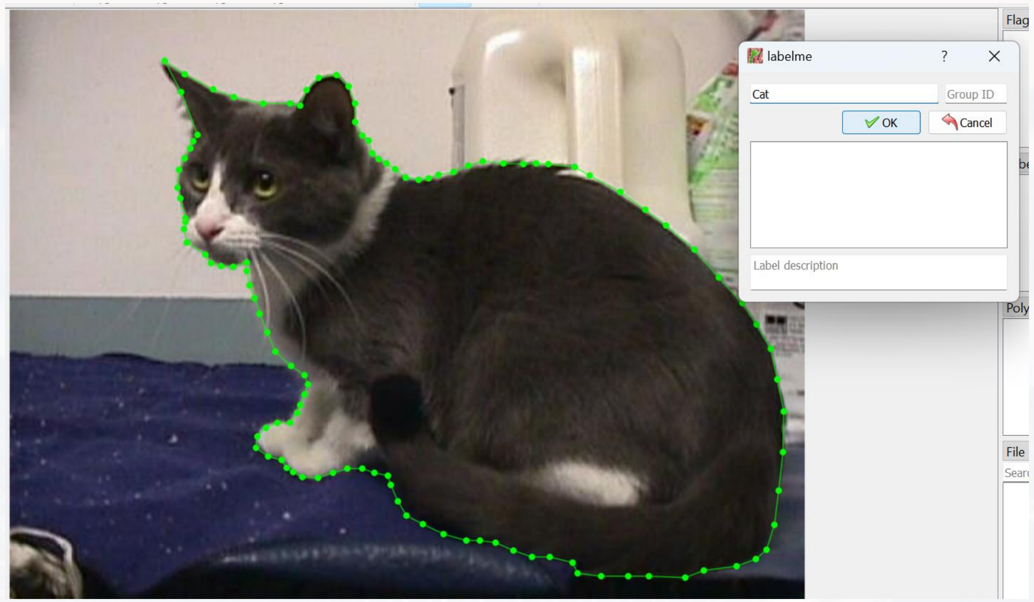
all grids (Cu, Au, …)
all cameras
all grid manufacturers
all resolutions

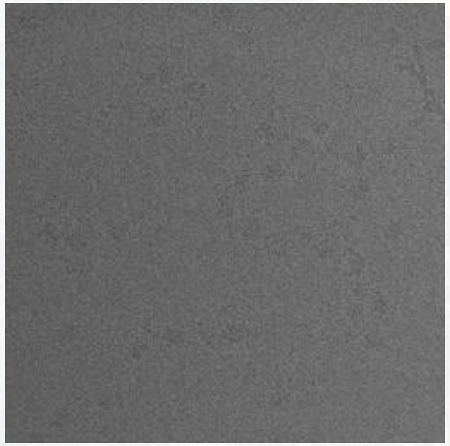
3) **augmentation:** blurred, skewed, fragmented, stretched, turned etc

tip: write your own augmentation routine!

data labeling

be as accurate as possible!





micrograph Cryo-EM image

→ good, medium and bad based on ice crystals

→ Undergrad, Grad, PostDoc, Senior Scientist

data preprocessing

scaling:

Image Input Size
331-by-331
256-by-256
224-by-224
224-by-224

All images have to be scaled to the input size of the CNN!

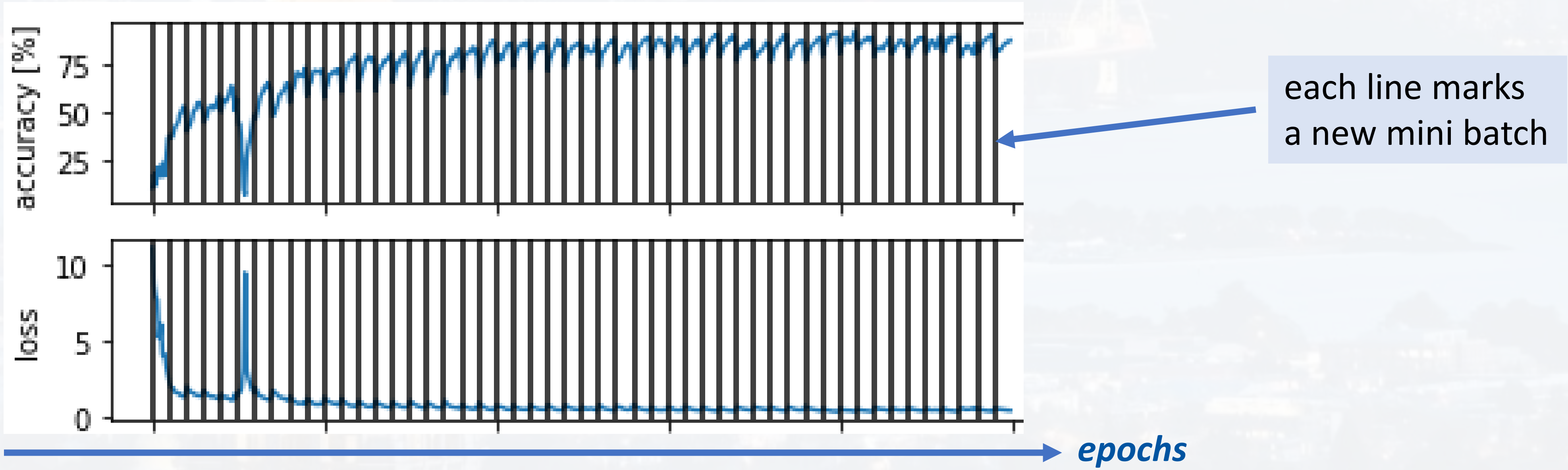
normalization: images can be

- logical (values are zero **or** one)
- gray scale (2D) → adding two more “color channels”
- 8bit (range 255), 16bit (range 512) etc

training

normalization: complex CNNs have many layers for normalization/re-centering/re-scaling
→ **batch normalization**

the training set is huge
→ loading only a few images at the time (**mini batch**)
→ the larger the mini batch, the better
→ run only **a few iterations** per mini batch (avoiding local minima)
→ check **training loss vs evaluation loss**



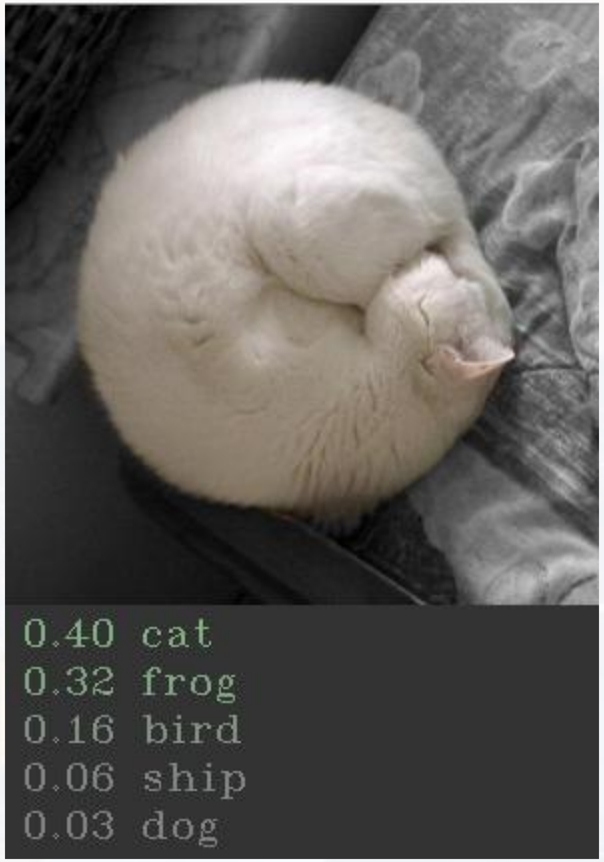
training

check out:

Training MLP

Training CNN 2D

Training CNN 3D



<u>Outline</u>

- The Problem
- What is Convolution
- The CNN Architectures
- Data Preparation & Training
- **A Simple Example**

Convolutional Neural Networks: Simple Example

constructing, running and testing LeNet → `LeNet.ipynb`

```
Model: "my_le_net_1"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 conv2d_3 (Conv2D)           (None, 28, 28, 6)         156

 average_pooling2d_2 (Avera  (None, 14, 14, 6)         0
 gePooling2D)

 conv2d_4 (Conv2D)           (None, 10, 10, 16)        2416

 average_pooling2d_3 (Avera  (None, 5, 5, 16)          0
 gePooling2D)

 conv2d_5 (Conv2D)           (None, 1, 1, 120)         48120

 flatten_1 (Flatten)         (None, 120)               0

 dense_2 (Dense)             (None, 84)                10164

 dense_3 (Dense)             (None, 10)                850

=================================================================
Total params: 61706 (241.04 KB)
Trainable params: 61706 (241.04 KB)
Non-trainable params: 0 (0.00 Byte)
```

input = (N images, 28 x 28 pixel, 3 colors)
output = (N images, 28 x 28 pixel, 6 Conv filter)

6 Conv filter * shape (5, 5) = 150
plus 1 bias for each filter → total 156

Each image is represented by a vector of length 120

output layer: one neuron for each class

constructing, running and testing LeNet → `LeNet.ipynb`

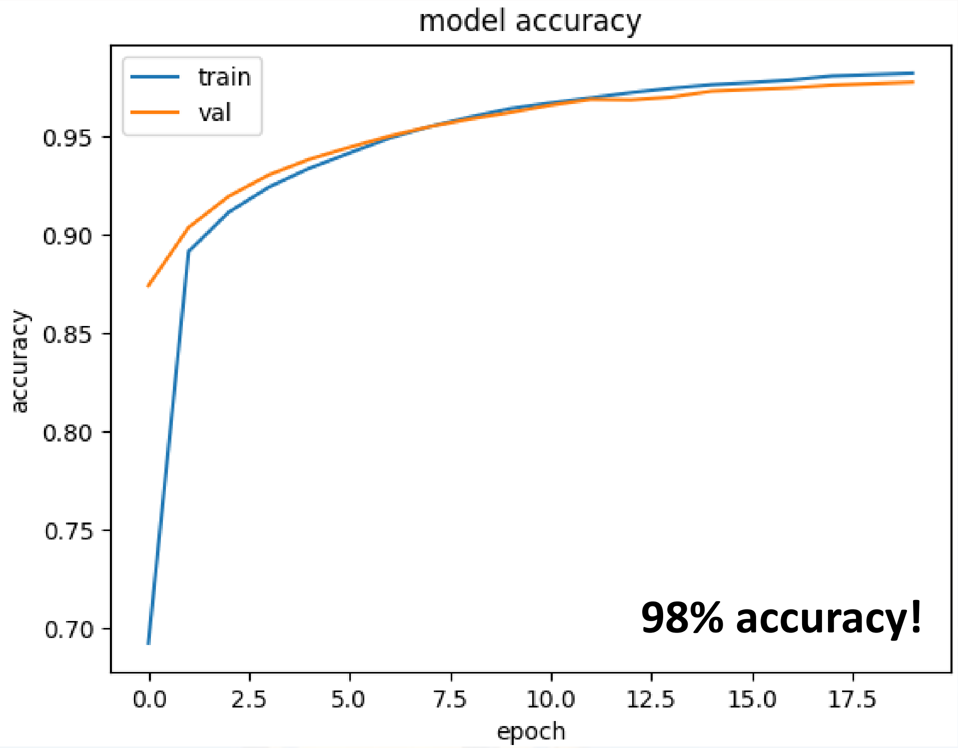
```
running model...
Epoch 1/20
94/94 [==============================] - 9s 92ms/step - loss: 1.1172 - accuracy: 0.7160 - val_loss: 0.4217 - val_accuracy: 0.8838
Epoch 2/20
94/94 [==============================] - 8s 88ms/step - loss: 0.3577 - accuracy: 0.8990 - val_loss: 0.3096 - val_accuracy: 0.9109
Epoch 3/20
94/94 [==============================] - 7s 73ms/step - loss: 0.2876 - accuracy: 0.9163 - val_loss: 0.2606 - val_accuracy: 0.9231
Epoch 4/20
94/94 [==============================] - 8s 90ms/step - loss: 0.2444 - accuracy: 0.9287 - val_loss: 0.2238 - val_accuracy: 0.9333
Epoch 5/20
94/94 [==============================] - 7s 69ms/step - loss: 0.2113 - accuracy: 0.9376 - val_loss: 0.1944 - val_accuracy: 0.9423
```

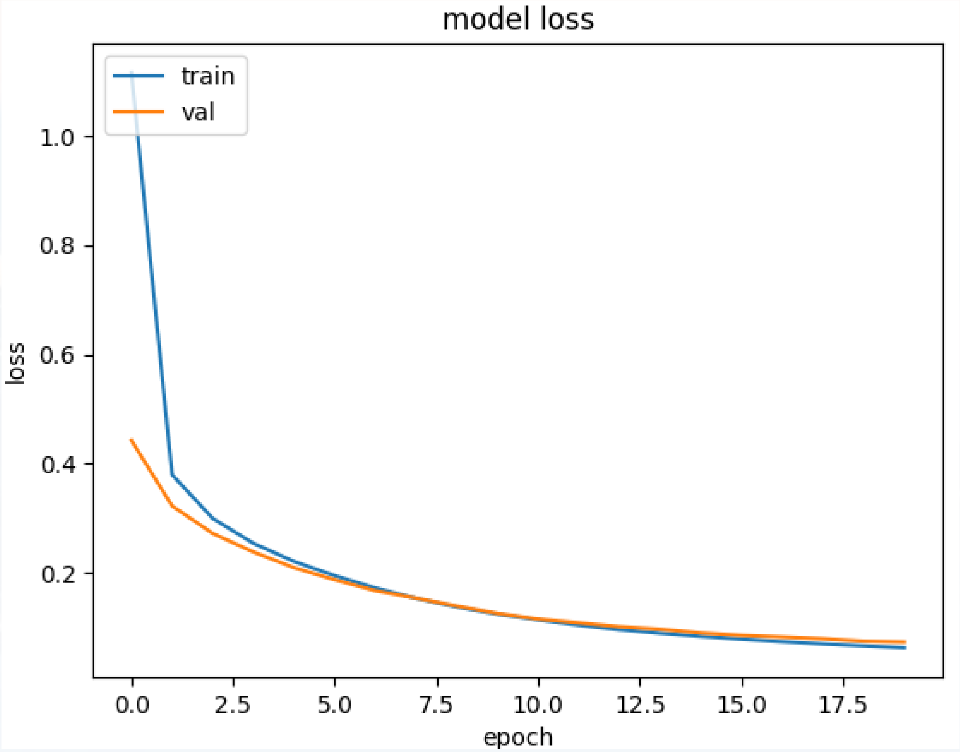
<u>epoch:</u> passing the entire dataset through the network

60, 000 images / batch size = **512** = 117 iterations per epoch
= **117 * 80**% for training = **94 iterations per epoch**

Convolutional Neural Networks:

constructing, running and testing LeNet → `LeNet.ipynb`

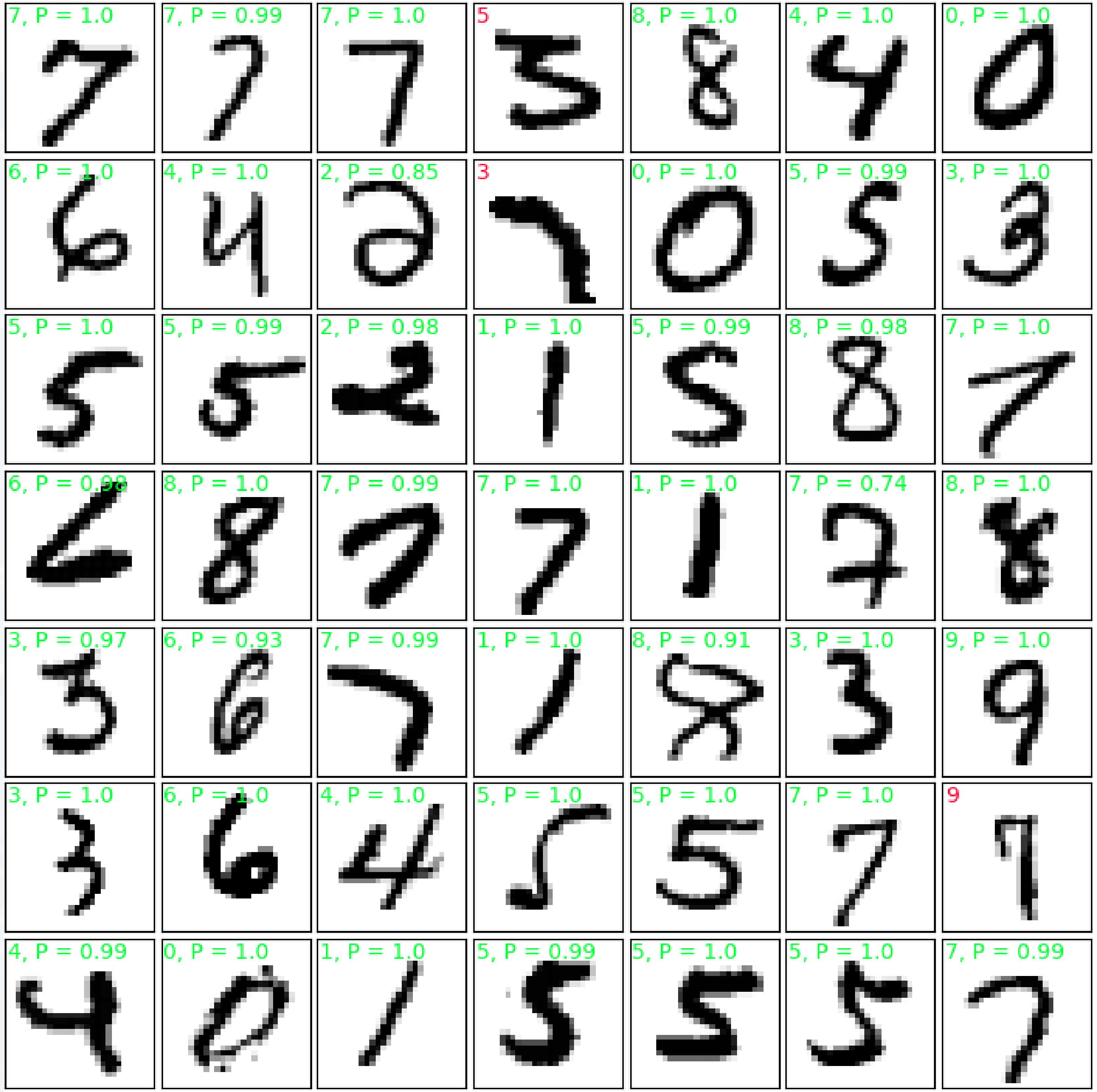




training loss should ≈ validation loss
if validation loss >> training loss → overfitting
- too many parameter
- too few images in batch
- too specific/unique batch)

Convolutional Neural Networks: Simple Example

constructing, running and testing LeNet → `LeNet.ipynb`



Thank you for your attention!