Lecture 09:

Convolutional Neural Networks (CNN)



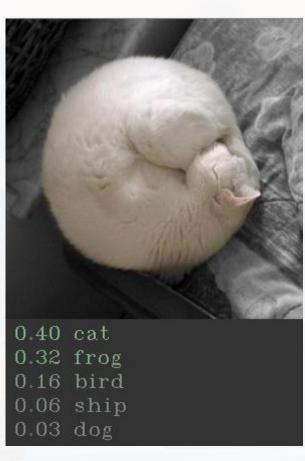
Markus Hohle
University California, Berkeley

Machine Learning Algorithms
MSSE 277B, 3 Units
Fall 2024



Berkeley Machine Learning Algorithms:





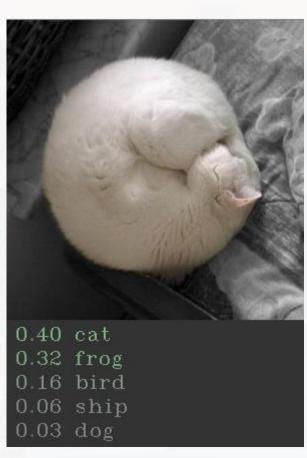
Outline

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



Berkeley Machine Learning Algorithms:



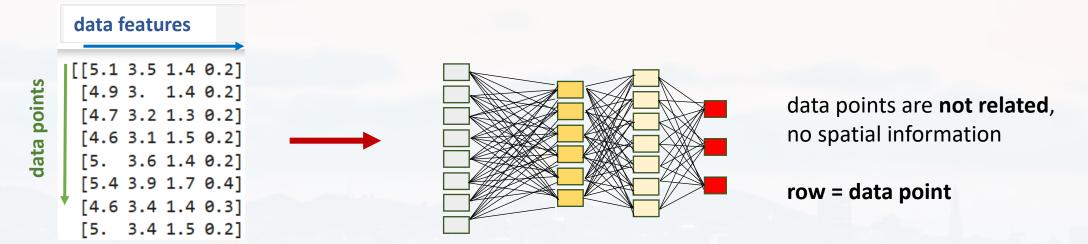


<u>Outline</u>

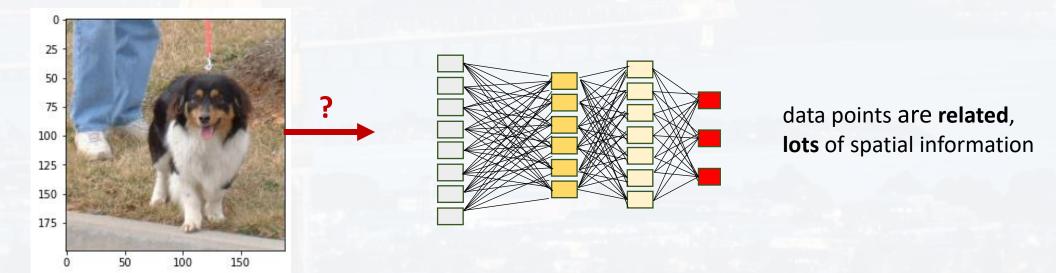
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so far:



now:

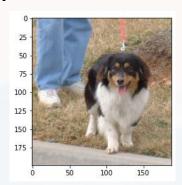


so far: now:

data features

[[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]

row = data point



matrix = data point

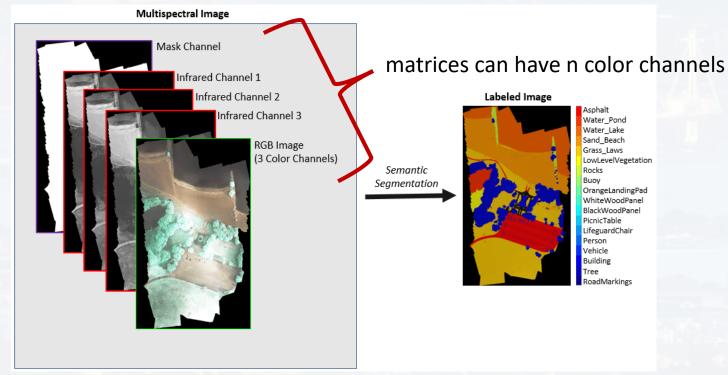
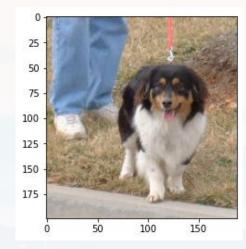


image curtesy: Mathworks



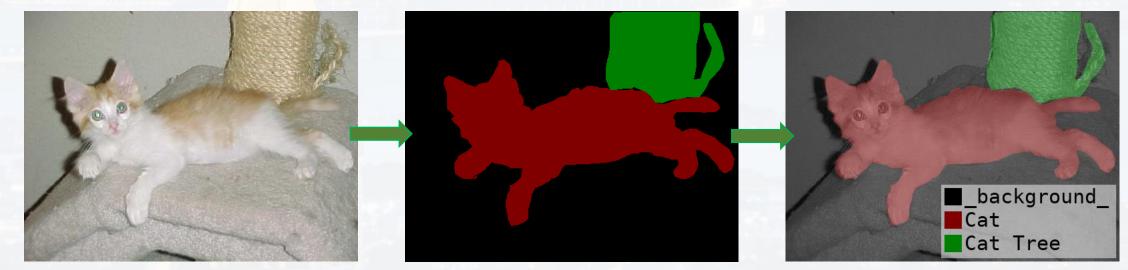
classification:

between different images



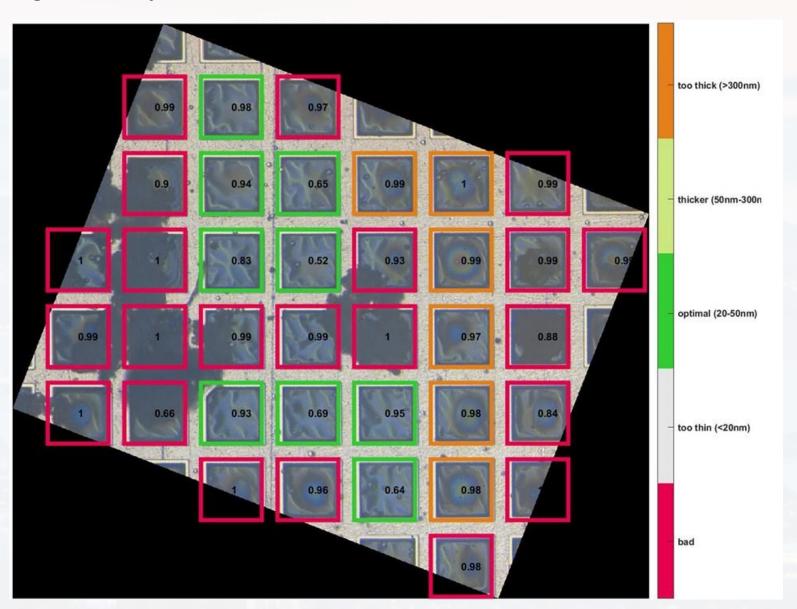


different pixel within images aka segmentation



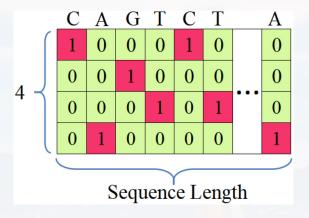


segmentation for classification

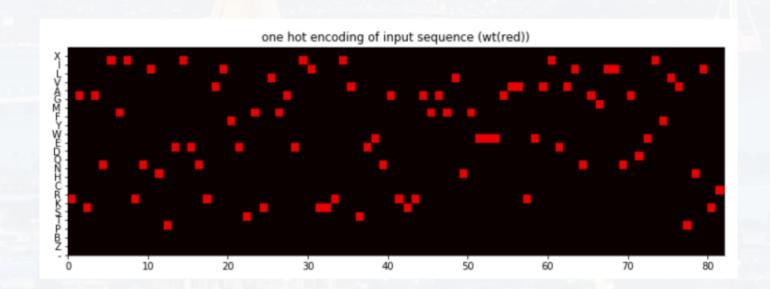




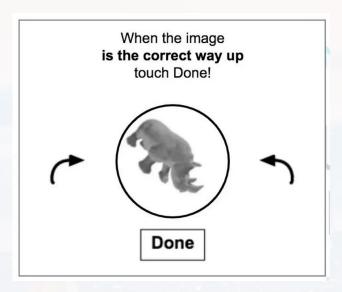
motif finding / sequence analysis



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

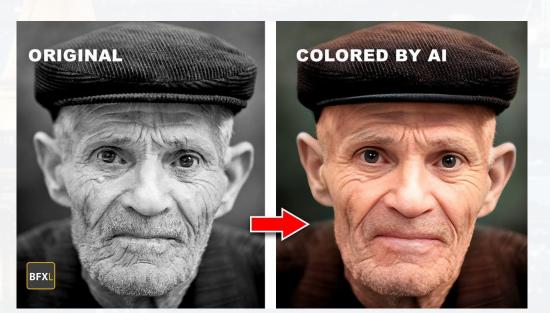


regression:



turning images the right way

part of GenAl:

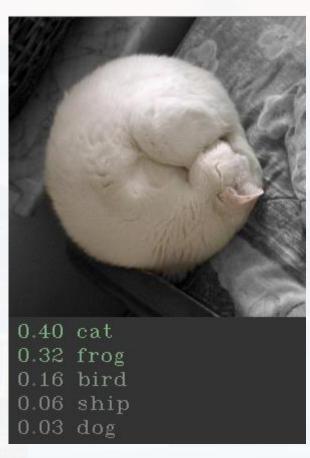


source: TopviewAl



Berkeley Machine Learning Algorithms:





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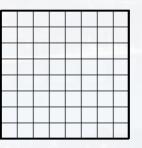
goal:

- maintaining the spatial information
- learning which features are important

- → convolution
- → training the convolution filter

What is convolution?

$$(f * g)(x) \coloneqq \int_{\mathbb{R}^n} f(\zeta) g(x - \zeta) d\zeta$$
 image f and filter g

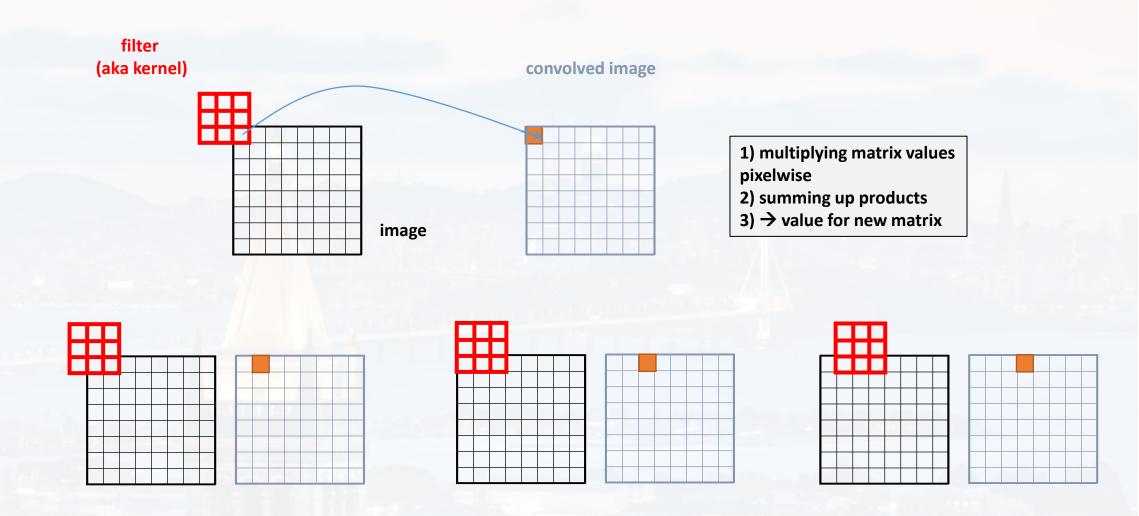




image

filter (aka kernel)

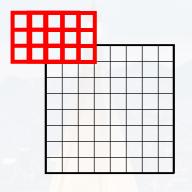
<u>What is convolution?</u> image ${\it f}$ and filter ${\it g}$

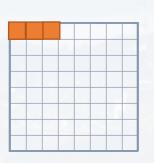


What is convolution?

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

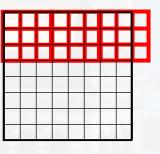
different techniques:





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

padding = 2; stride length = 1





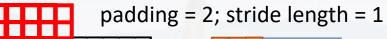
padding = 0; stride length = 3

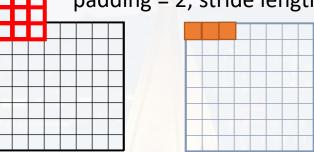


What is convolution?

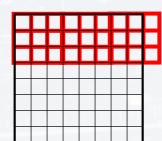
image **f** and filter **g**

different techniques:





padding = 0; stride length = 3





1) multiplying matrix values pixelwise

2) summing up products

3) → value for new matrix

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

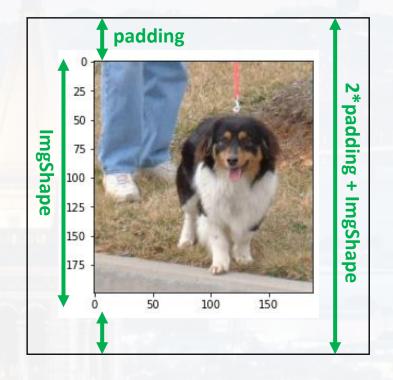
$$N_{out} = \frac{\left(N_{in} - N_{filt} + 2 * padding\right)}{stride\ length} + 1$$

What is convolution?

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

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

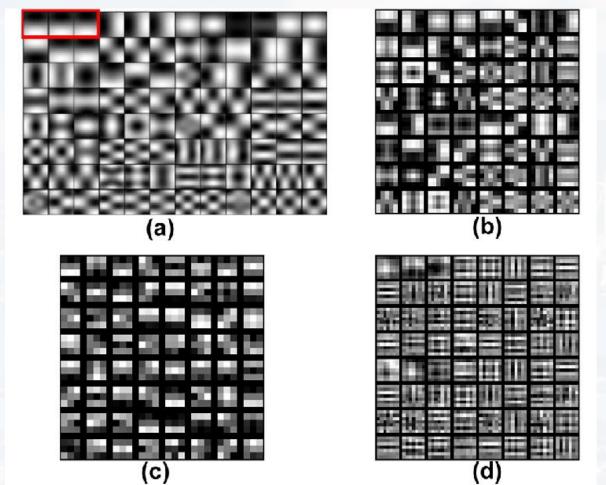
$$N_{out} = \frac{\left(N_{in} - N_{filt} + 2 * padding\right)}{stride\ length} + 1$$



What is convolution?

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

filters:



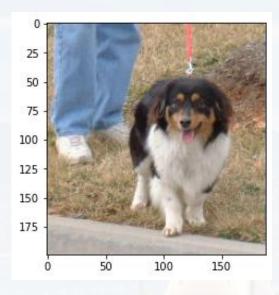
- 1) multiplying matrix values pixelwise
- 2) summing up products
- 3) → value for new matrix

DOI:10.1016/j.actbio.2017.09.025

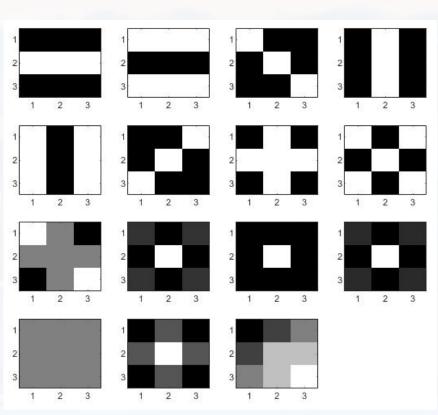


see Convolution.ipynb for the impact of different convolution filter on the image

image



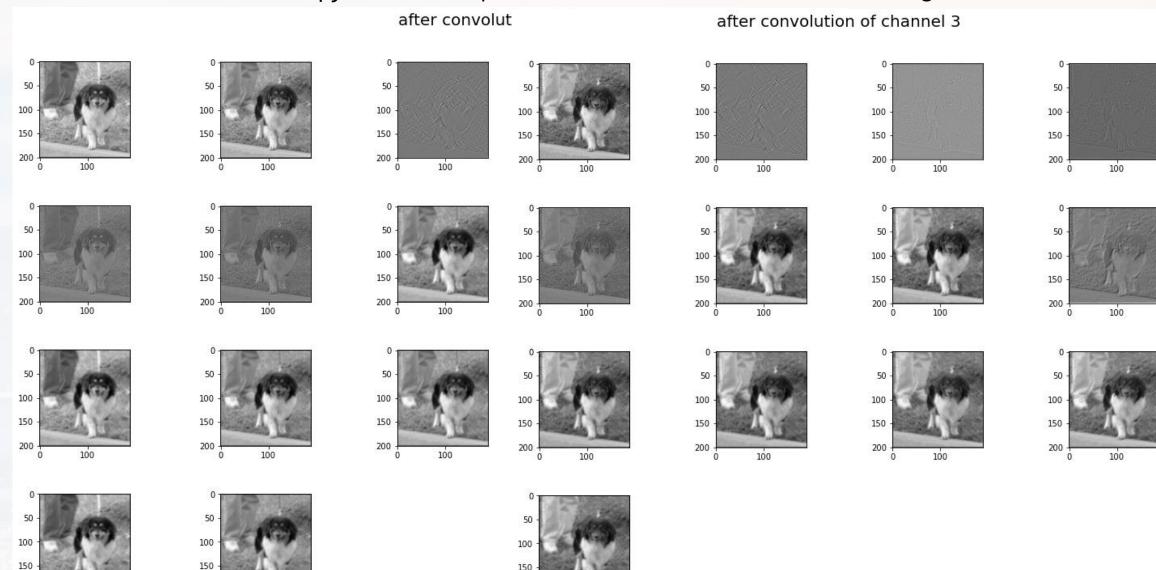
filter



200

Convolution

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

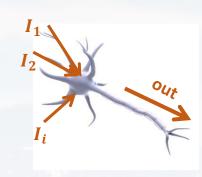




CNN:

- 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

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



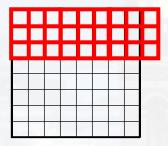
$$net = \sum_{i} I_i \cdot w_i + b$$

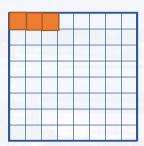
inputs are pixel values

kernel weights

$$\sum_{i} I_{i} \mathbf{w_{i}} + \mathbf{l}$$

can be interpreted as a neuron!







Berkeley Machine Learning Algorithms:

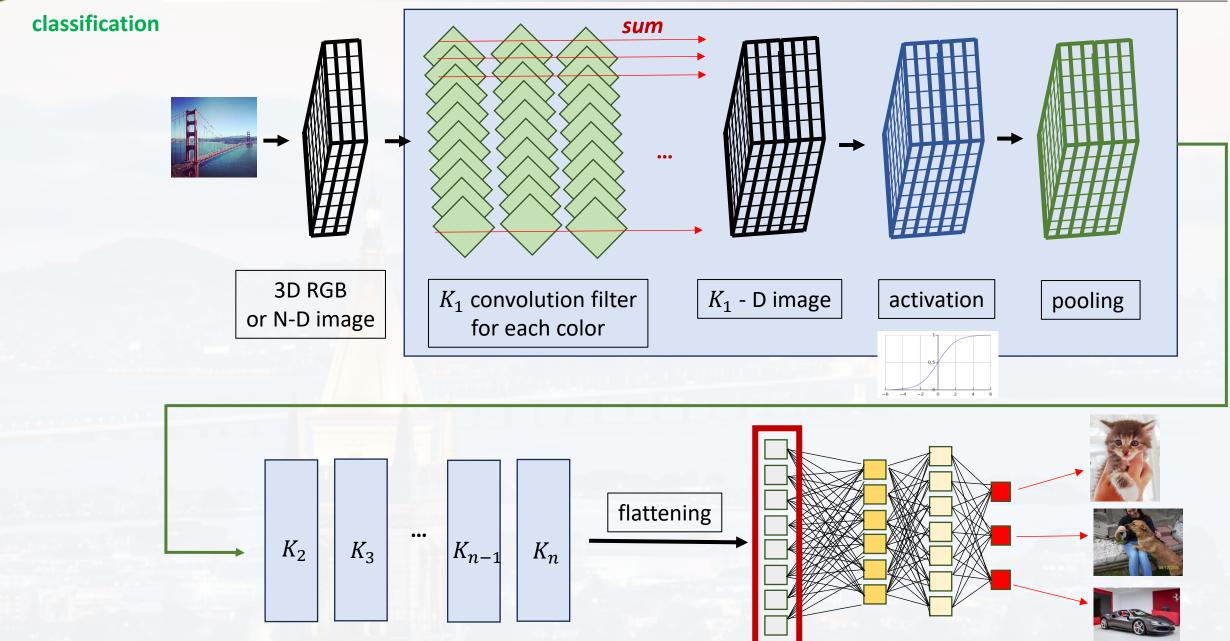




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classification pooling:

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

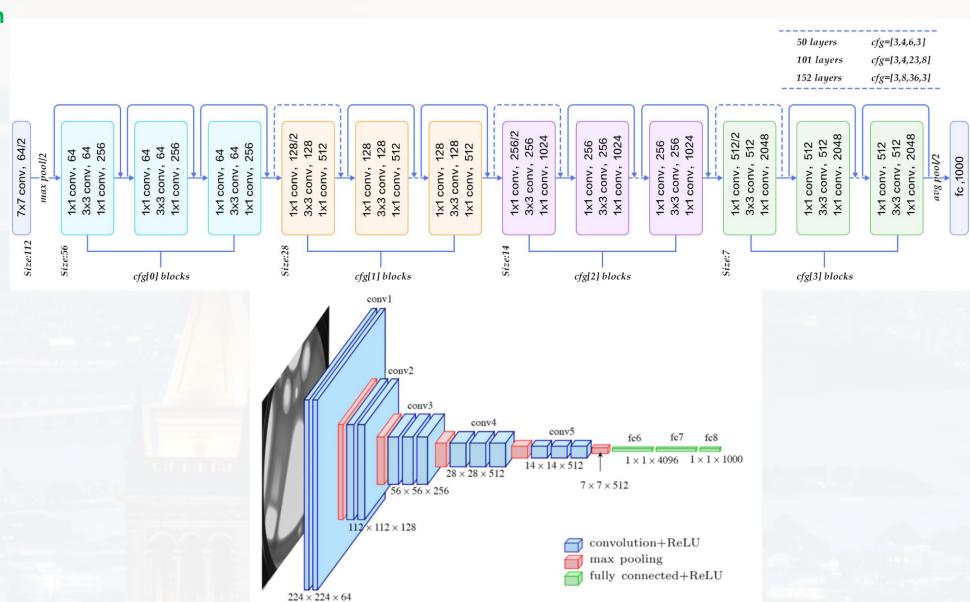
values are usually low) and enhances

brighter foreground objects (exactly what we need here)

→ min pool: does the opposite of max pool

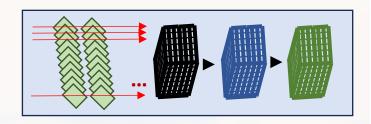


classification

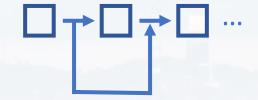


classification

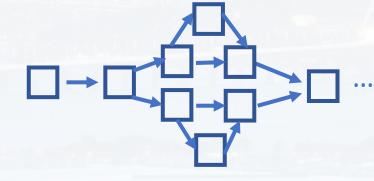
sequential CNNs \longrightarrow \longrightarrow \longrightarrow ...



Residual**Net**



Inception Net



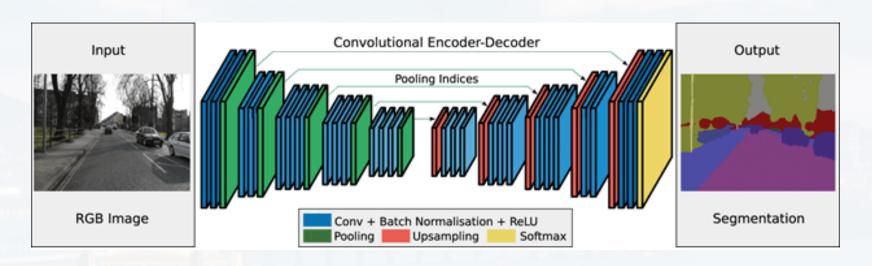
many others...

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

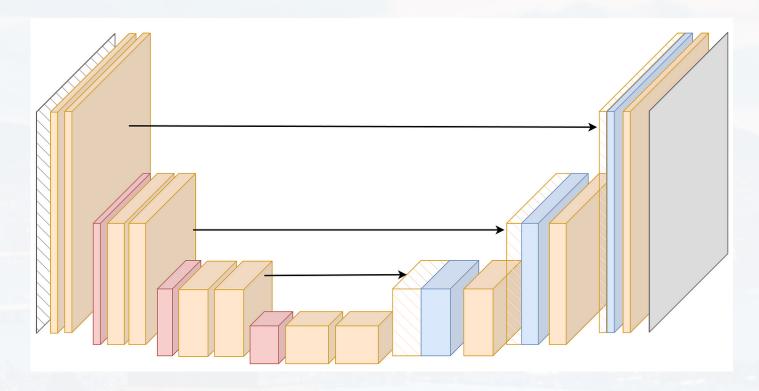
segmentation



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

segmentation

U-net segmentation CNN



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

segmentation

common pretrained segmentation CNNs

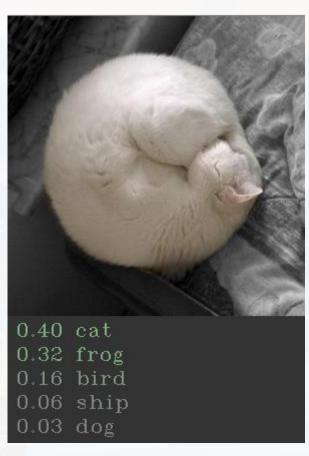
note: the input size is usually 5 – 10 times larger than compared to a classification CNN!

Туре	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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data acquisition

- 1) classes should be well balanced
- 2) dataset should be diverse





example Cryo-EM:

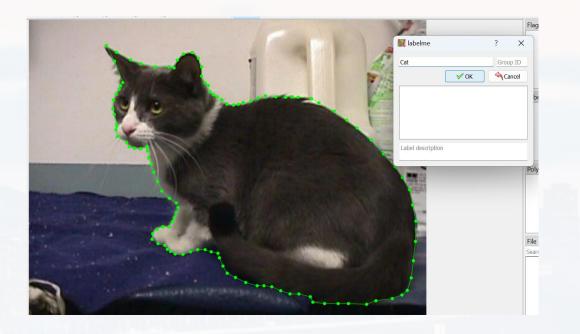
all grids (Cu, Au, ...)
all cameras
all grid manufacturers
all resolutions

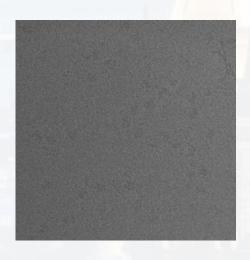
3) augmentation: blurred, skewed, fragmented, stretched, turned etc

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

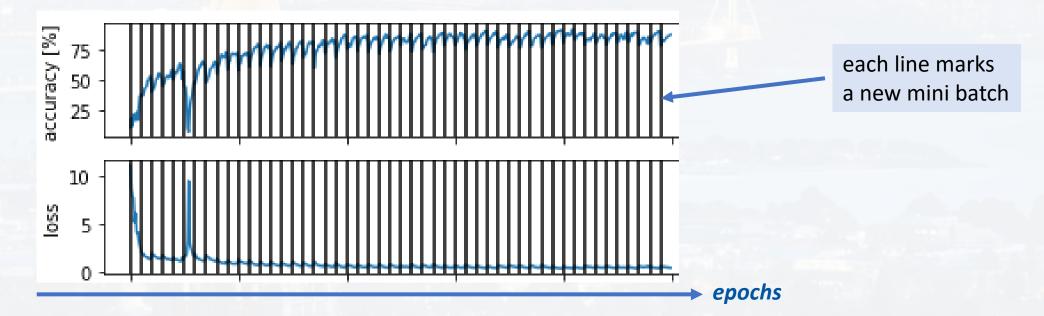
training

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

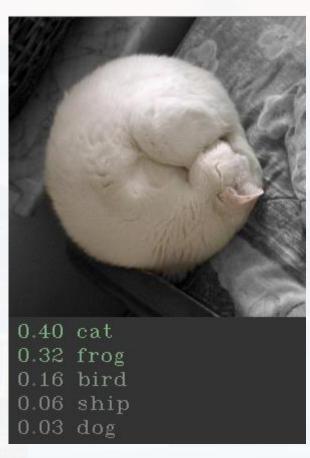
Training CNN 2D

Training CNN 3D



Berkeley Machine Learning Algorithms:



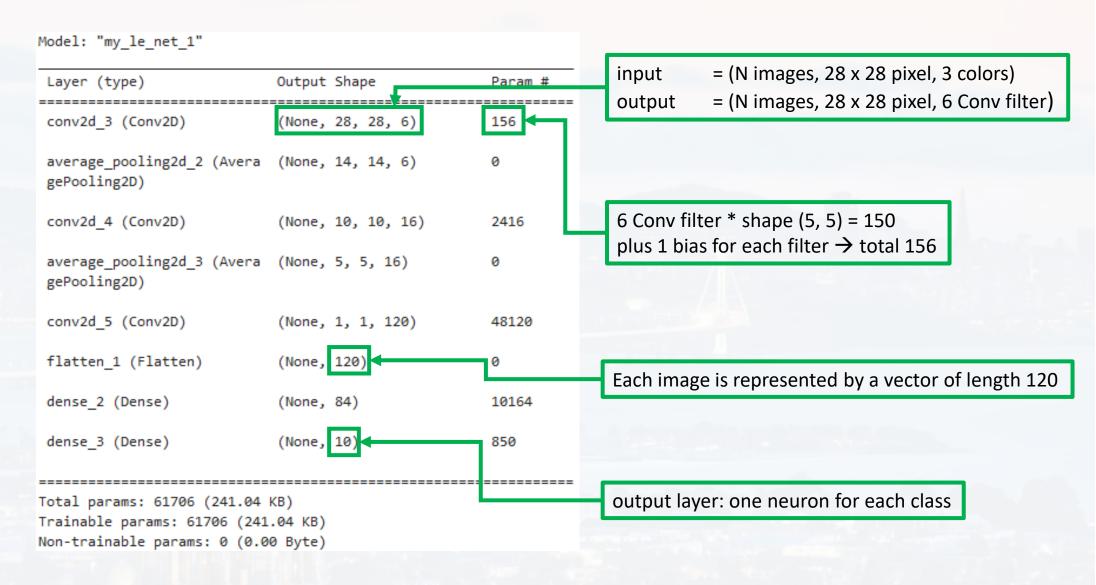


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constructing, running and testing LeNet → LeNet.ipynb



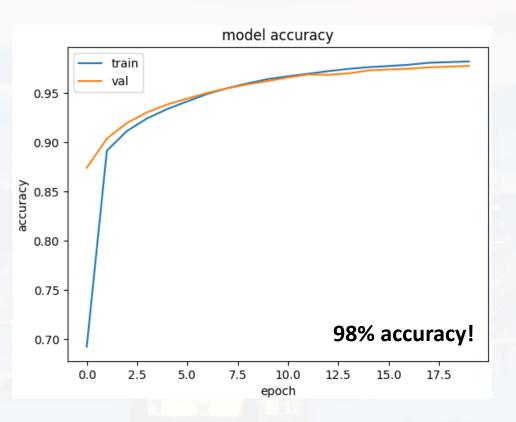
constructing, running and testing LeNet → LeNet.ipynb

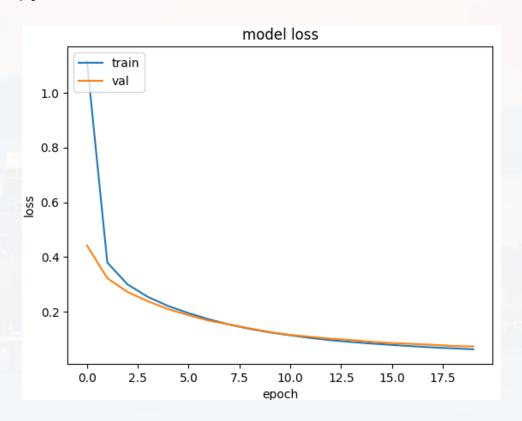
epoch: passing the entire dataset through the network

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



constructing, running and testing LeNet → LeNet.ipynb





training loss should \approx validation loss if validation loss \Rightarrow overfitting

- too many parameter
- too few images in batch
- too specific/unique batch)



constructing, running and testing LeNet → LeNet.ipynb

7, P = 1.0	7, P = 0.99	7, P = 1.0	5	8, P = 1.0	4, P = 1.0	0, P = 1.0
6, P = 10	4, P = 1.0	2 , P = 0.85	3	0, P = 1.0	5, P = 0.99	3 , P = 1.0
5, P = 1.0	5, P = 0.99	2, P = 0.98	1, P = 1.0	5, P = 0.99	8, P = 0.98	7, P = 1.0
6, P = 0.00	8, P = 1.0	7, P = 0.99	7, P = 1.0	1, P = 1.0	7, P = 0.74	8, P = 1.0
3, P = 0.97	6, P = 0.93	7, P = 0.99	1, P = 1.0	S, P = 0.91	3, P = 1.0	9, P = 1.0
3, P = 1.0	6, P = 3.0	4, P = 1.0	5, P = 1.0	5, P = 1.0	7, P = 1.0	9
4, P = 0.99	P	1, P = 1.0	5, P = 0.99	5, P = 1.0	5, P = 1.0	7, P = 0.99



Berkeley Machine Learning Algorithms:

Thank you for your attention!



