

Lecture 11:

Convolution and Image Classification & Segmentation



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Bayesian Data Analysis and
Machine Learning for Physical
Sciences



Course Map

Module 1	Maximum Entropy and Information, Bayes Theorem
Module 2	Naive Bayes, Bayesian Parameter Estimation, MAP
Module 3	MLE, Lin Regression
Module 4	Model selection I: Comparing Distributions
Module 5	Model Selection II: Bayesian Signal Detection
Module 6	Variational Bayes, Expectation Maximization
Module 7	Hidden Markov Models, Stochastic Processes
Module 8	Monte Carlo Methods
Module 9	Machine Learning Overview, Supervised Methods & Unsupervised Methods
Module 10	ANN: Perceptron, Backpropagation, SGD
Module 11	Convolution and Image Classification and Segmentation
Module 12	RNNs and LSTMs
Module 13	RNNs and LSTMs + CNNs
Module 14	Transformer and LLMs
Module 15	Graphs & GNNs



Outline

The Problem

Convolution

CNN Architectures

Data Preparation & Training

Example

- LeNet numpy only
- LeNet TensorFlow
- sequences as images
- segmentation



```
0.40 cat
0.32 frog
0.16 bird
0.06 ship
0.03 dog
```

Outline

The Problem

part I

Convolution

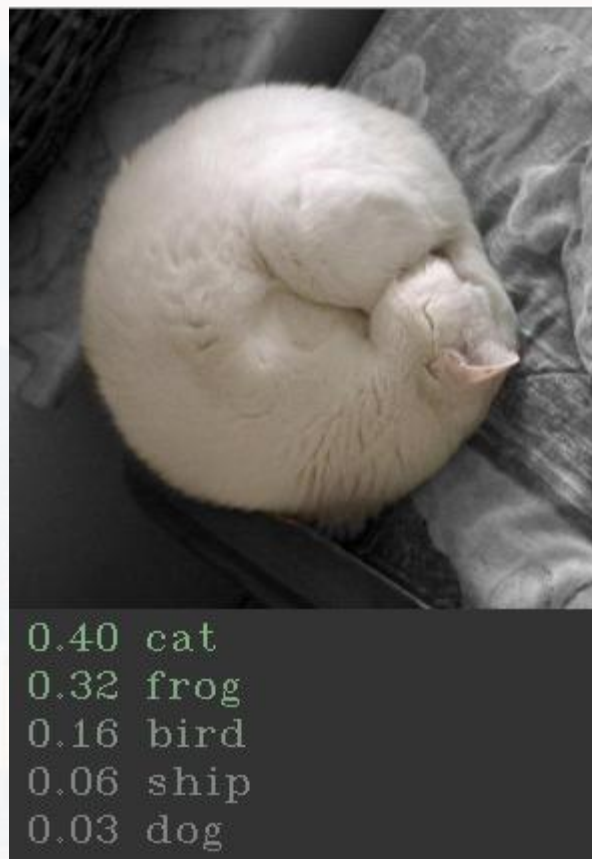
CNN Architectures

Data Preparation & Training

Example

part II

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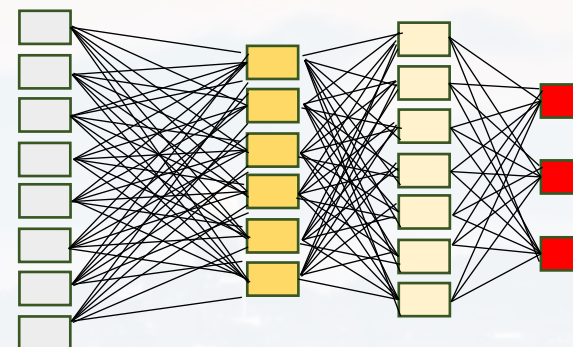
Example

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- sequences as images
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so far:

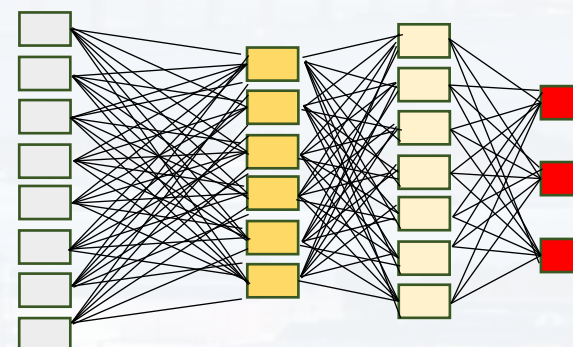
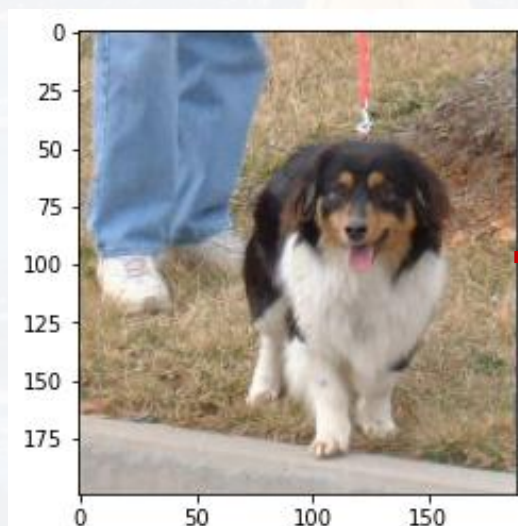
	data features				
data points ↓	[5.1	3.5	1.4	0.2]
	[4.9	3.	1.4	0.2]
	[4.7	3.2	1.3	0.2]
	[4.6	3.1	1.5	0.2]
	[5.	3.6	1.4	0.2]
	[5.4	3.9	1.7	0.4]
	[4.6	3.4	1.4	0.3]
	[5.	3.4	1.5	0.2]



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

row = data point

now:



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



so far:

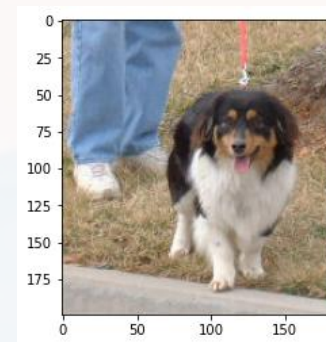
data features

data points ↓

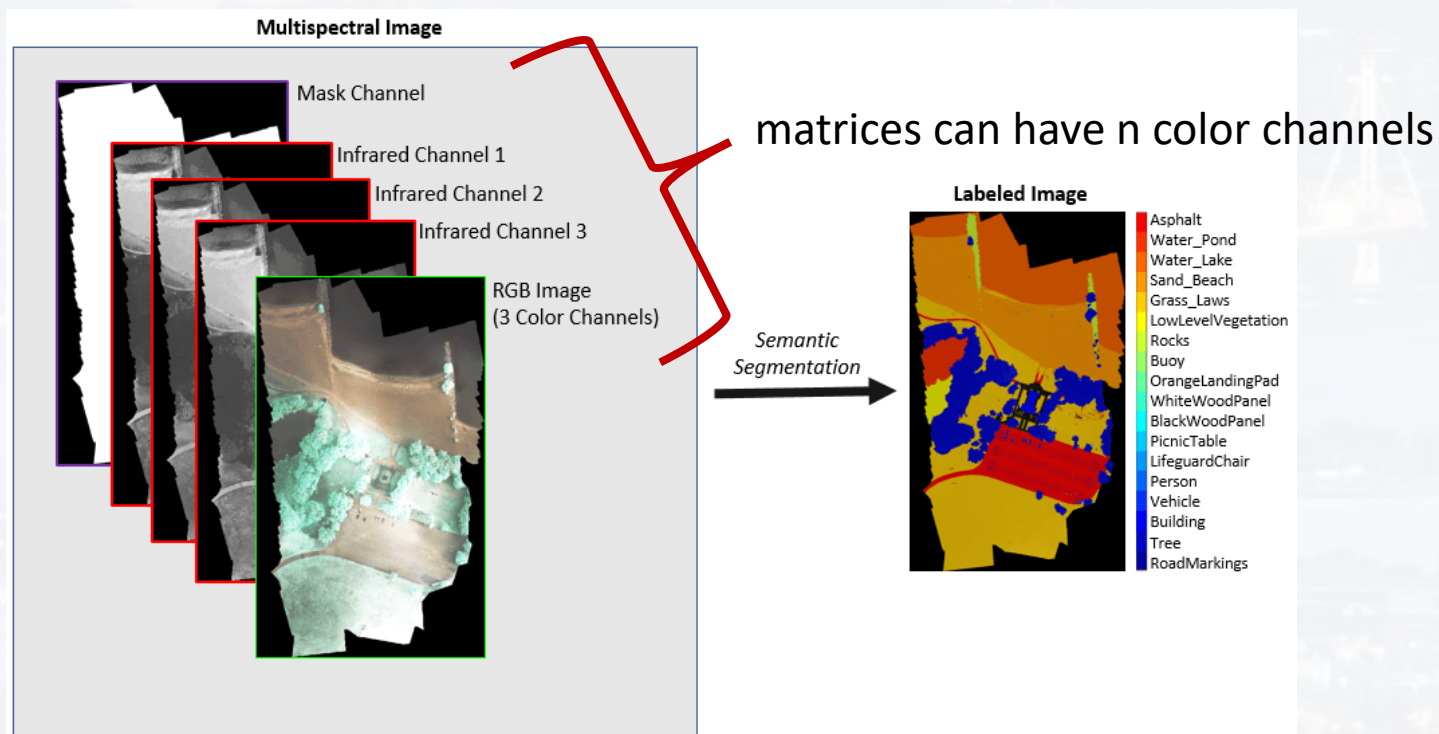
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[4.9	3.	1.4	0.2]
[4.7	3.2	1.3	0.2]
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[5.4	3.9	1.7	0.4]
[4.6	3.4	1.4	0.3]
[5.	3.4	1.5	0.2]

row = data point

now:

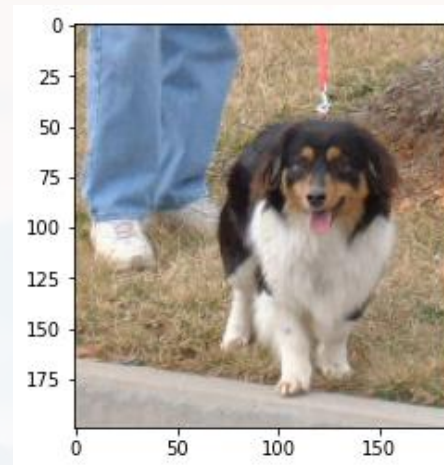


matrix = data point

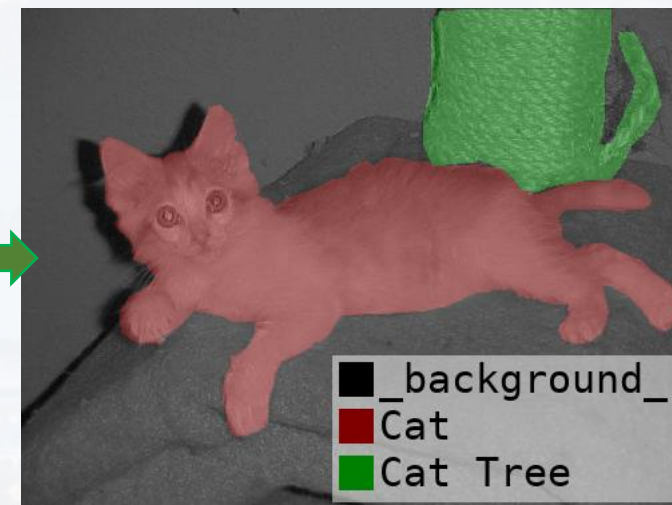
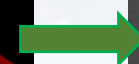
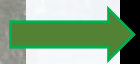




1) **classification:** between different images



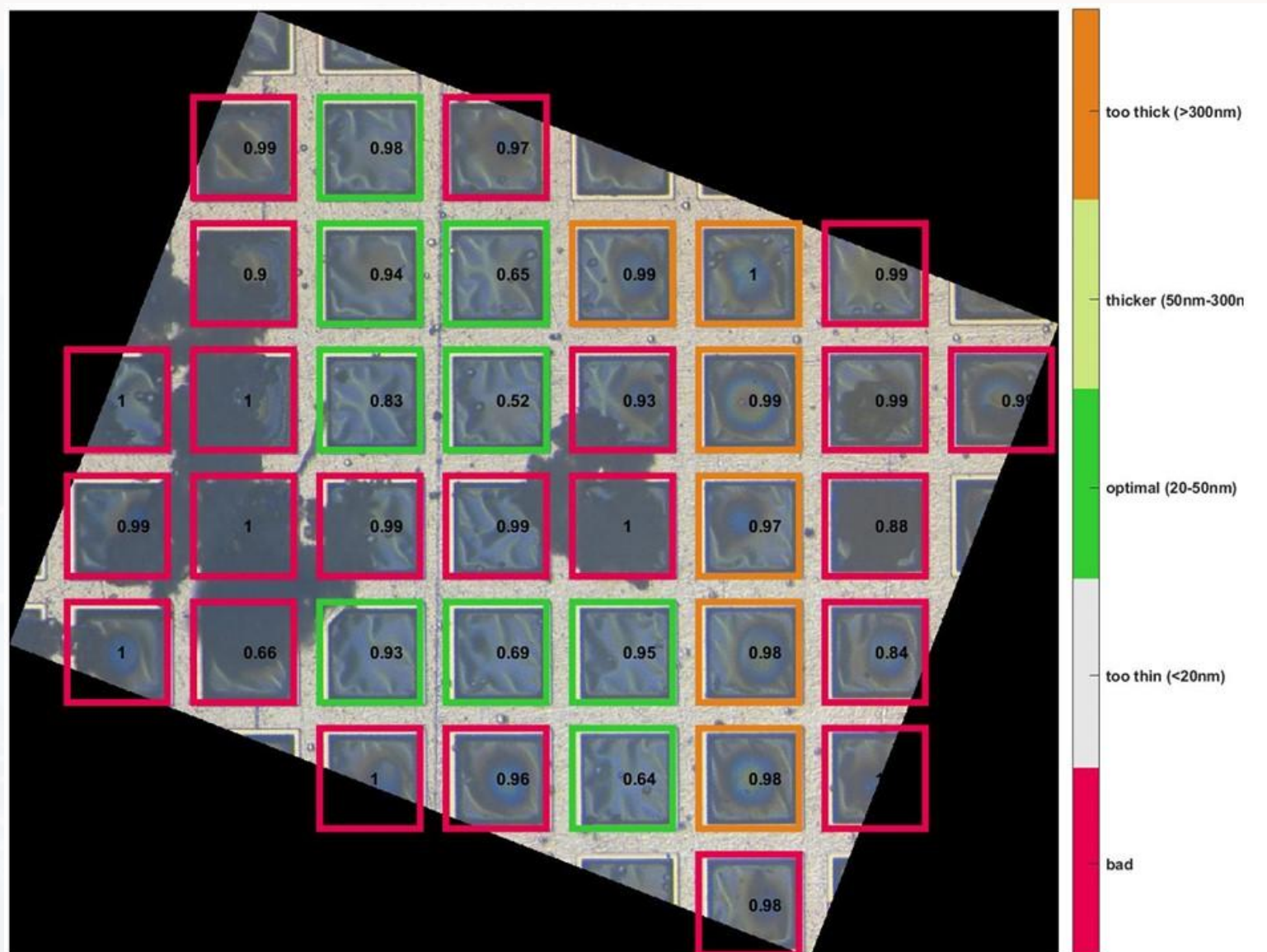
different pixel within images aka 2) **segmentation**



■ _background_
■ Cat
■ Cat Tree



segmentation *for* classification



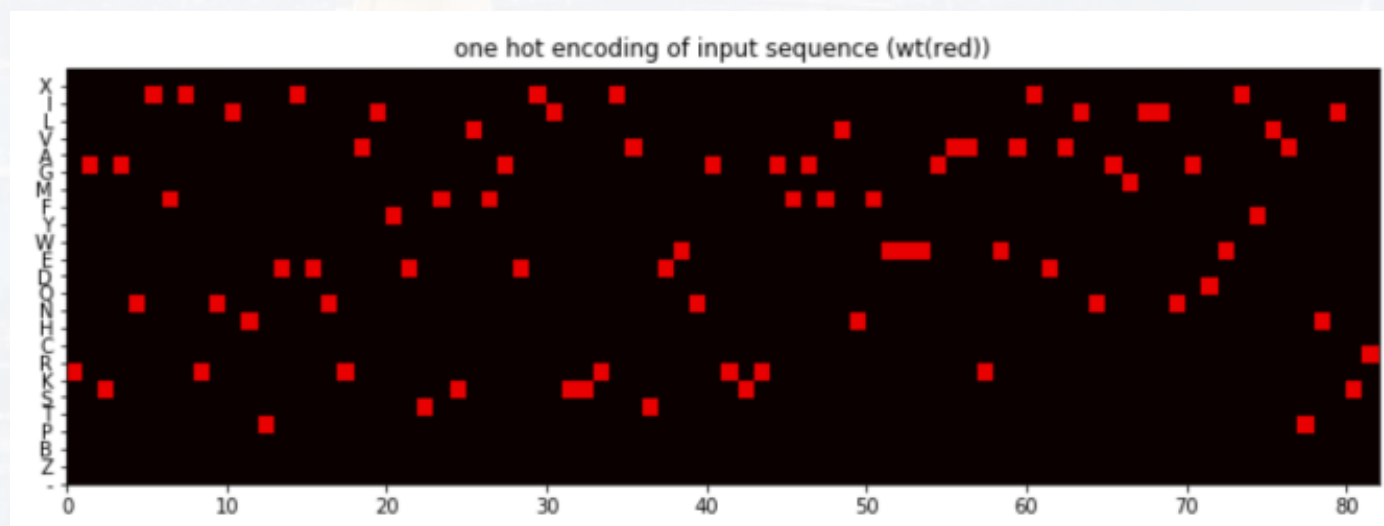
see [here](#)



motif finding / sequence analysis

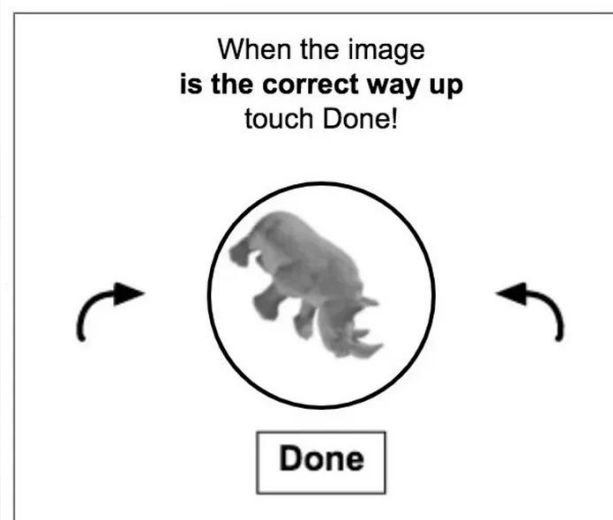
	C	A	G	T	C	T	A
4	1	0	0	0	1	0	0
	0	0	1	0	0	0	0
	0	0	0	1	0	1	0
	0	1	0	0	0	0	1
	Sequence Length						

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



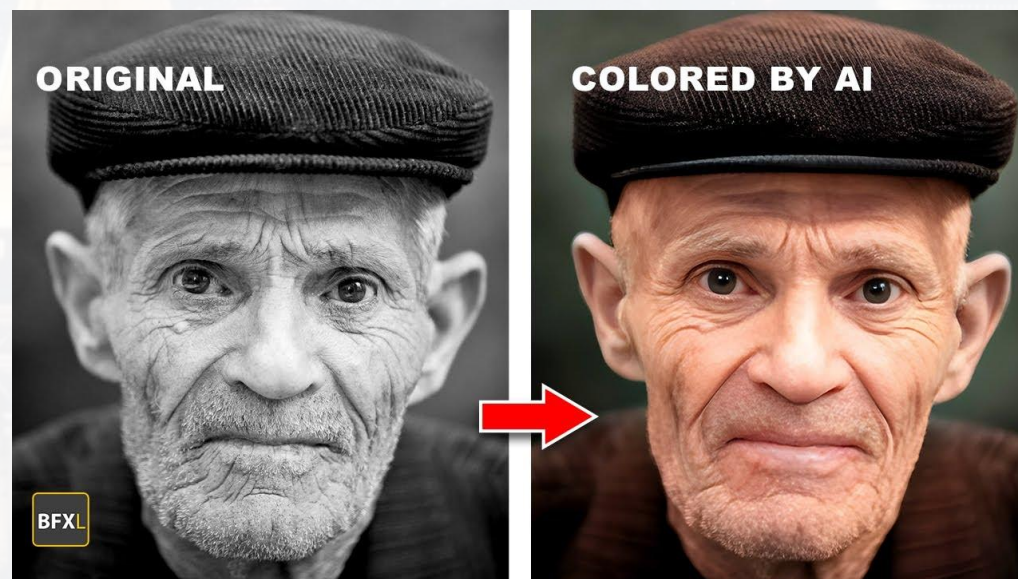


3) regression:



turning images the right way

4) generation



source: TopviewAI



before we had CNNs: k-means for segmentation & classification:

```
rows, cols, channels = Image.shape  
x_flat              = Image.reshape(rows * cols, channels)
```

```
kmeans              = KMeans(n_clusters = k)  
pxl_labels          = kmeans.fit_predict(x_flat)  
colors              = kmeans.cluster_centers_
```

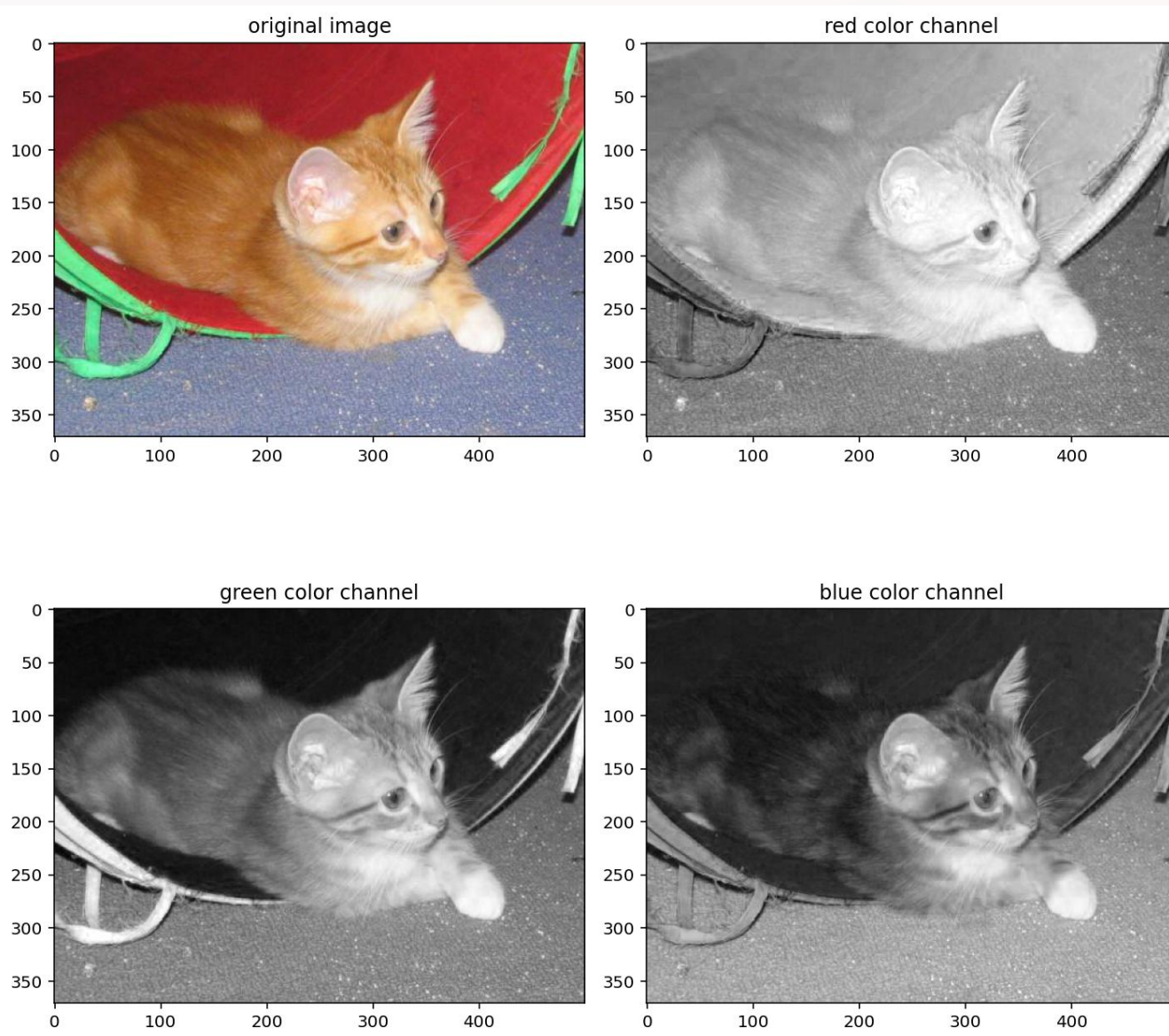
turning image into table
(**spatial information is lost!**)

- labels are assigned according to cluster in **color space** (RGB, HSV etc)
- cluster means are mean colors

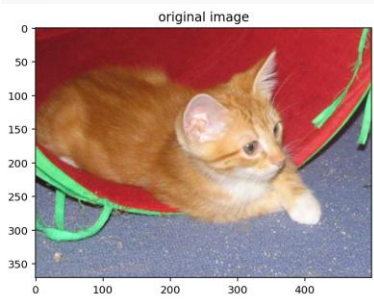
see `KMeansSegmentation.py`



see `KMeansSegmentation.py`

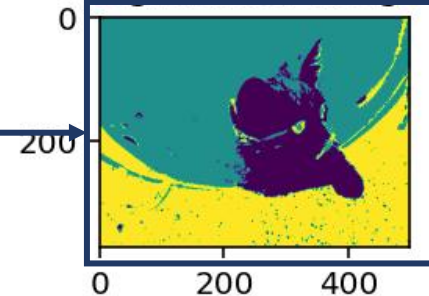


```
K = KMeansSegmentation()
```

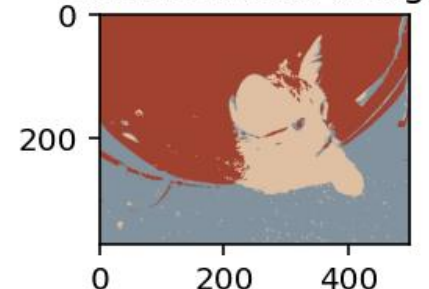



K.Segment()

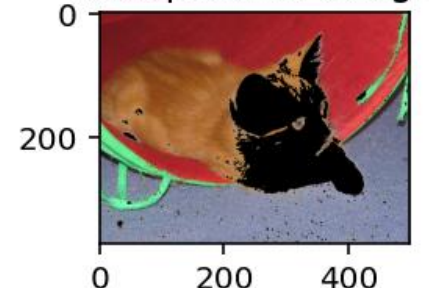
segmented image



reconstructed image

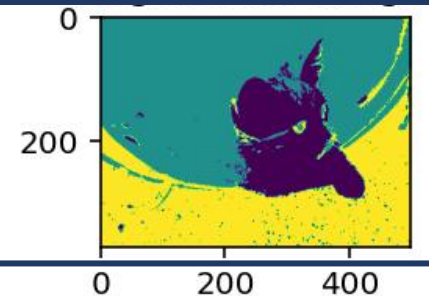


manipulated image

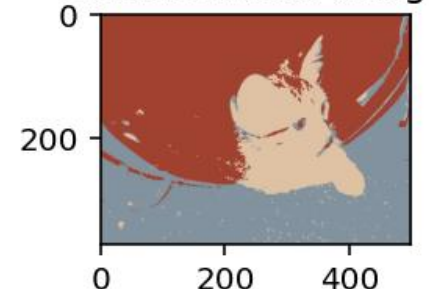


K.Segment(values\
= [255, 255, 255])

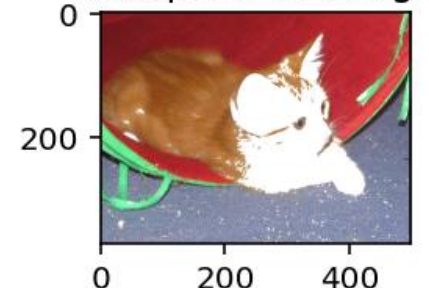
segmented image



reconstructed image

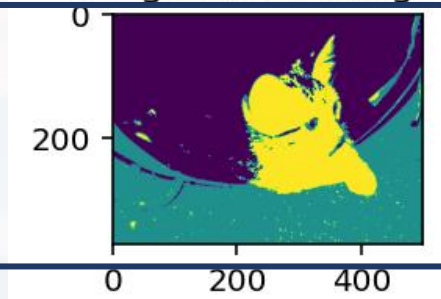


manipulated image

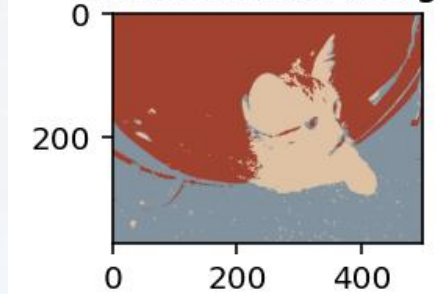


K.Segment(values\
= [255, 0, 0], label = 1)

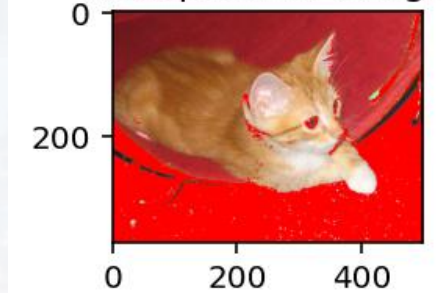
segmented image



reconstructed image



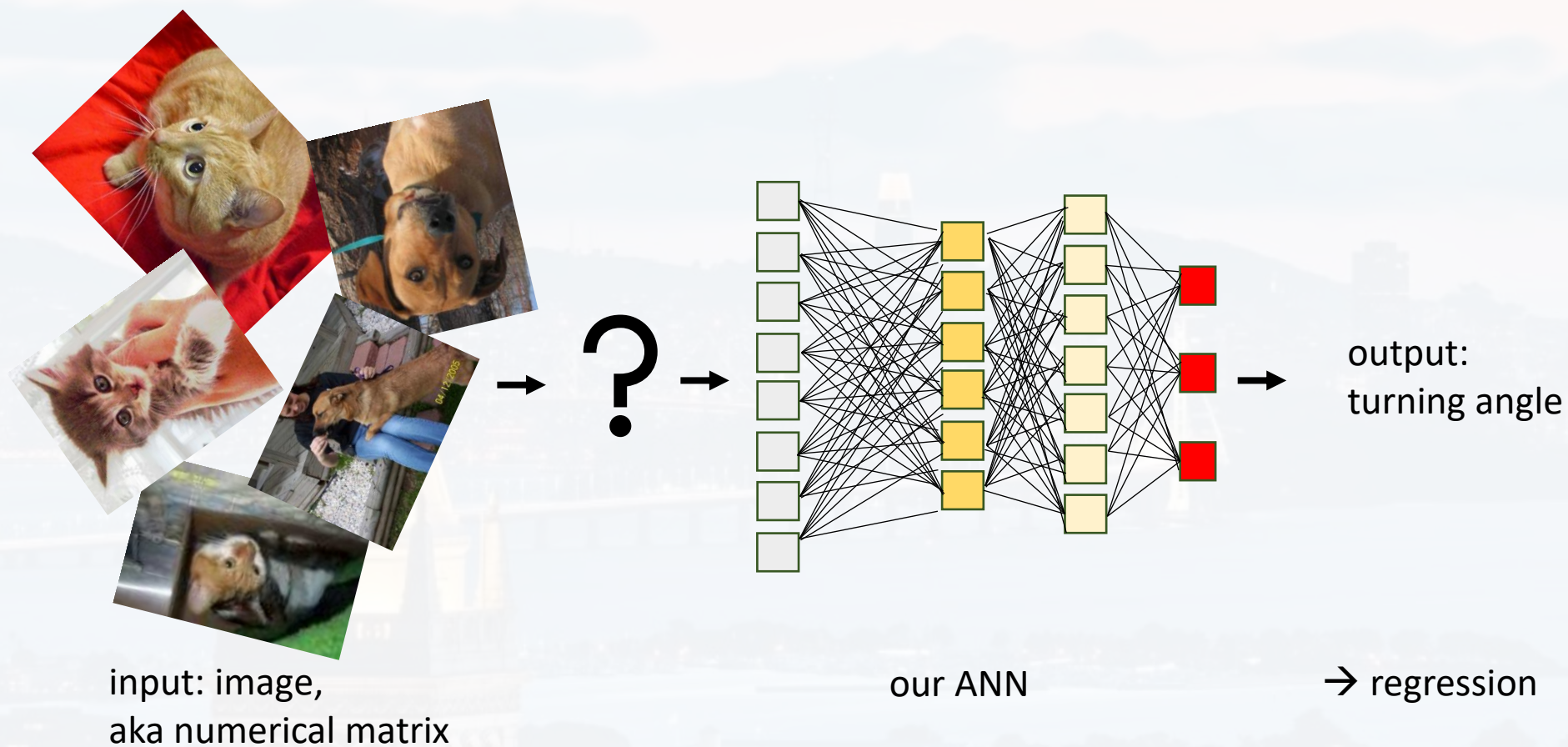
manipulated image



labels can swap
(k-means is
unsupervised)

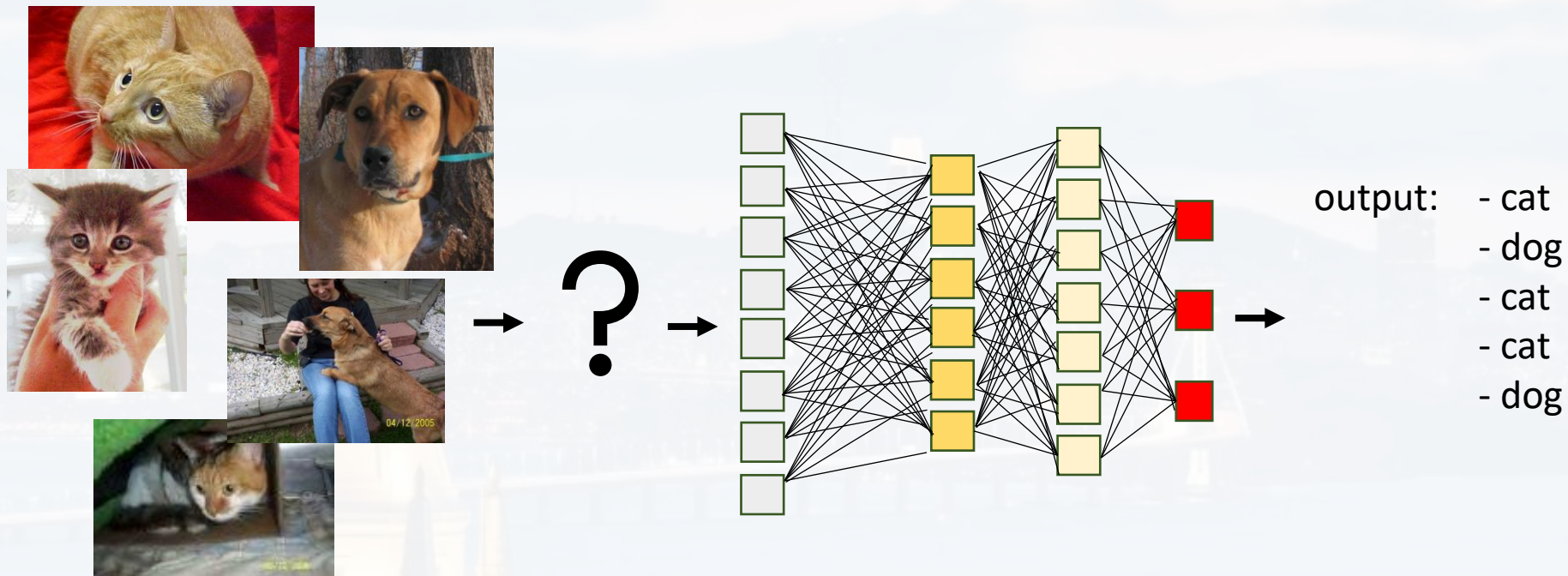


task: find a way to keep both: **color** and **spatial** information and link the image to our ANN





task: find a way to keep both: color and spatial information and link the image to our ANN

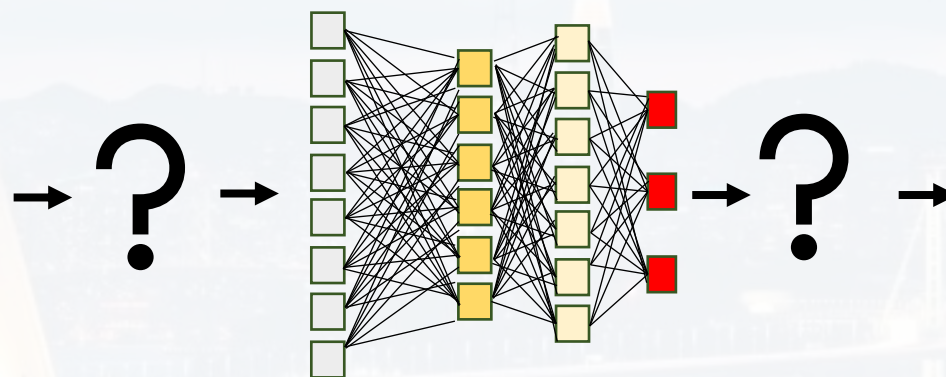




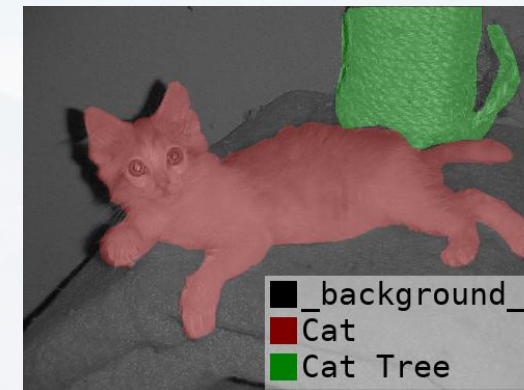
task: find a way to keep both: color and spatial information and link the image to our ANN



input: image,
aka numerical matrix



our ANN



segmented image



```
0.40 cat
0.32 frog
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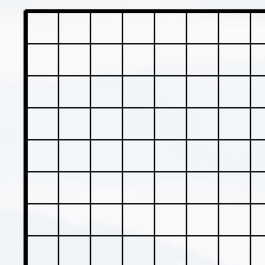


- goal:
- maintaining the spatial information
 - learning which features are important

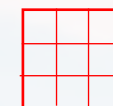
- convolution
- training the convolution filter

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

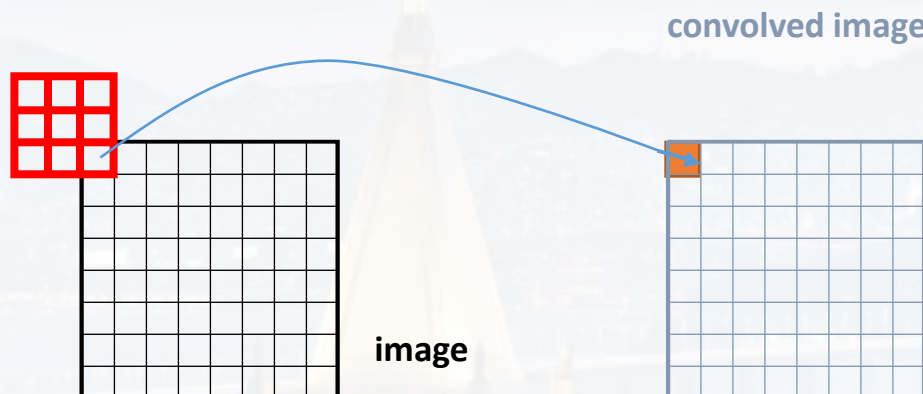
image f and filter g



image



filter
(aka kernel)



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



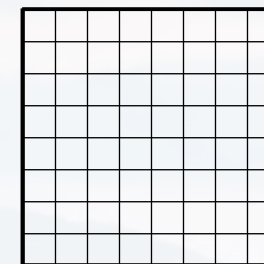


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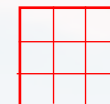
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image \mathbf{f} and filter \mathbf{g}

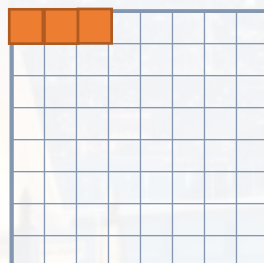
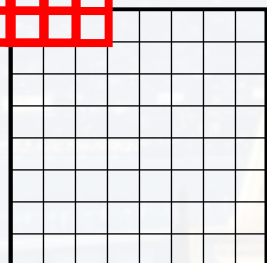
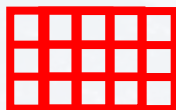


image

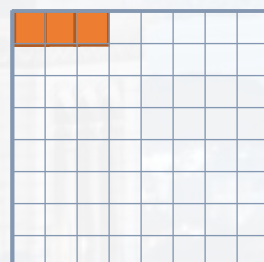
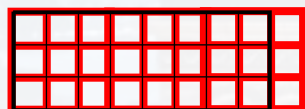


filter
(aka kernel)

different techniques:



padding = 2; stride length = 1



padding = 0; stride length = 3

N: number of rows/columns

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

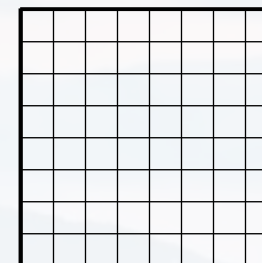


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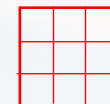
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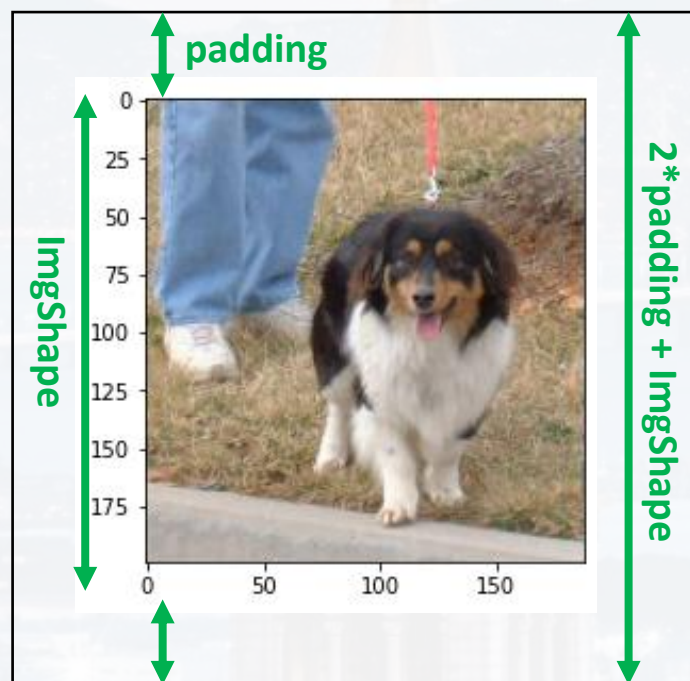
image \mathbf{f} and filter \mathbf{g}



image



filter
(aka kernel)

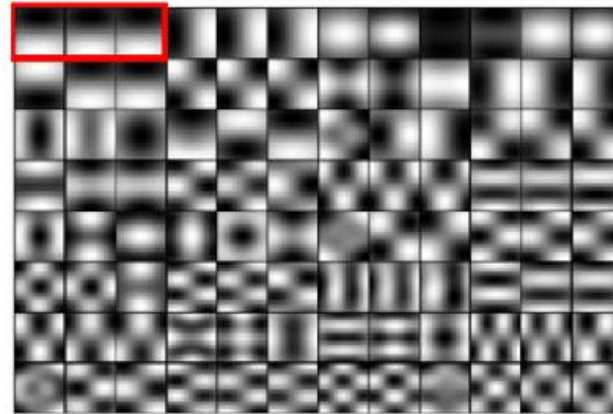


N: number of rows/columns

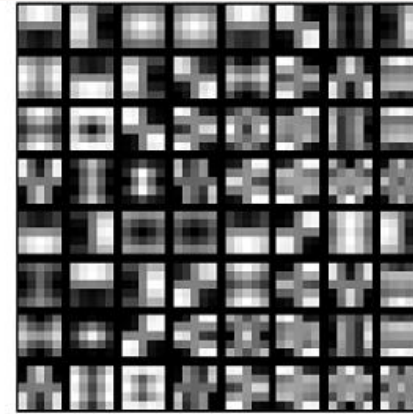
$$N_{out} = \frac{(N_{in} - N_{filt} + 2 * padding)}{stride\ length} + 1$$



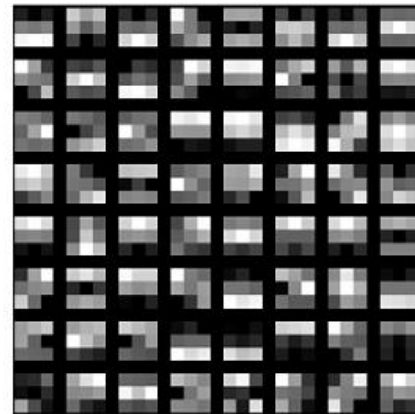
filters:



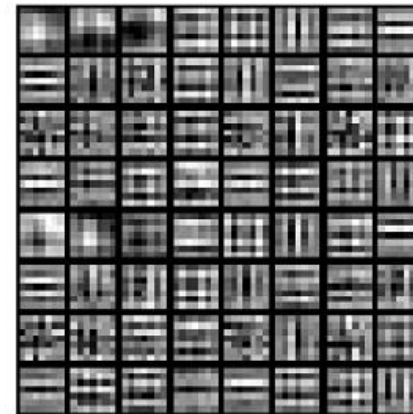
(a)



(b)



(c)



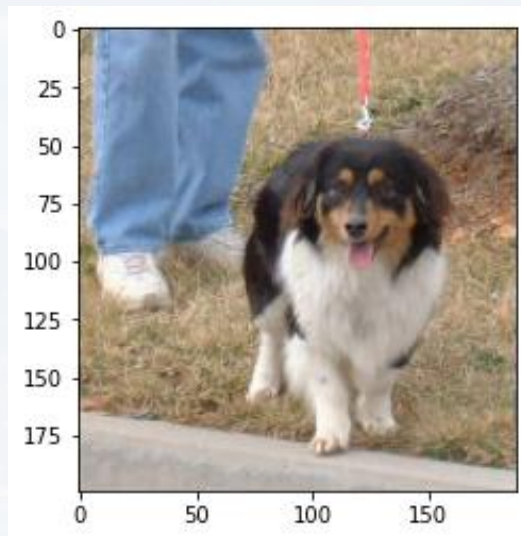
(d)

DOI:10.1016/j.actbio.2017.09.025

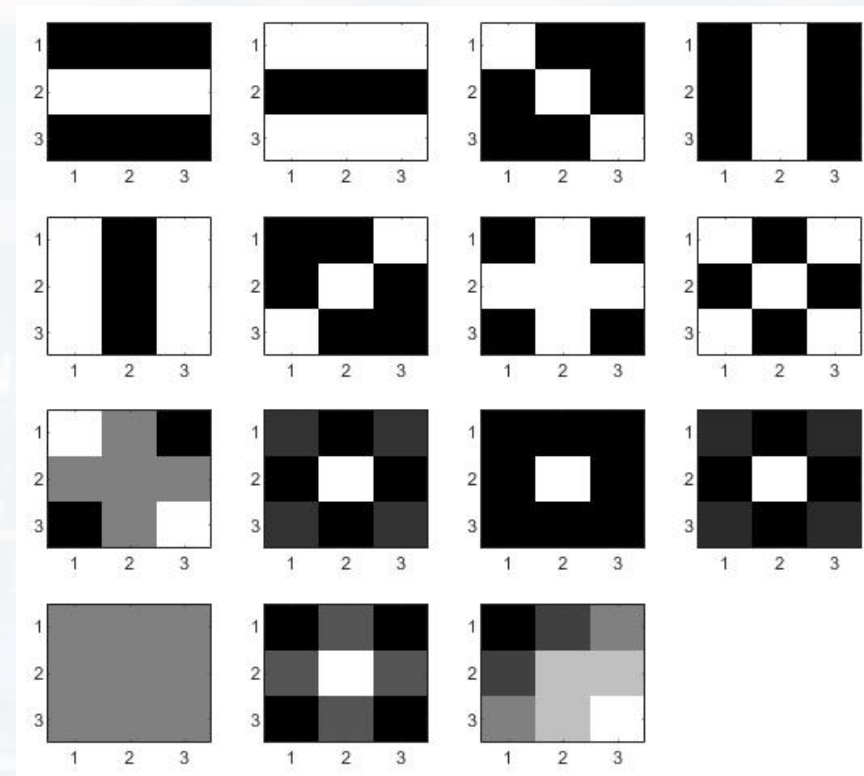


see `Convolution.ipynb` for visualizing the impact of different convolution filter on the image

image

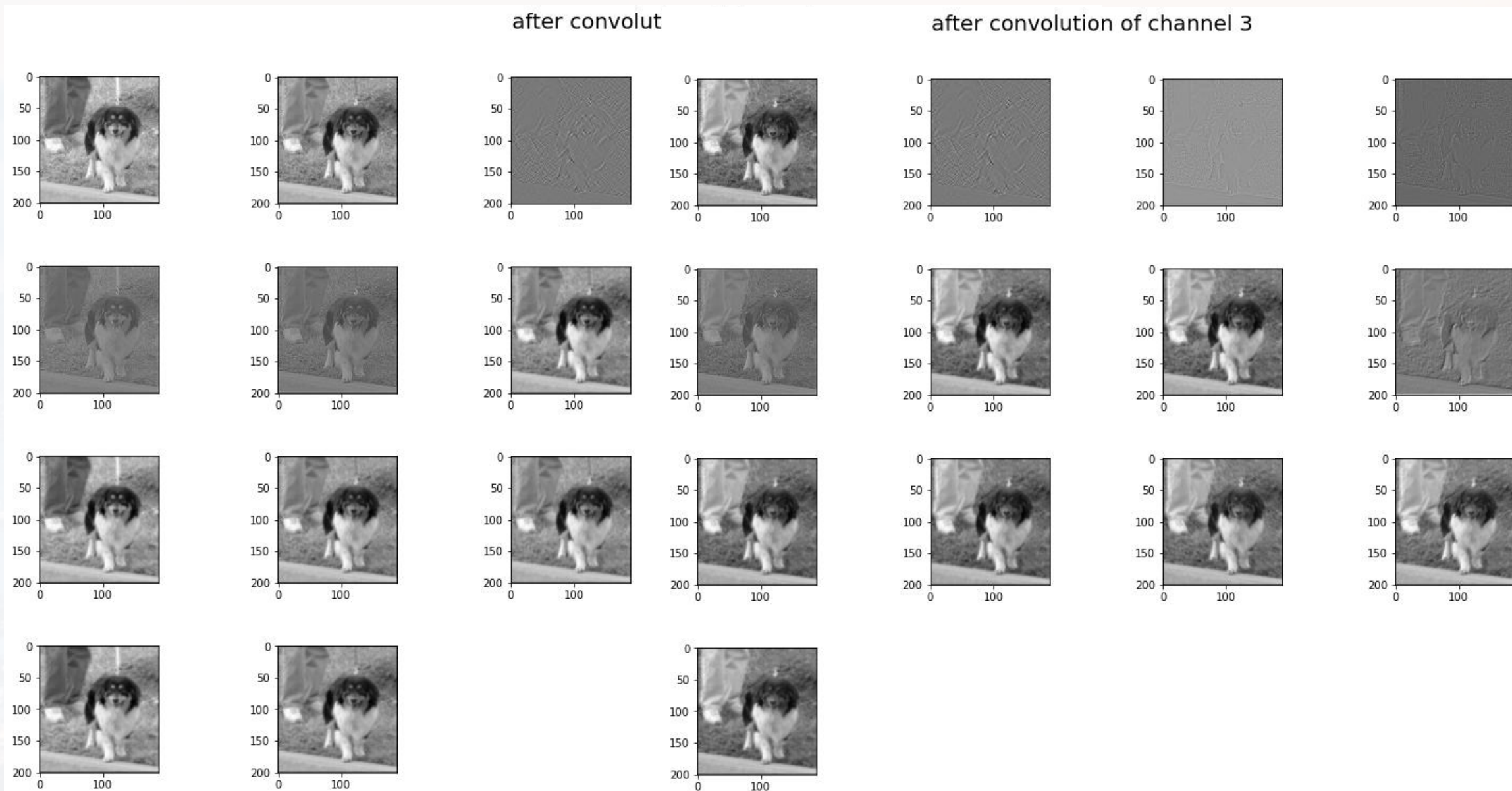


filter



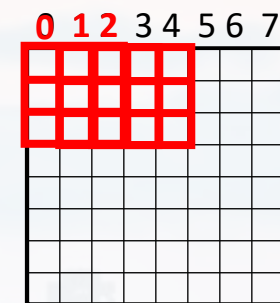


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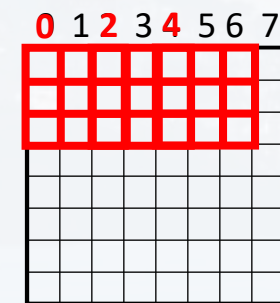




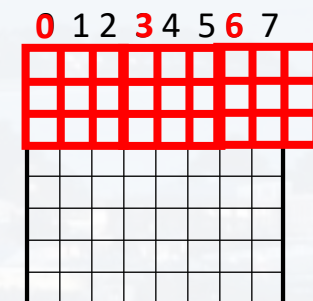
```
def ConvSelfMade(*Image, K, padding = 0, stride = 1):  
    ...  
  
    for c in range(numChans):# loop over channels  
        for y in range(yOutput):# loop over y axis of output  
            for x in range(xOutput):# loop over x axis of output  
  
                # finding corners of the current "slice"  
                y_start = y*stride  
                y_end   = y*stride + yK  
                x_start = x*stride  
                x_end   = x*stride + xK  
  
                #selecting the current part of the image  
                current_slice = imagePadded[x_start:x_end,\  
                                             y_start:y_end, c]  
  
                #the actual convolution part  
                s              = np.multiply(current_slice, K)  
                output[x,y,c] = np.sum(s)
```



stride = 1



stride = 2

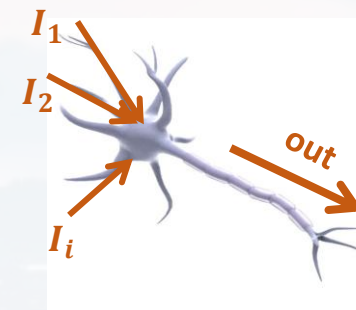


stride = 3



- 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

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



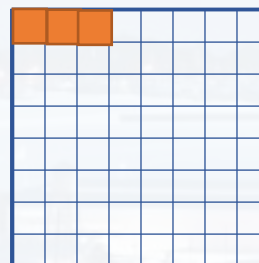
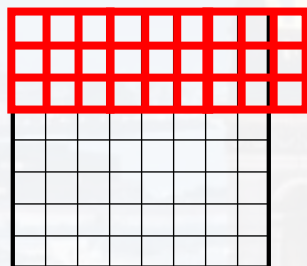
$$net = \sum_i I_i \cdot w_i + b$$

inputs are pixel values

kernel weights

$$\sum_i I_i \mathbf{w}_i + b$$

can be interpreted as a neuron!



i. e. a filter of shape $N \times N$
has $N^2 + 1$ learnables (N^2 weights + bias)



```
0.40 cat
0.32 frog
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CNN Architectures

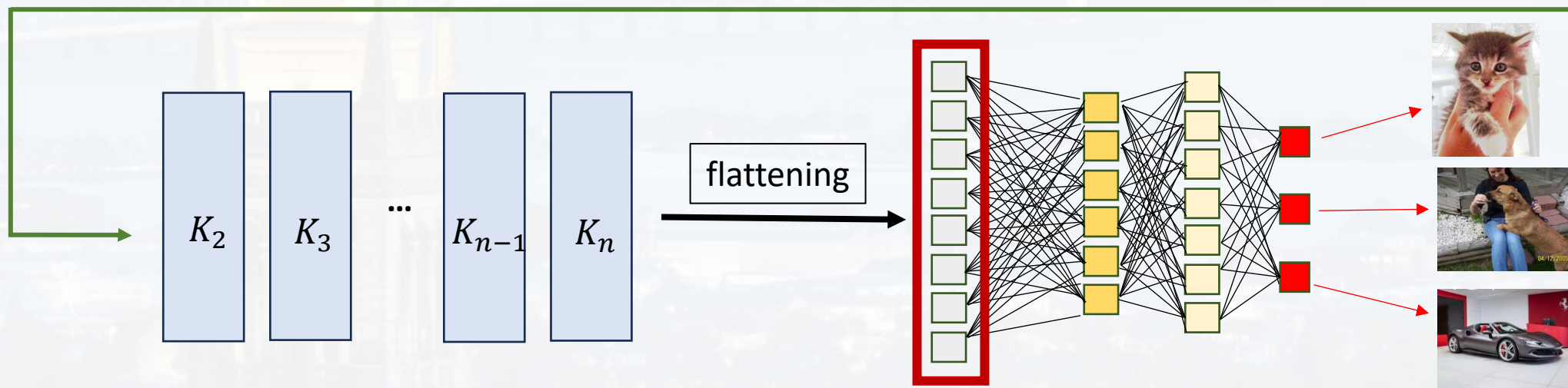
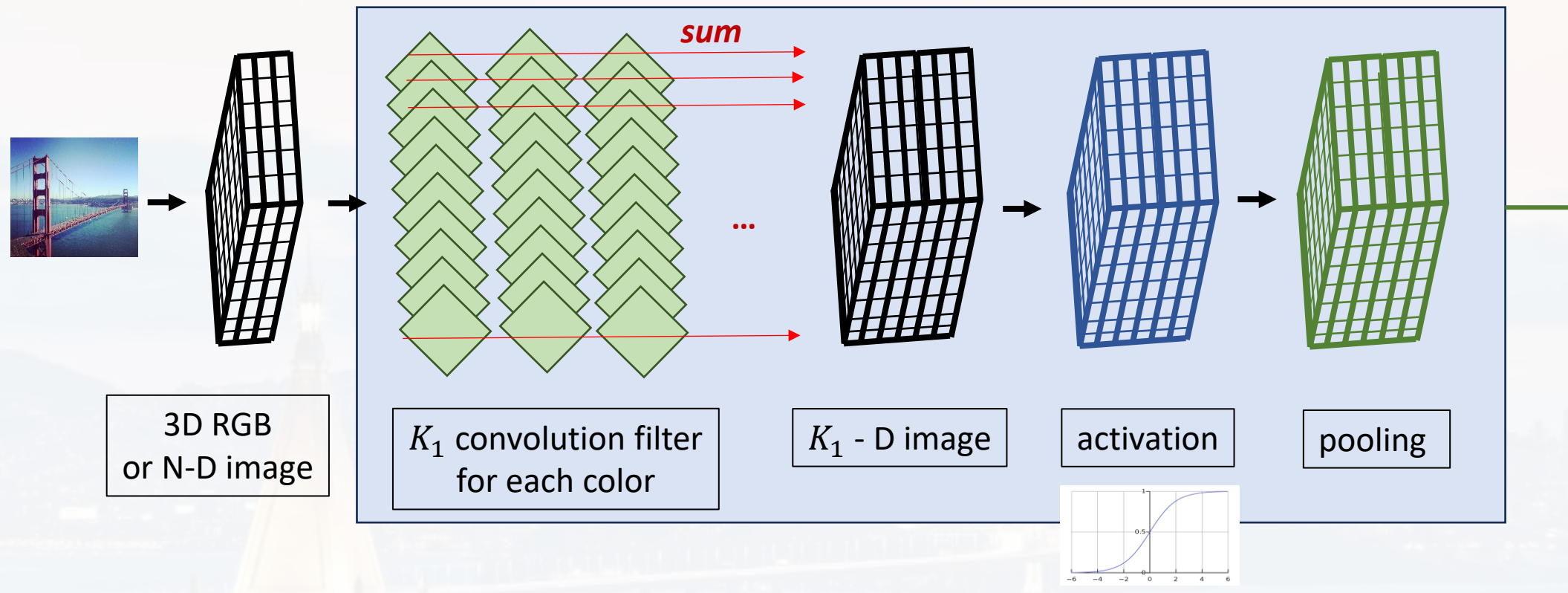
Data Preparation & Training

Example

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- Segmentation



classification





classification pooling:

there are three different main pooling methods

→ **average pool:**

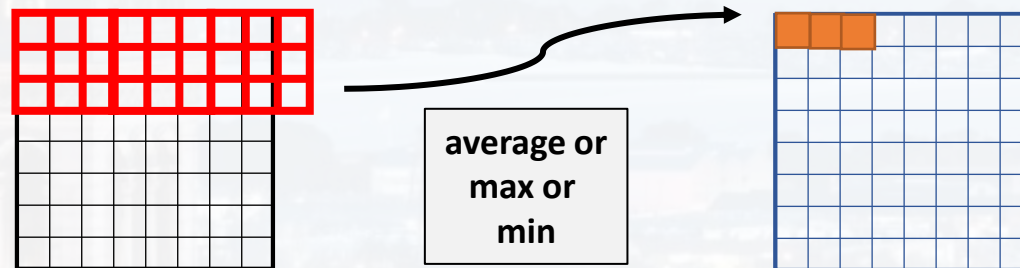
blurs the image, reduces edges
(not what we want here)

→ **max pool:**

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

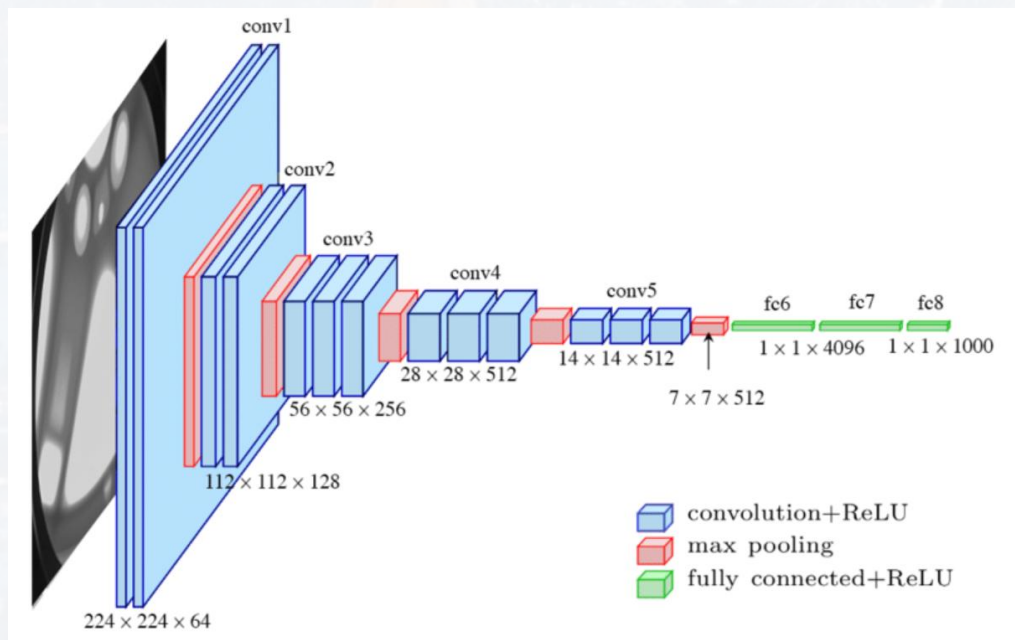
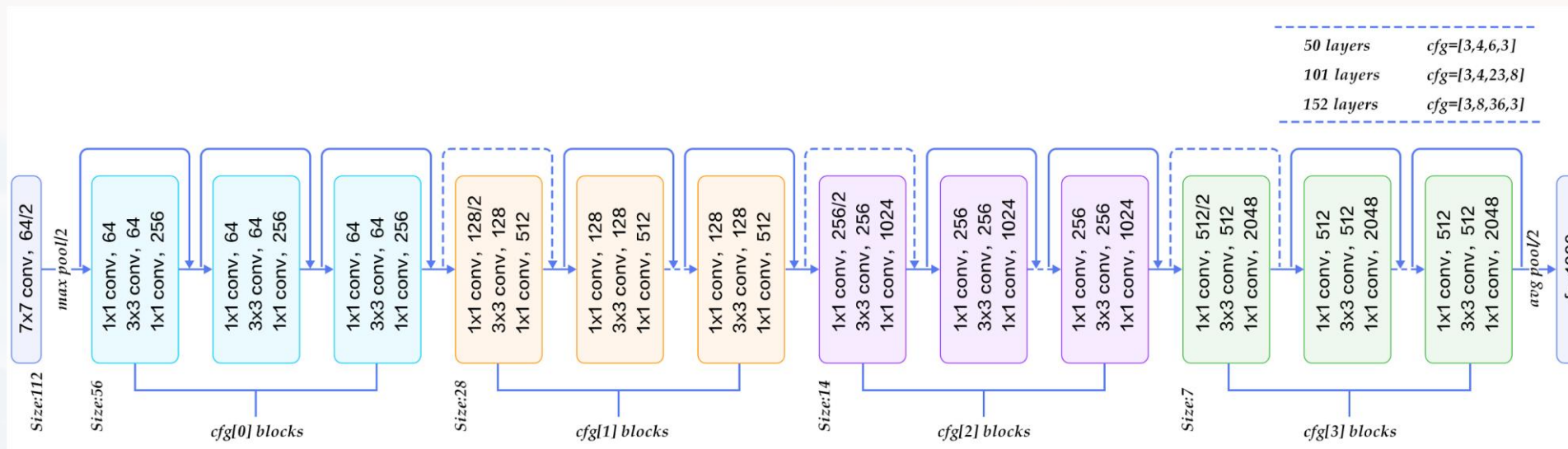
→ **min pool:**

does the opposite of max pool





classification



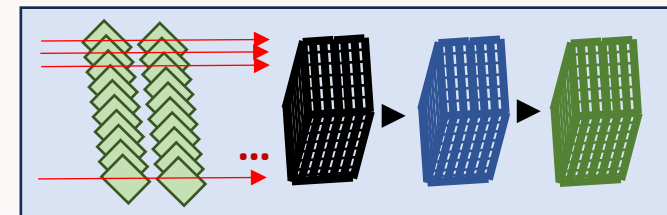
convolution process down-samples the image

- network focuses on important features
- reduces computational cost

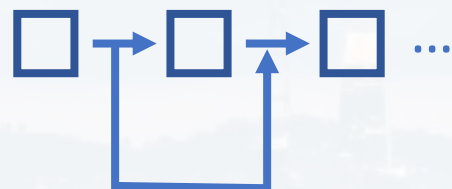


classification

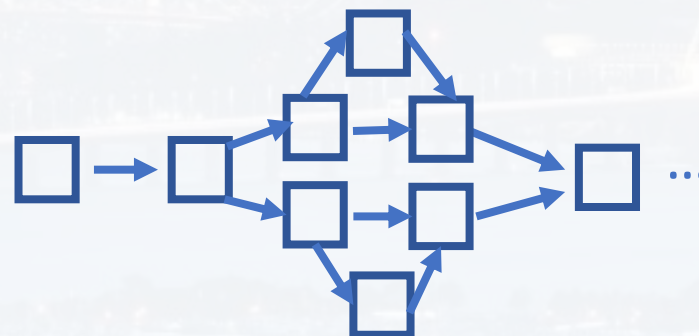
sequential CNNs



ResidualNet



Inception Net



many others...



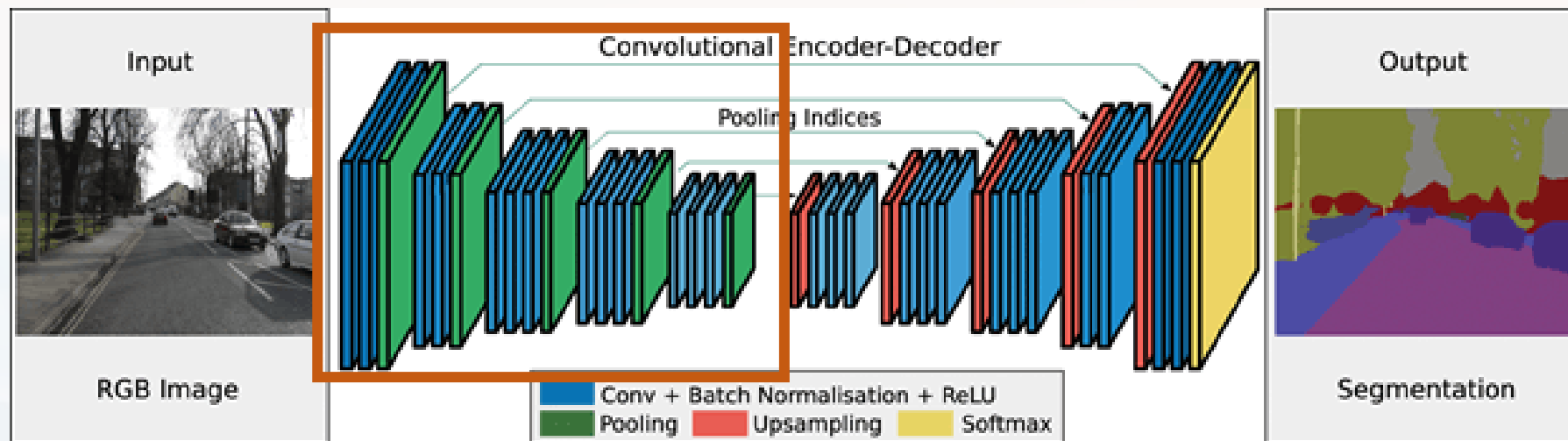
classification

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

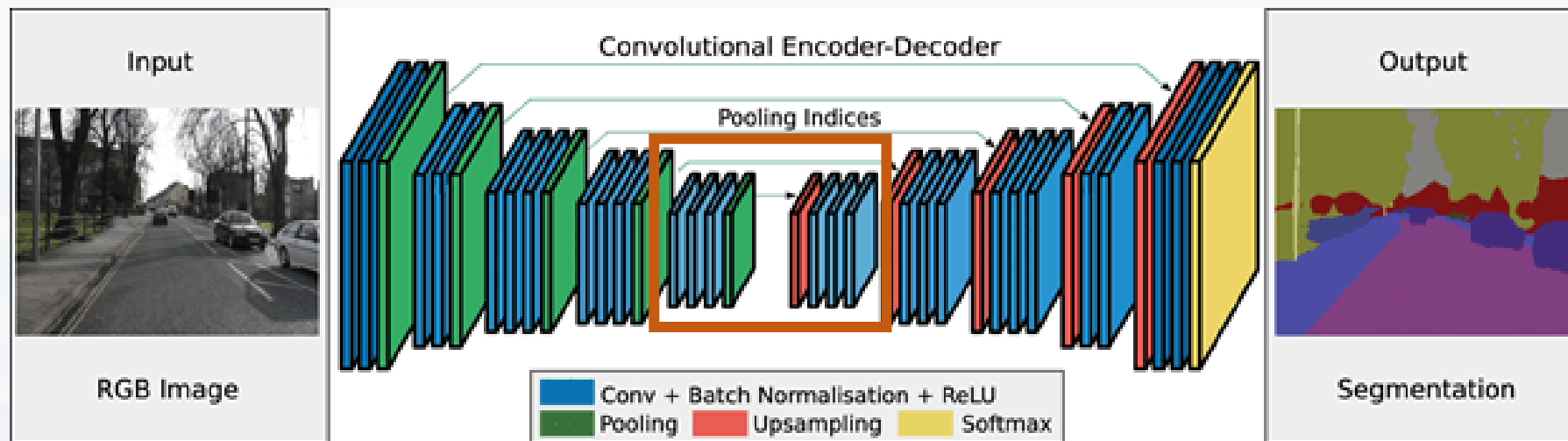


Vijay Badrinarayanan et. al 2017 "SegNet: A Deep Convolutional Encoder-Decoder Architecture for Image Segmentation"

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



segmentation

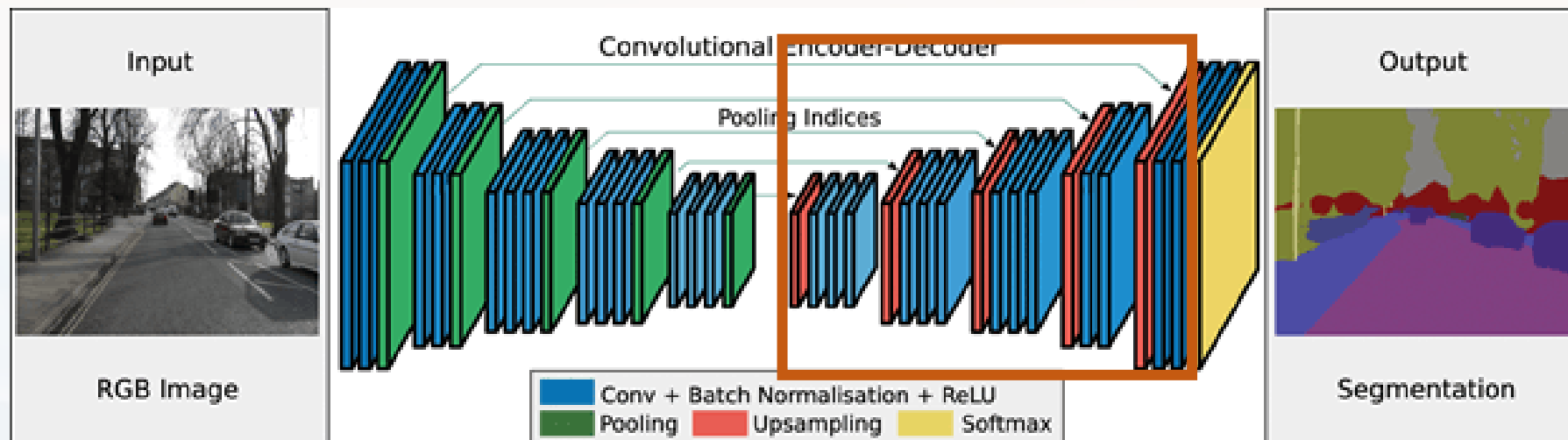


Vijay Badrinarayanan et. al 2017 "SegNet: A Deep Convolutional Encoder-Decoder Architecture for Image Segmentation"

- 1) down-sampling as before (= **encoder**)
- 2) down to bottle neck



segmentation

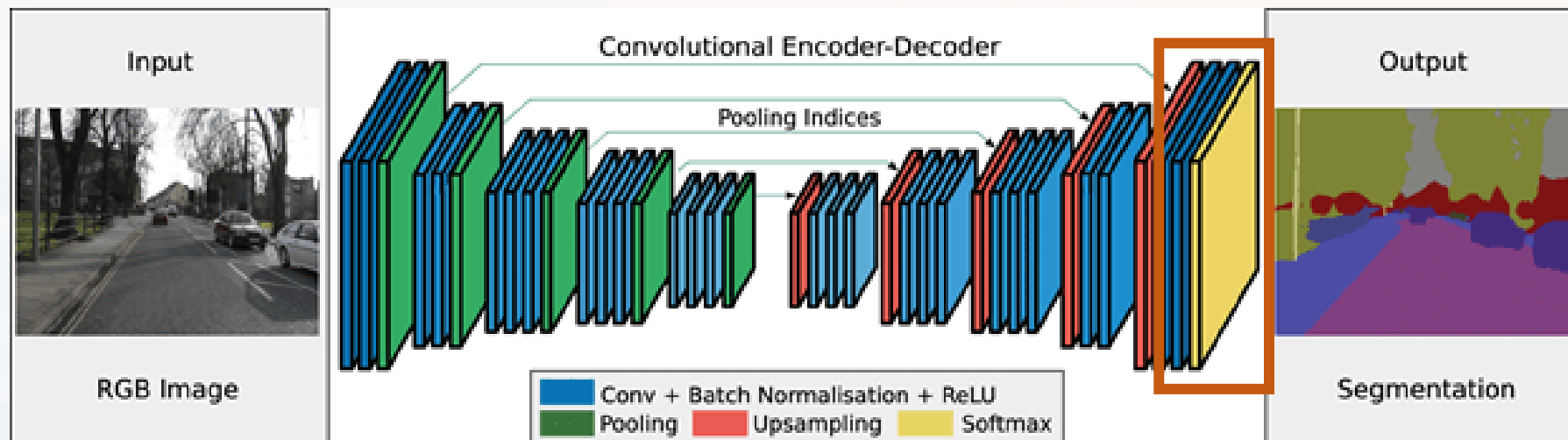


Vijay Badrinarayanan et. al 2017 "SegNet: A Deep Convolutional Encoder-Decoder Architecture for Image Segmentation"

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



segmentation

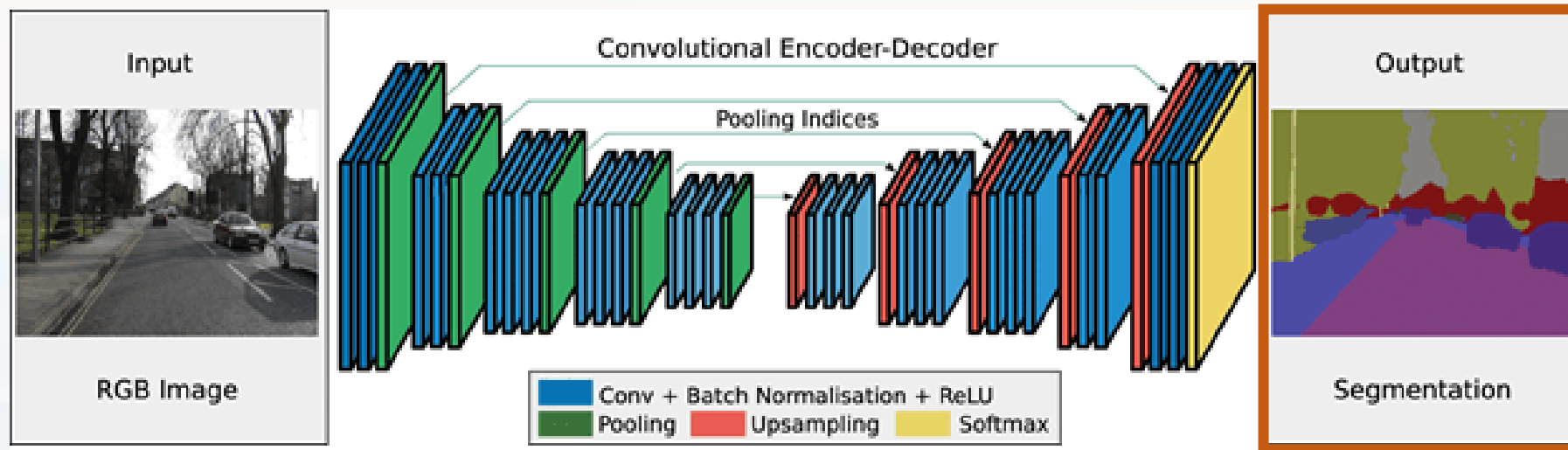


Vijay Badrinarayanan et. al 2017 "SegNet: A Deep Convolutional Encoder-Decoder Architecture for Image Segmentation"

- 1) down-sampling as before (= **encoder**)
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- 4) softmax, in order to turn output of last layer into probabilities



segmentation

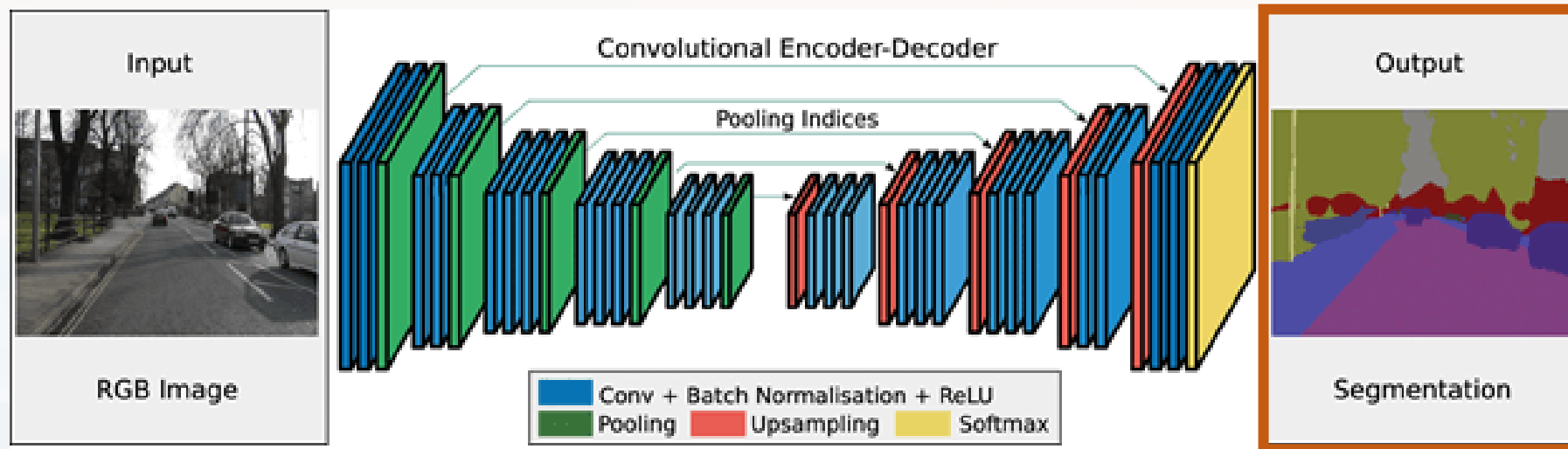


Vijay Badrinarayanan et. al 2017 "SegNet: A Deep Convolutional Encoder-Decoder Architecture for Image Segmentation"

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



segmentation



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

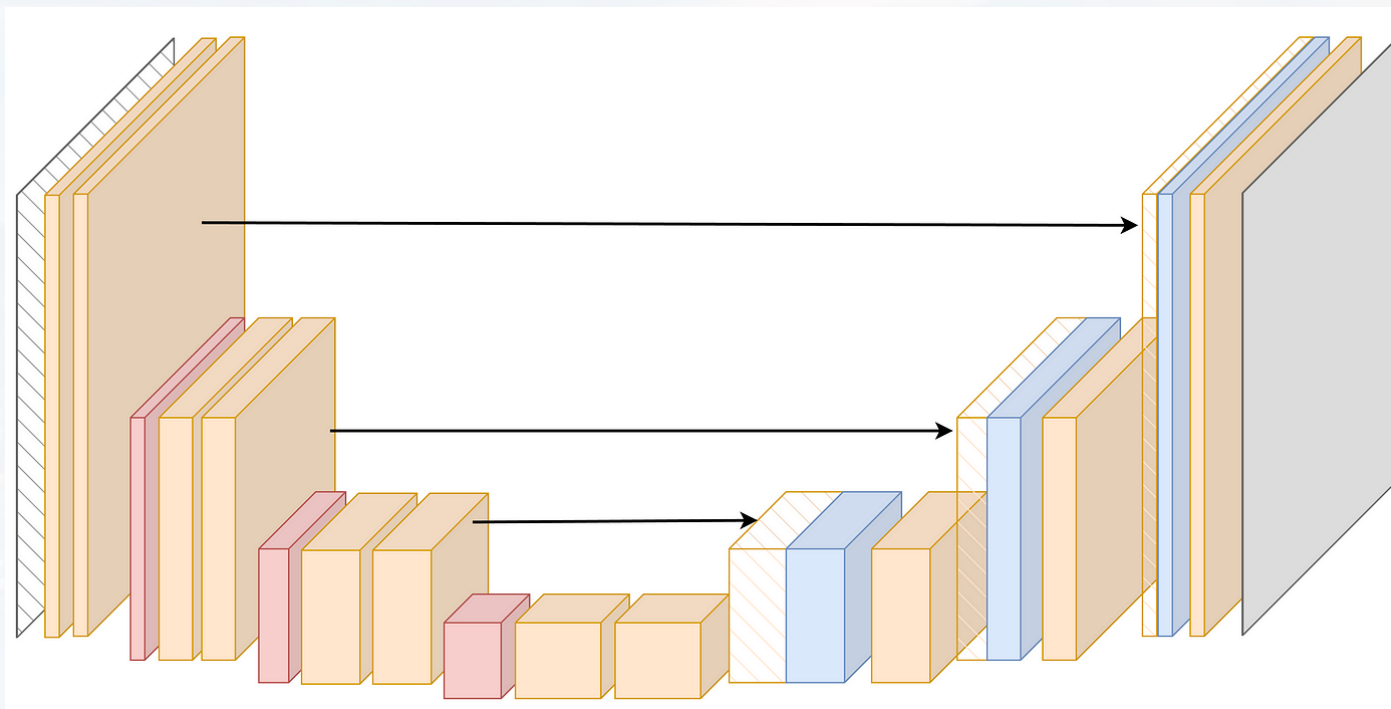
depending on the architecture, the decoder has **different learning mechanisms**

- 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>

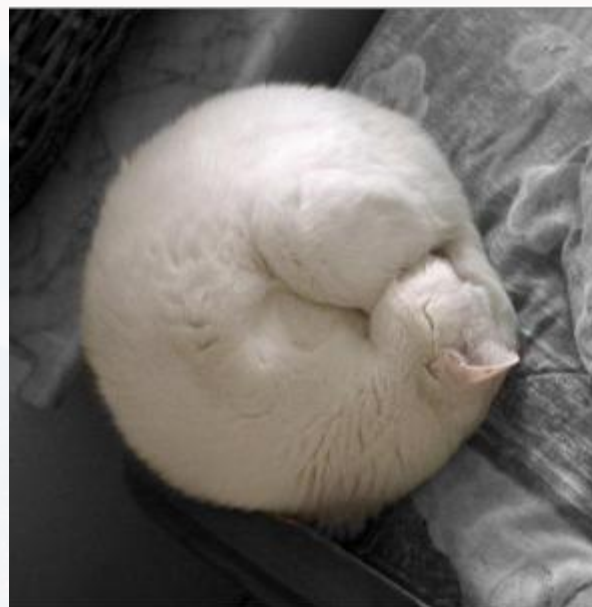


segmentation

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'



```
0.40 cat
0.32 frog
0.16 bird
0.06 ship
0.03 dog
```

Outline

The Problem

Convolution

CNN Architectures

Data Preparation & Training

Example

- LeNet numpy only
- LeNet TensorFlow
- sequences as images
- segmentation



data acquisition

1) classes should be **well balanced**

2) dataset should be **diverse**



example Cryo-EM:

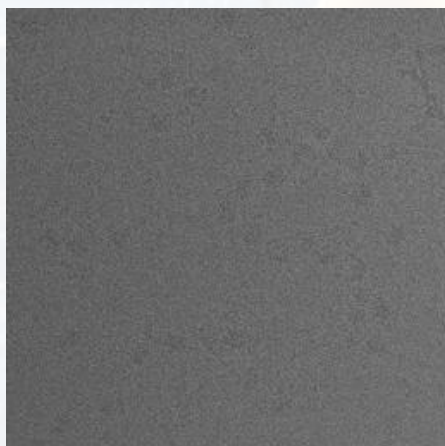
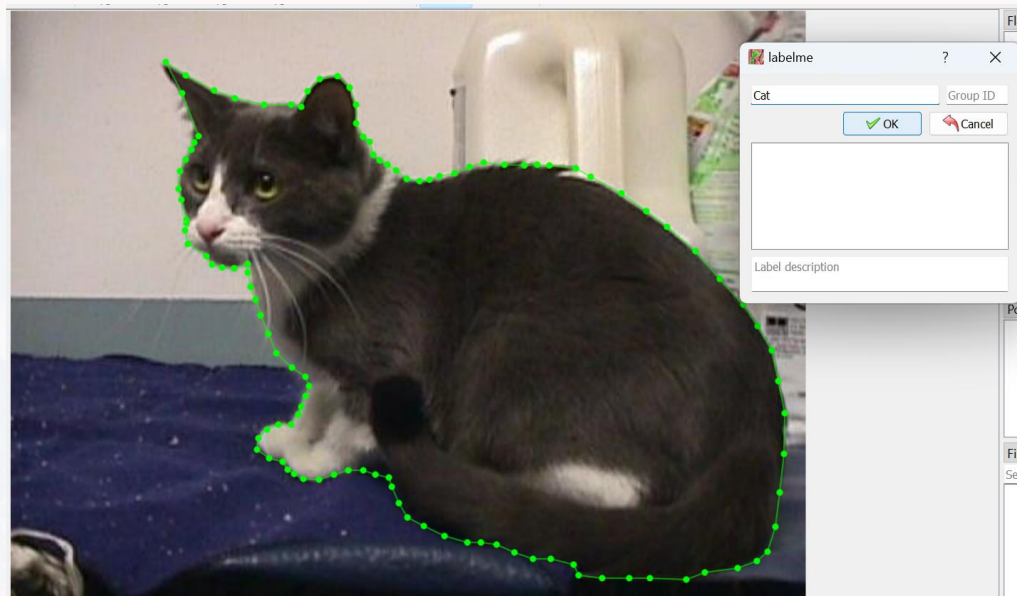
all grids (Cu, Au, ...)
all cameras
all grid manufacturers
all resolutions

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**

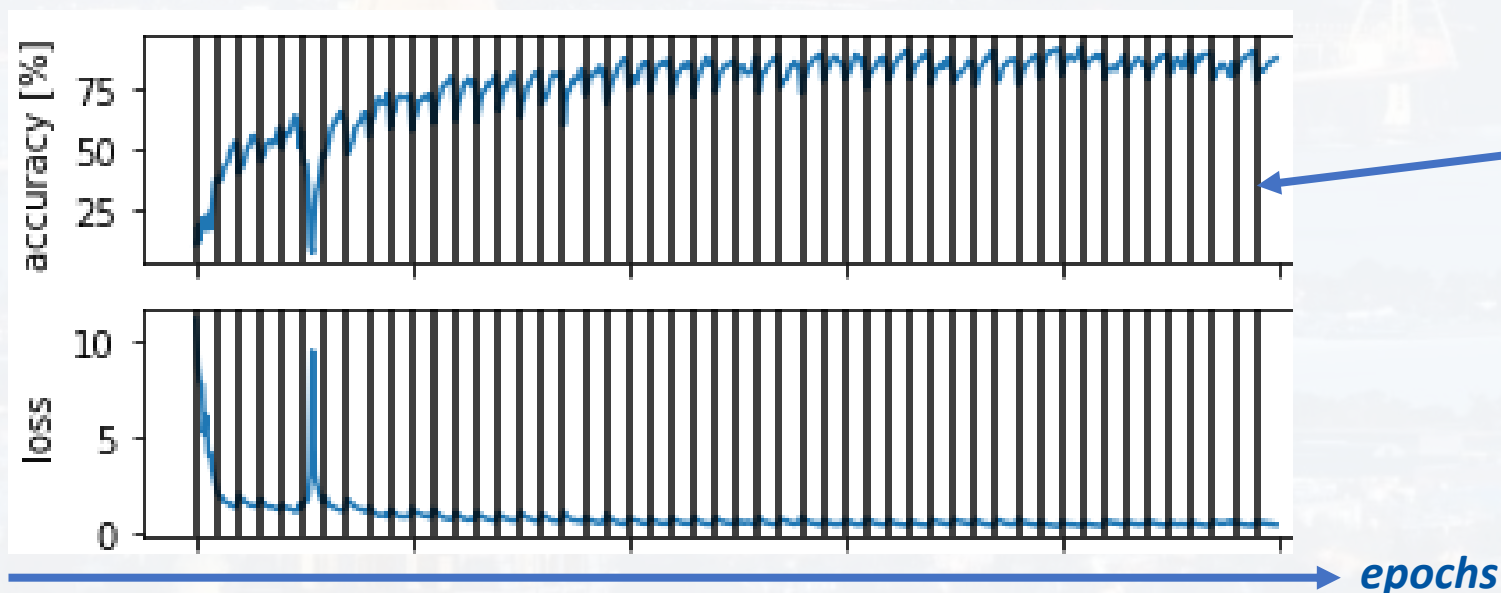
the training set is huge

→ loading only a few images at the time (**batches**)

→ the larger the batch, the better

→ run only **a few iterations** per batch (avoiding local minima)

→ check **training loss vs evaluation loss**



each line marks
a new batch



training

check out:

[Training MLP](#)

[Training CNN 2D](#)

[Training CNN 3D](#)



End of Part I

