Introduction to High Performance Machine Learning

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Today's schedule

9:15 - 9:45		Introduction to deep learning
9:45 - 10:15	lab	Your first neural network
10:15 - 10:30		**Break**
10:30 - 11:00		Deep learning's knobs and dials
11:00 - 12:00	lab	Improving your network - hyperparameter tuning
12:00 - 13:00		**Lunch break**
13:00 - 13:30		Convolutional neural networks
13:30 - 14:30	lab	Your first convolutional neural network
14:30 - 14:45		**Break**
14:45 - 15:15		Regularisation and advanced techniques
15:15 - 16:15	lab	Improving neural networks
16:15 - 17:00		Open discussion: questions / hands-on

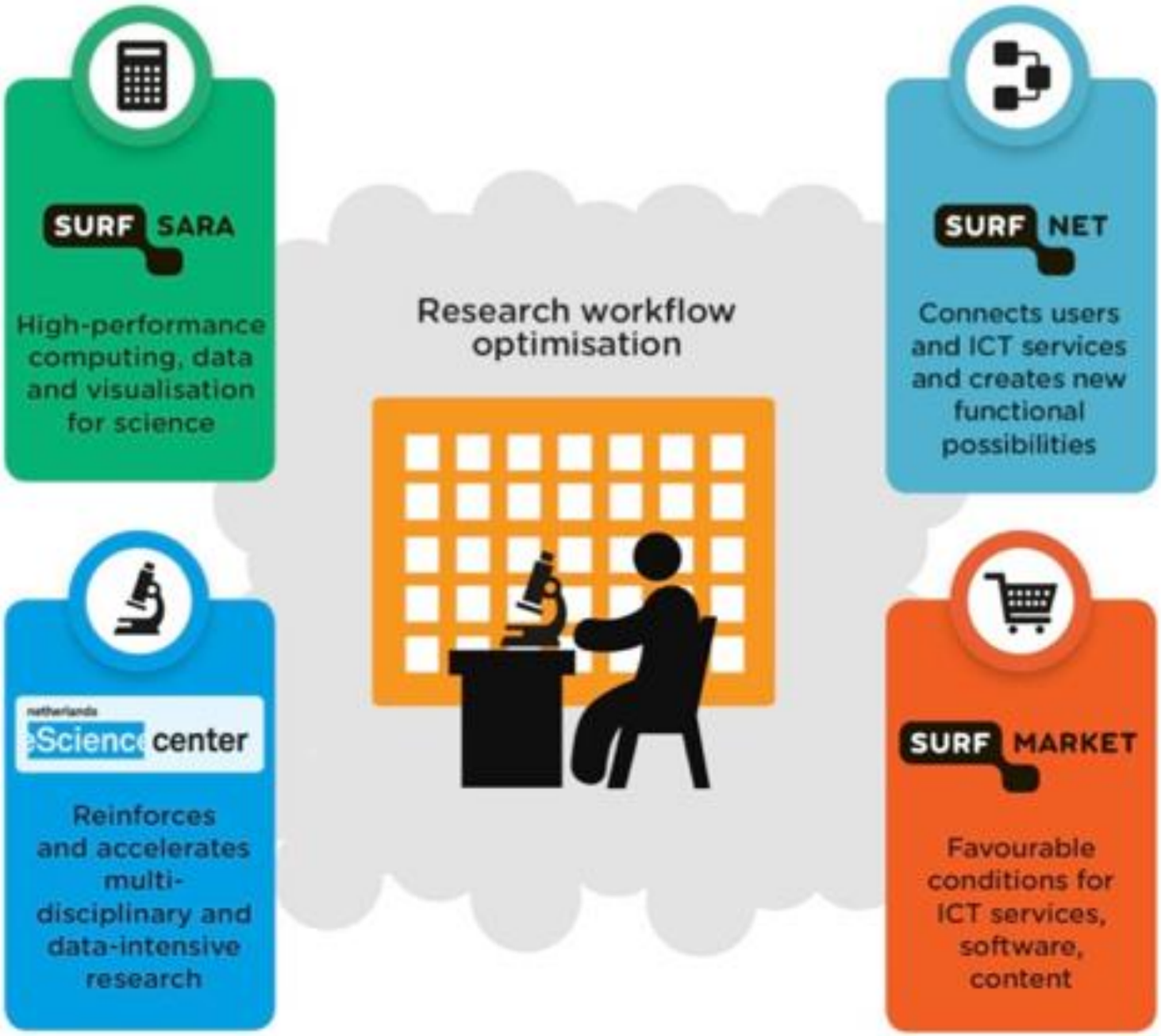
Preparation for hands-on

Go to http://github.com/sara-nl/PRACE-intro-dl

Please follow the instructions in the README.

After the first session the Jupyter notebooks will be accessible…

SURF

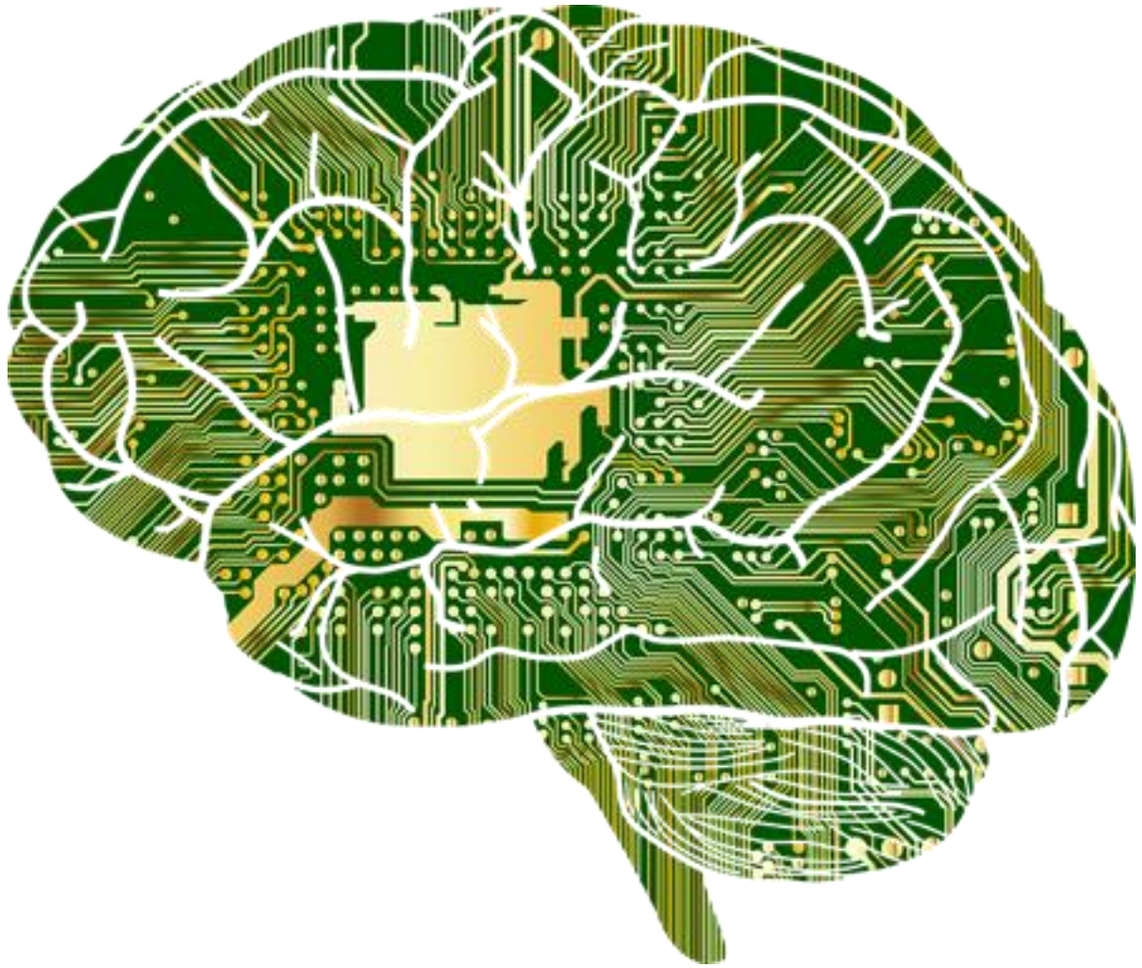

SURF SARA
High-performance computing, data and visualisation for science
Research workflow optimisation
SURF NET
Connects users and ICT services and creates new functional possibilities
netherlands eScience center
Reinforces and accelerates multi-disciplinary and data-intensive research
SURF MARKET
Favourable conditions for ICT services, software, content

SURF services

- High-end computing in different flavours
- Data storage and management solutions
- Fast networks for data transfer and scaling out
- Federated access management solutions
- Facilities to share data and to collaborate online
- Visualisation services

Deep learning @ SURF

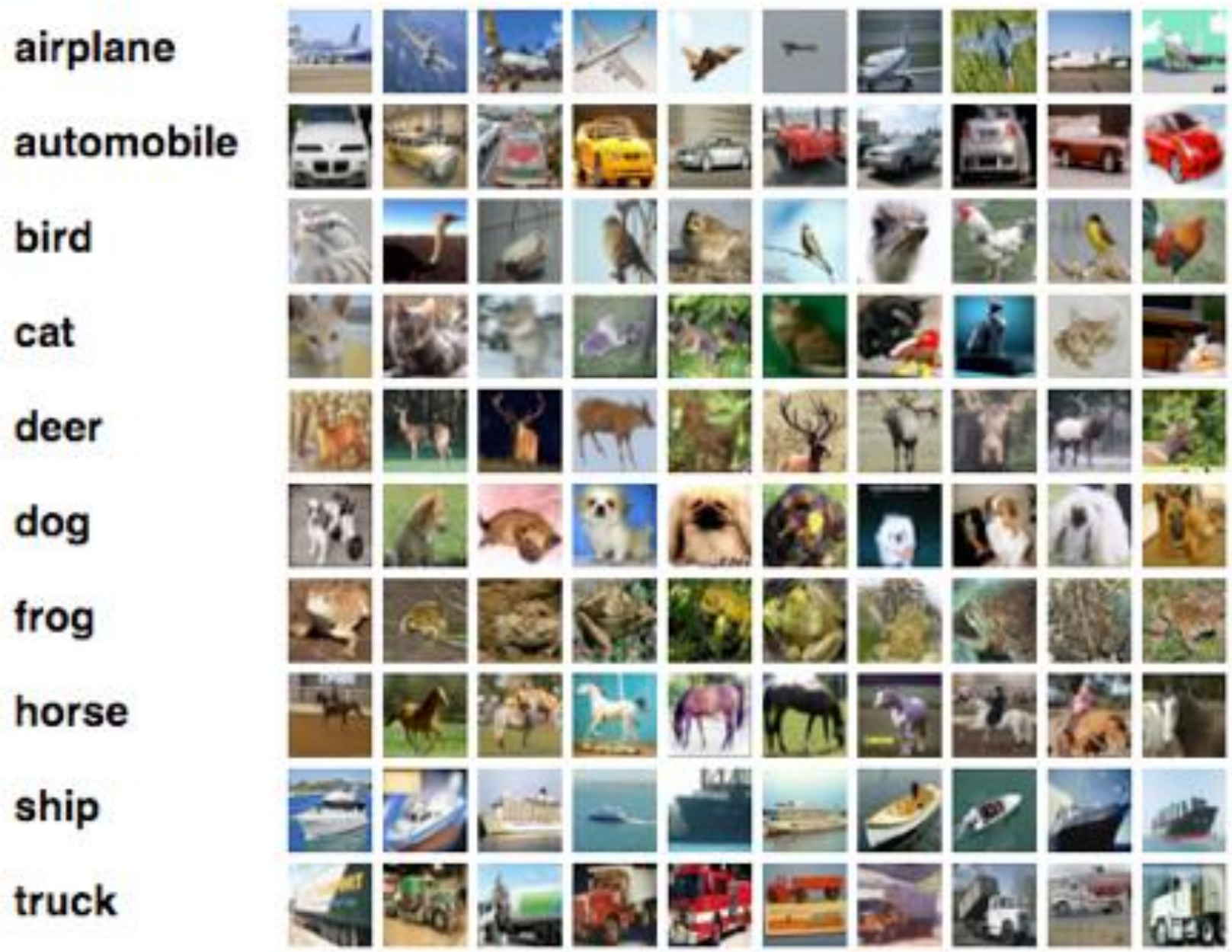
- GPUs on different infrastructures
- HPC Cloud
- LISA cluster
- Cartesius supercomputer
- Innovation projects
- Upscaling of deep learning models
- Deep learning for simulation
- Workshops & courses



Goals

- Find out what deep learning can do
- Understand the components of a neural network
- Solve a real-life image classification problem

Deep learning



Style transfer

Source: [Deep Dream Generator]

Text generation

DeepDrumpf
@DeepDrumpf

Follow

Replying to @jimjefferies

If I win, I'm going to instruct my attorney general to put racists in charge. We are going to do great crimes with my programs.@jimjefferies

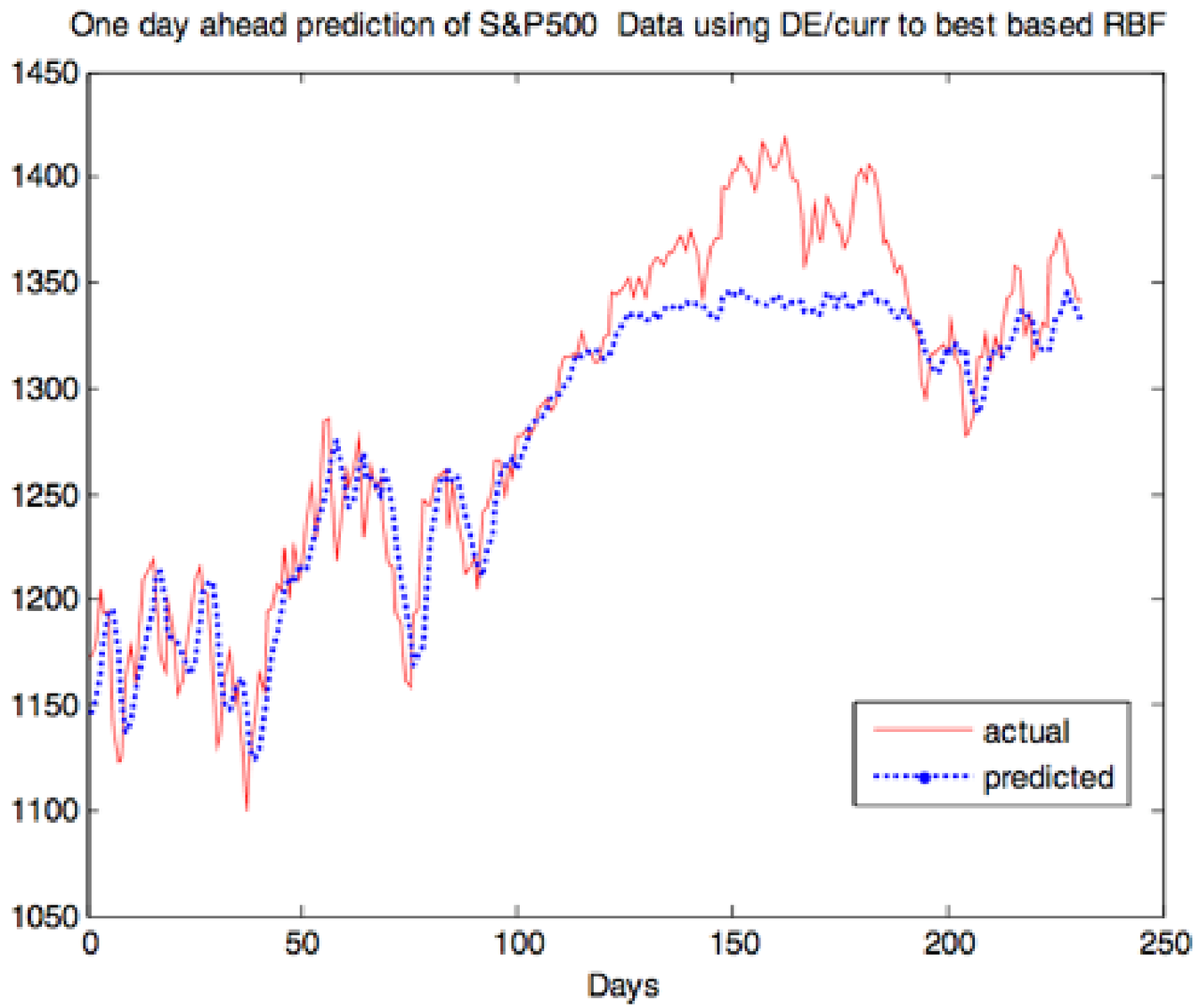
6:31 PM - 9 Oct 2016

157 Retweets **266** Likes

3 157 266

Source: Deep Drumpf

Time series prediction

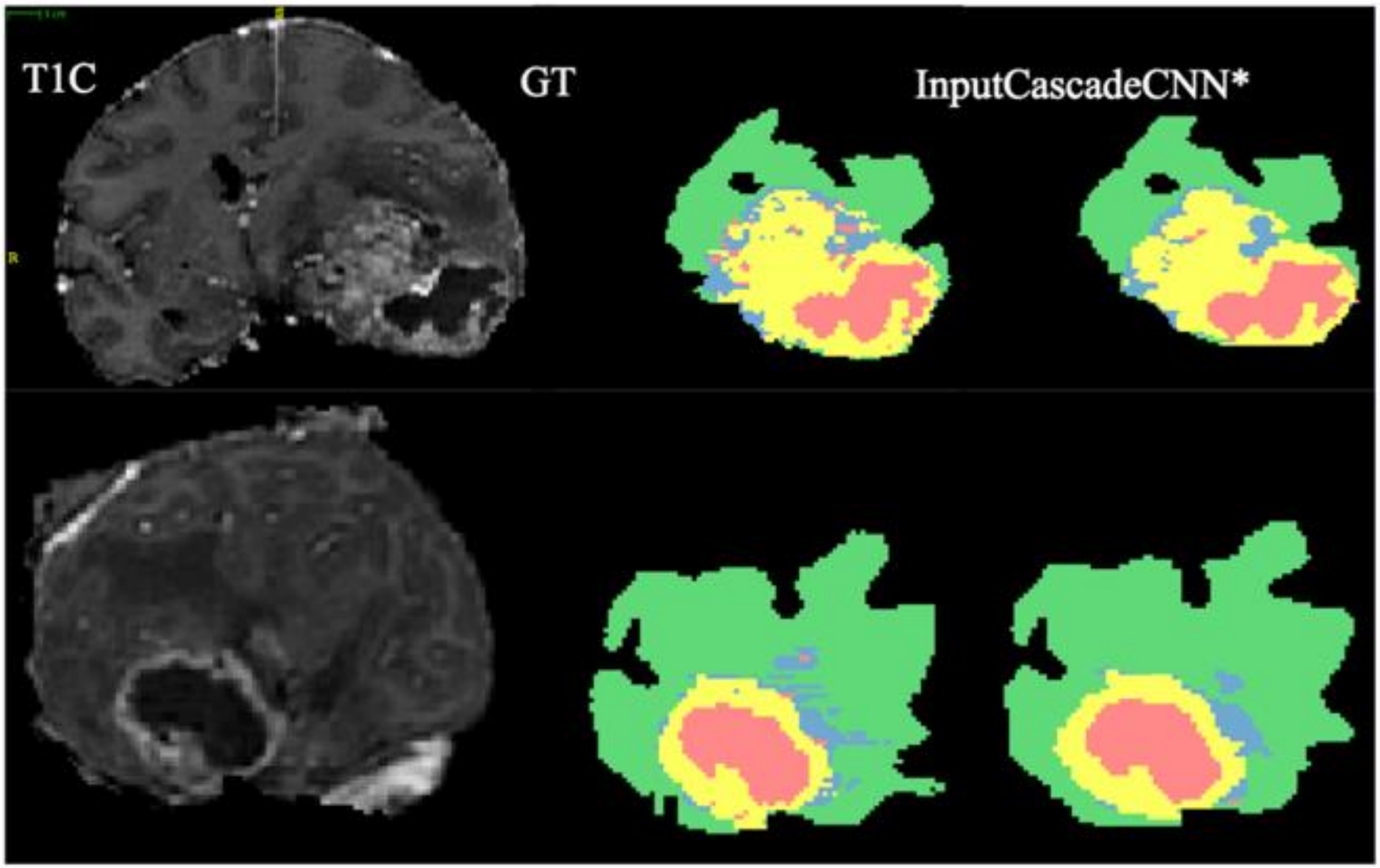


Source: [Forecasting financial time series using a low complexity recurrent neural network and evolutionary learning approach,] **Rout et al., 2015**

Reinforcement learning

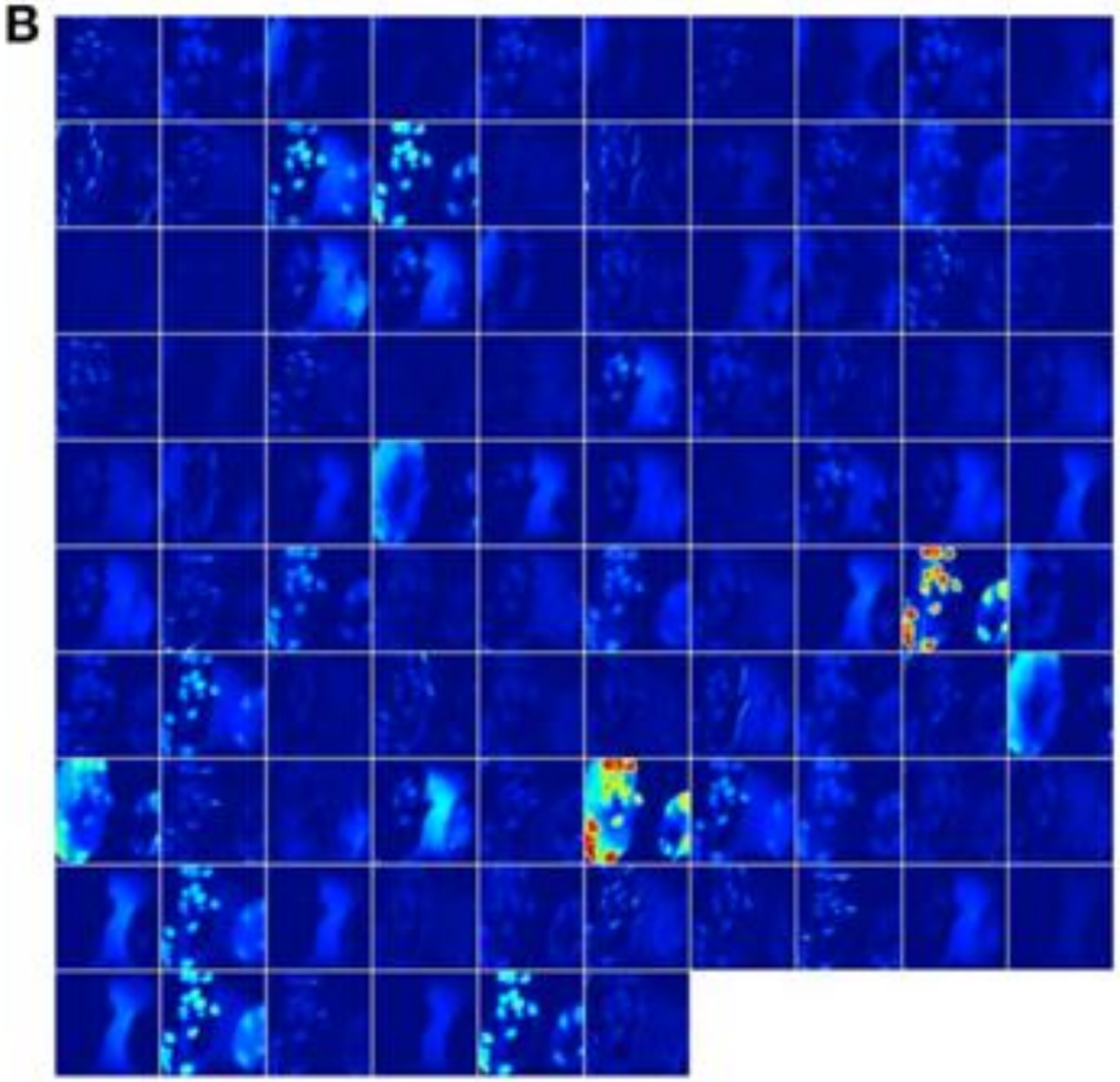
Source: [Emergence of Locomotion Behaviours in Rich Environments](), DeepMind, 2017

Medical image segmentation



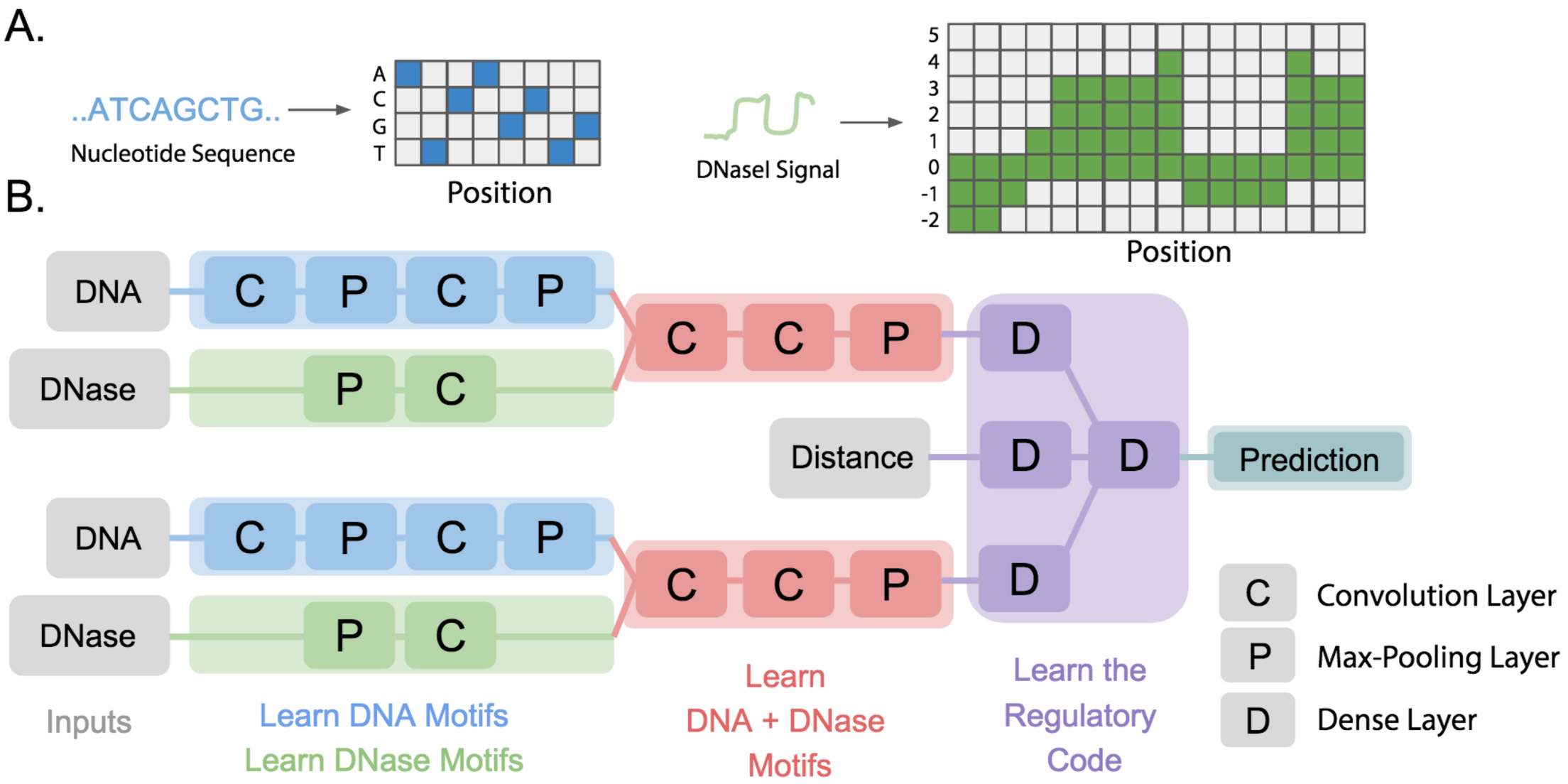
Source: [Brain Tumor Segmentation with Deep Neural Networks](), Havaei et al., 2016

Disease detection



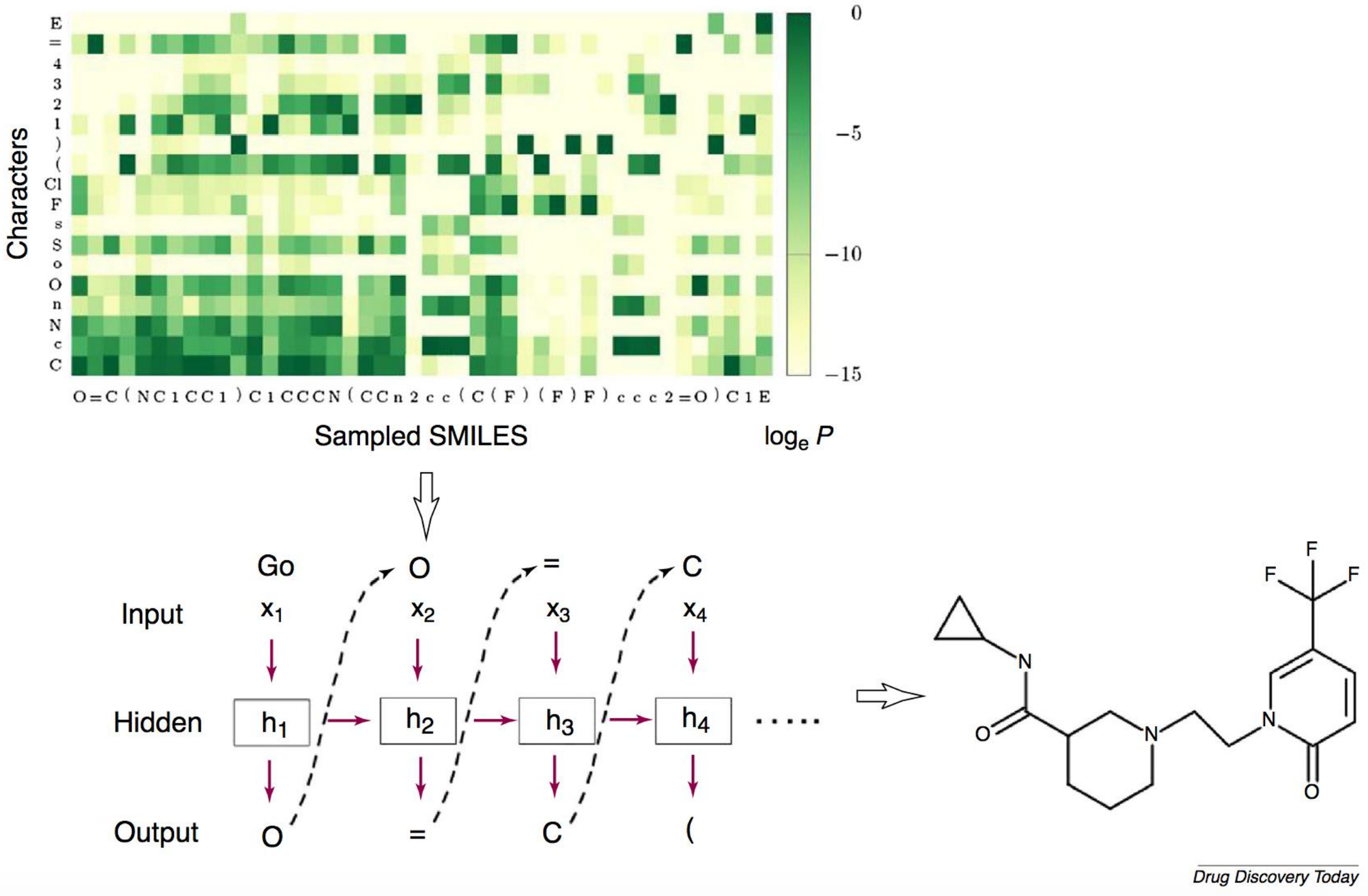
Source: [Using Deep Learning for Image-Based Plant Disease Detection](), Mohanty et al., 2016

Omics



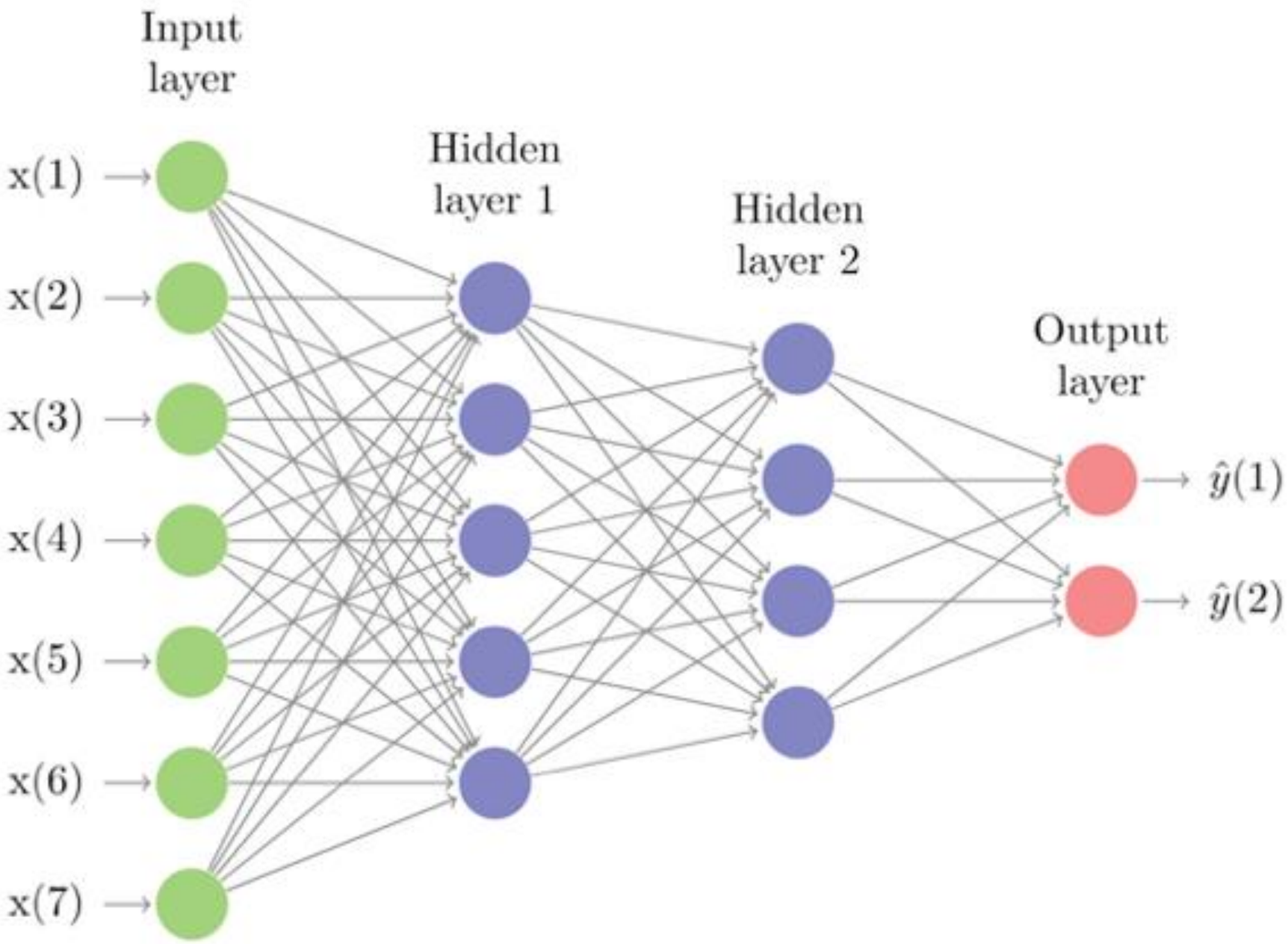
Source: [Nucleotide sequence and DNaseI sensitivity are predictive of 3Dchromatin architecture](), Schreiber et al., 2017

Drug design

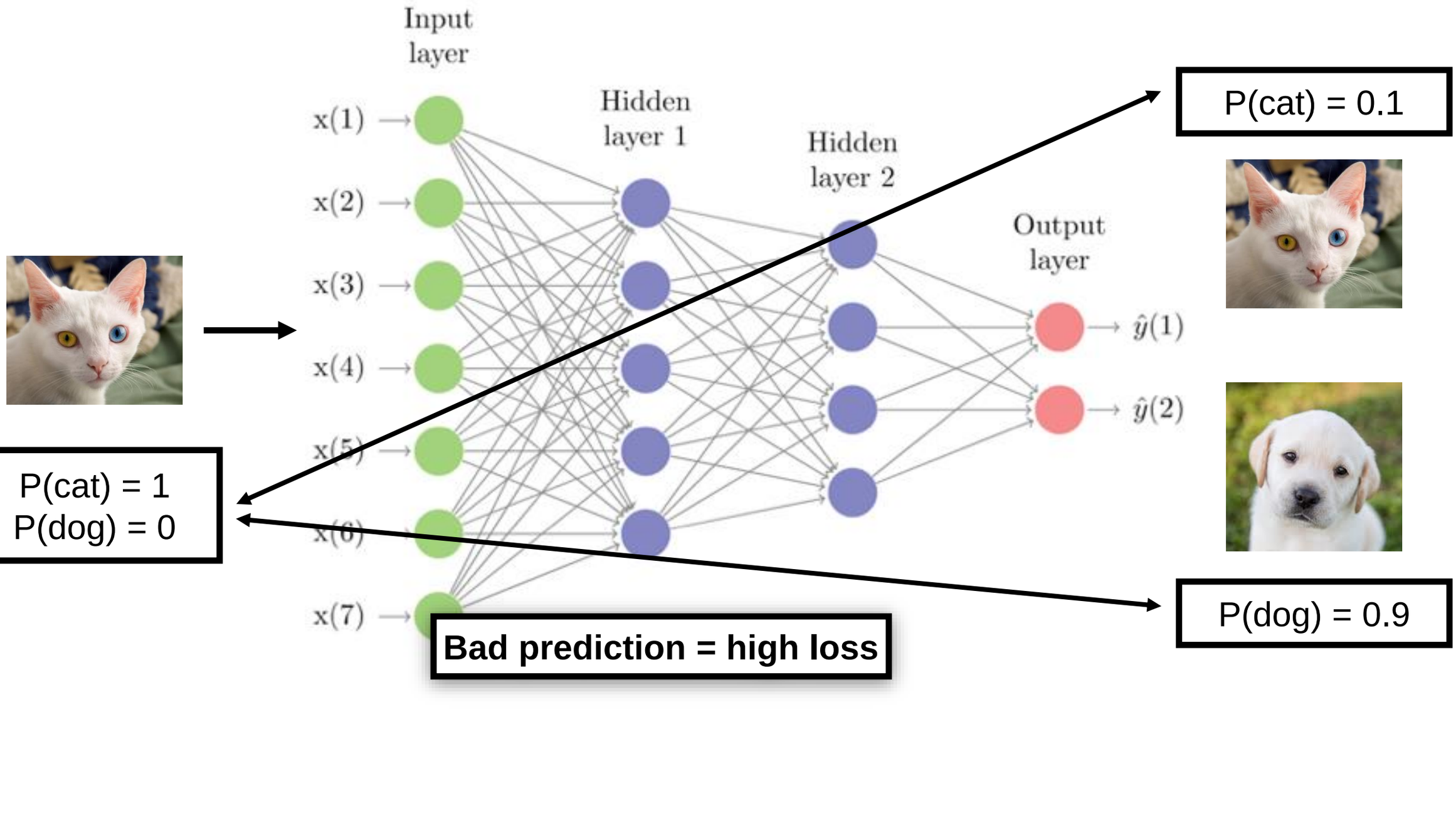


Source: [The rise of deep learning in drug discovery](). Chen et al., 2018

Neural networks

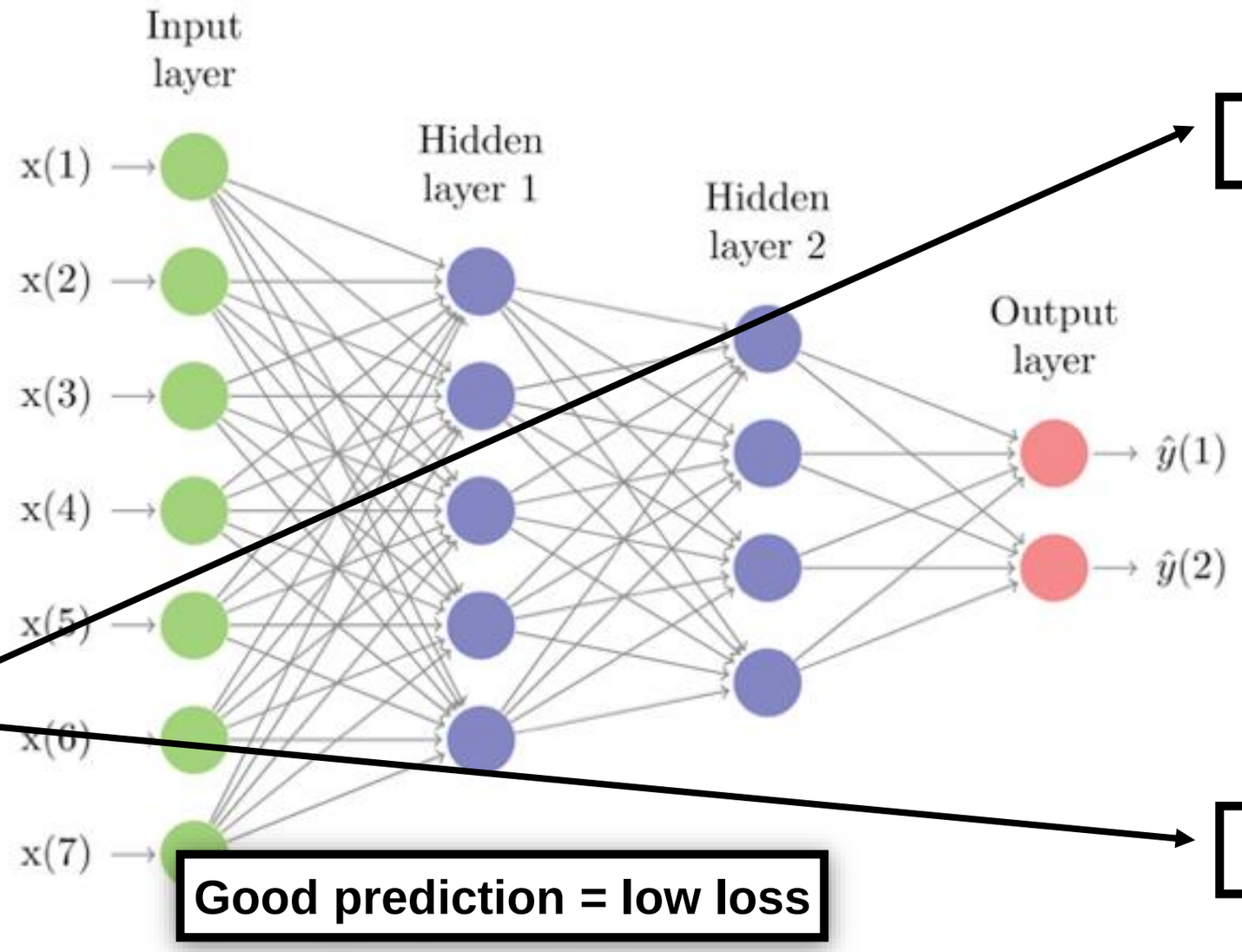


Example


Input layer
Hidden layer 1
Hidden layer 2
Output layer
x(1)
x(2)
x(3)
x(4)
x(5)
x(6)
x(7)
ŷ(1)
ŷ(2)
P(cat) = 0.1
P(cat) = 1
P(dog) = 0
P(dog) = 0.9
Bad prediction = high loss

Example

P(cat) = 1
P(dog) = 0



P(cat) = 0.9

P(dog) = 0.1

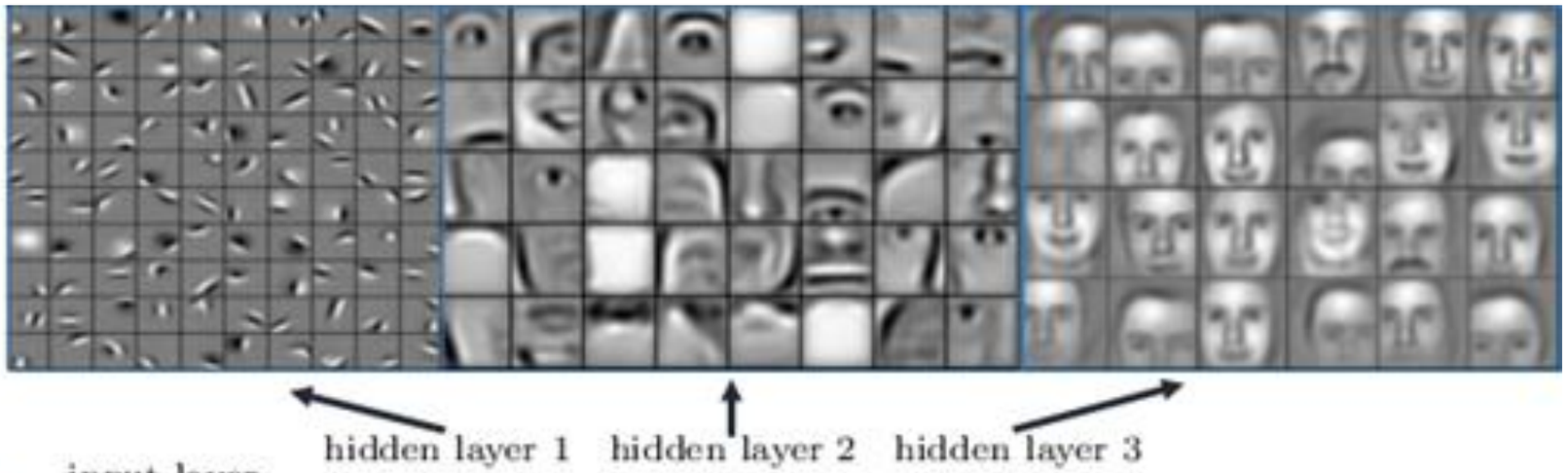
Good prediction = low loss

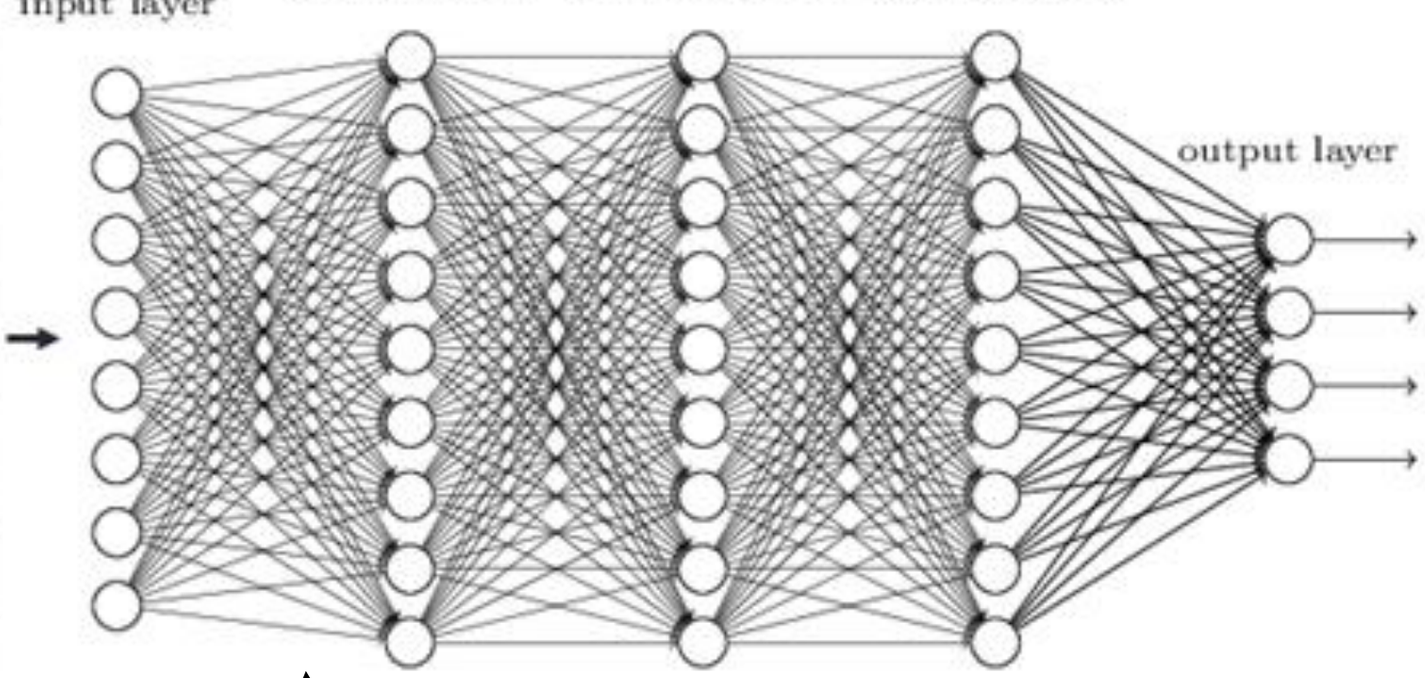
Learners and loss functions

- A neural network can learn to solve a problem
- Learn representations from data
- Every layer applies a simple mathematical function
- Adapt parameters of network to reduce loss

Feature hierarchy

Deep neural networks learn hierarchical feature representations



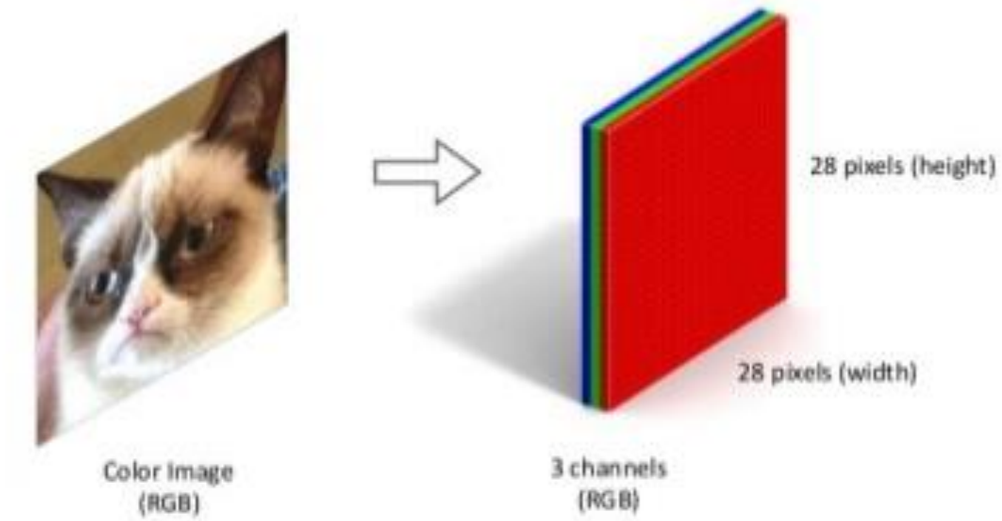


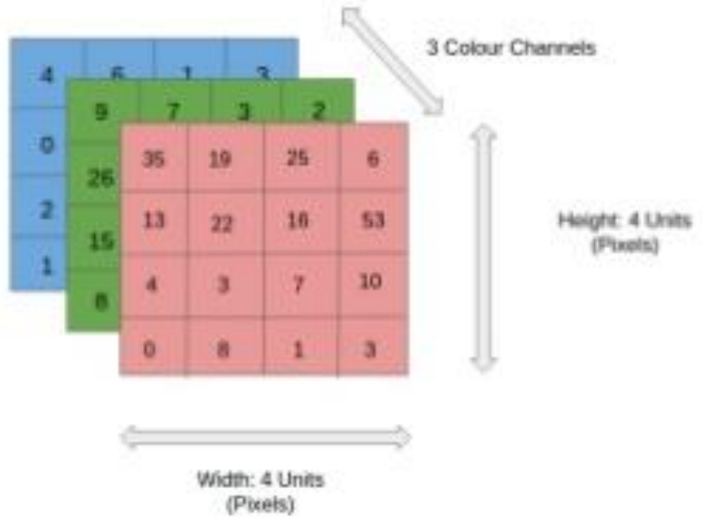
(even though not exactly with this type of network…)

Image data

color image is 3rd-order tensor

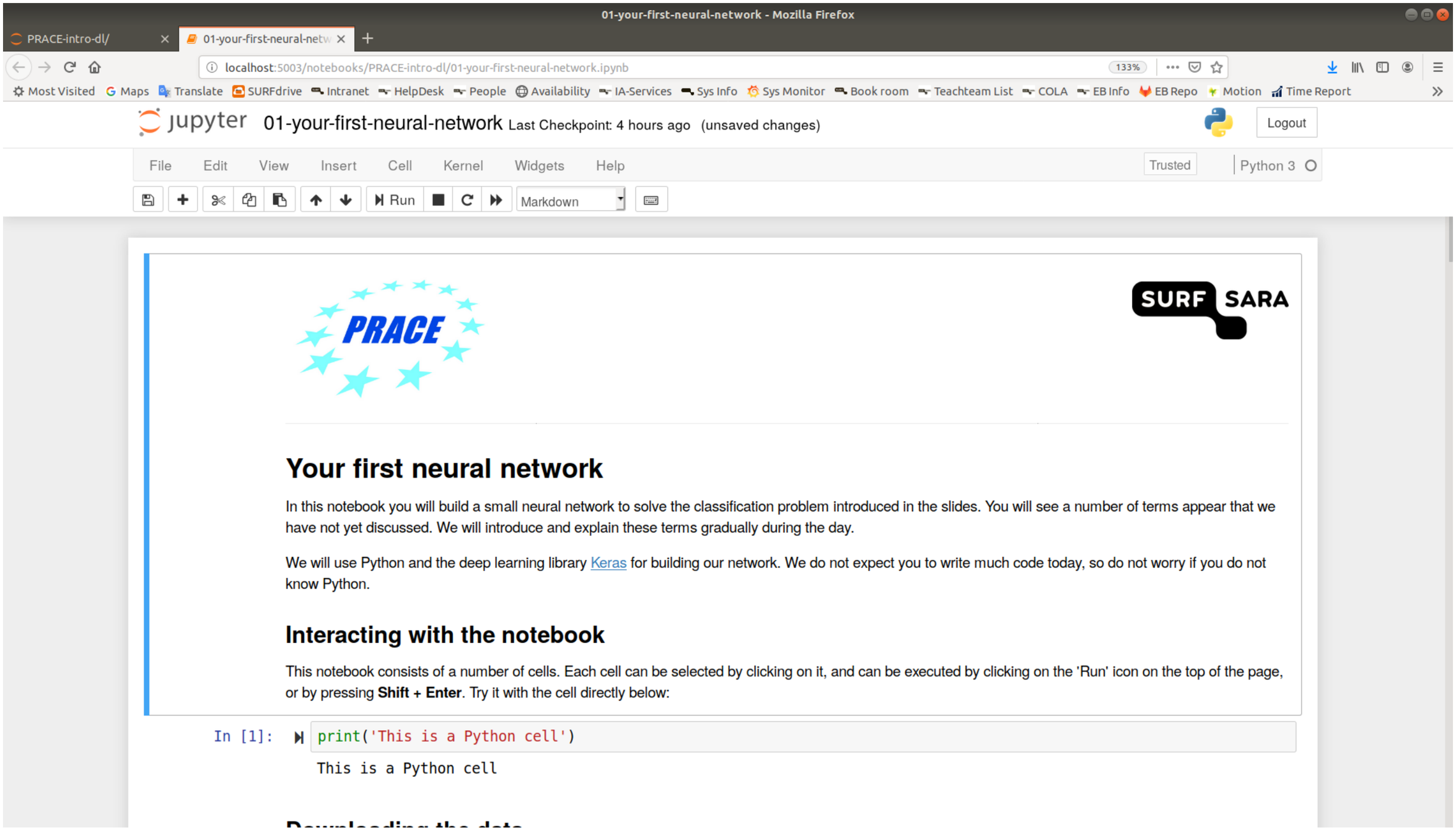
- With colours = 3D
- 3 color channels
- Instead of just storing single value between 0-255 we store 3 such values.



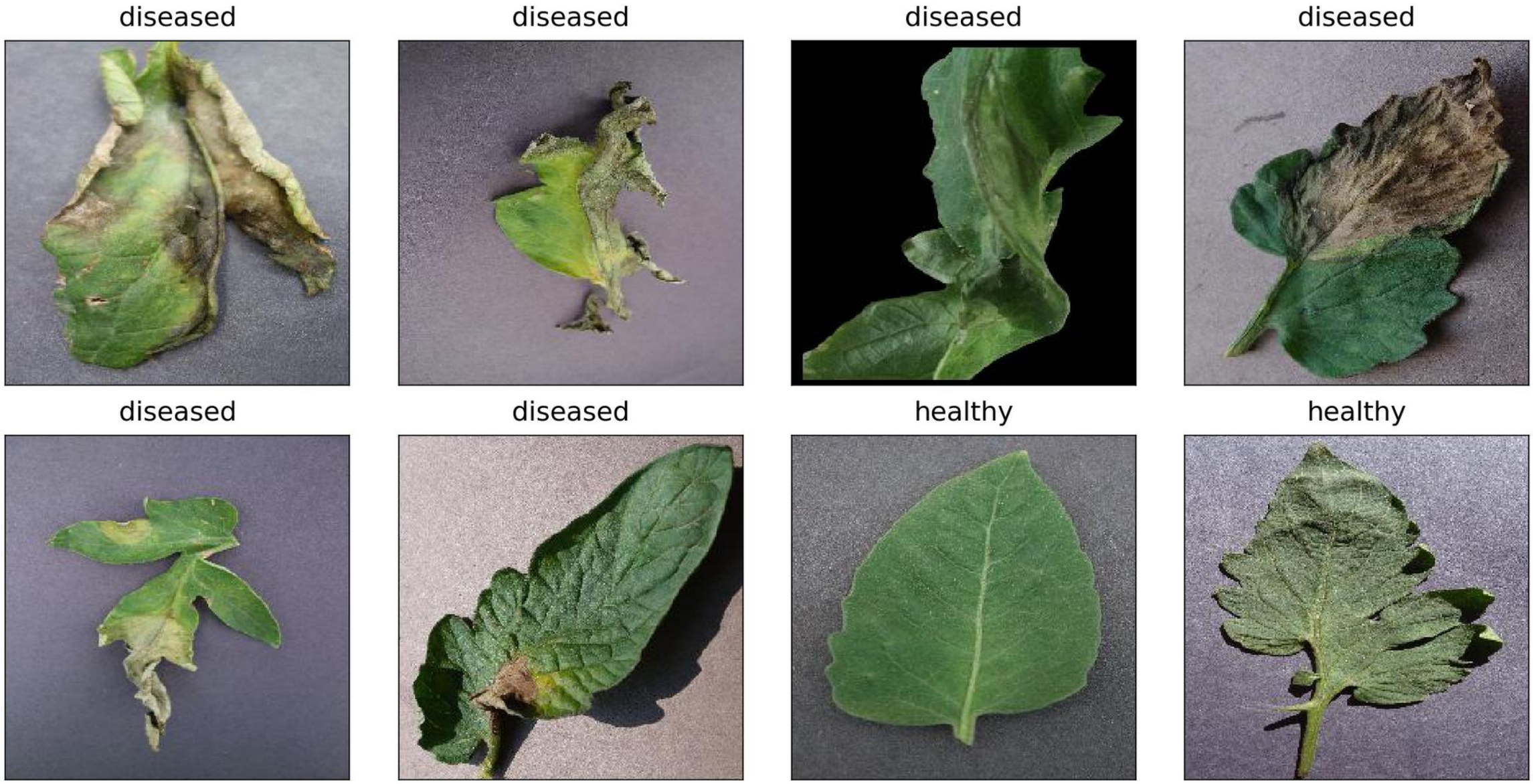


Source: https://www.slideshare.net/pabitramani/digital-image-processing-and-interpretation

Jupyter notebooks



The problem


diseased
diseased
diseased
diseased
diseased
diseased
healthy
healthy

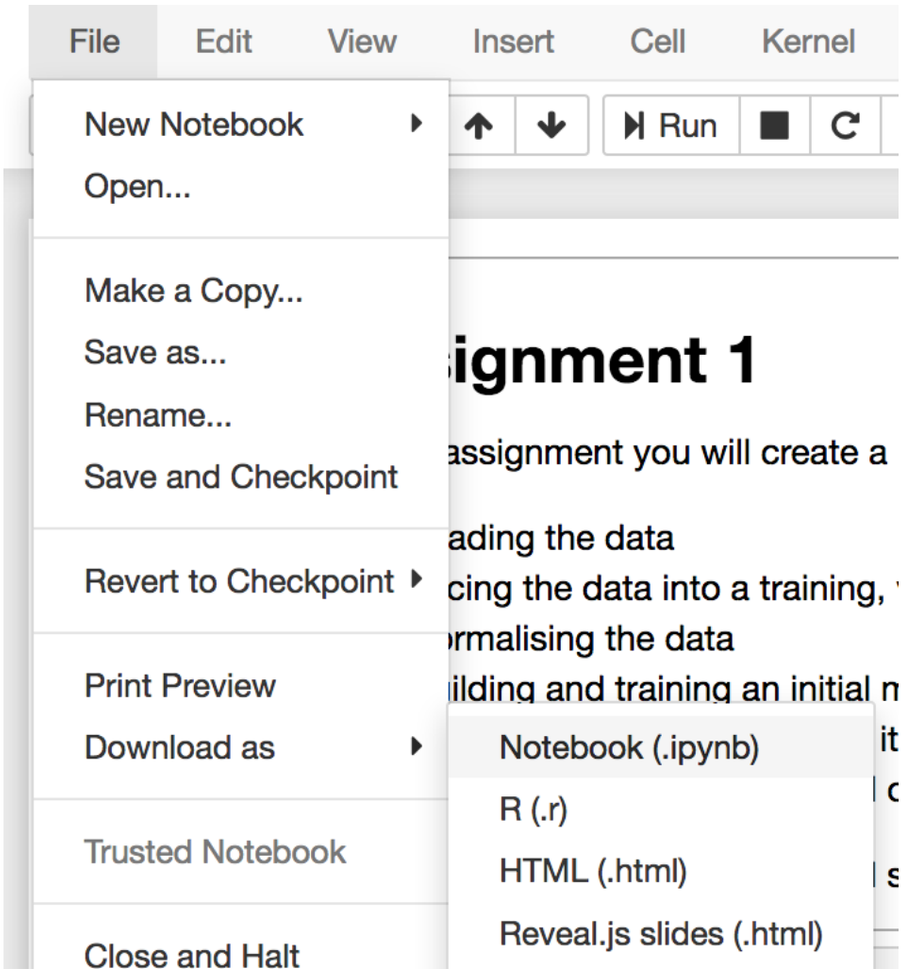
Hands-on

Go to https://localhost:5XXX (where XXX comes from “ptcXXX”)

Notebook: 01-your-first-neural-network.ipynb

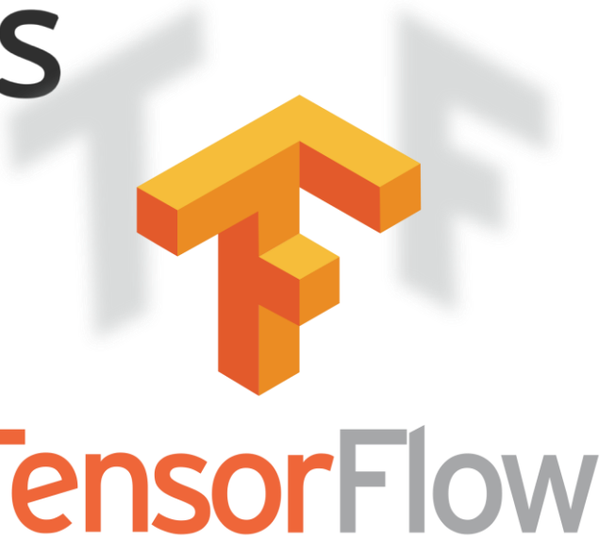
Break at 10:15

Workshop material



https://github.com/sara-nl/PRACE-intro-dl

Creating neural networks

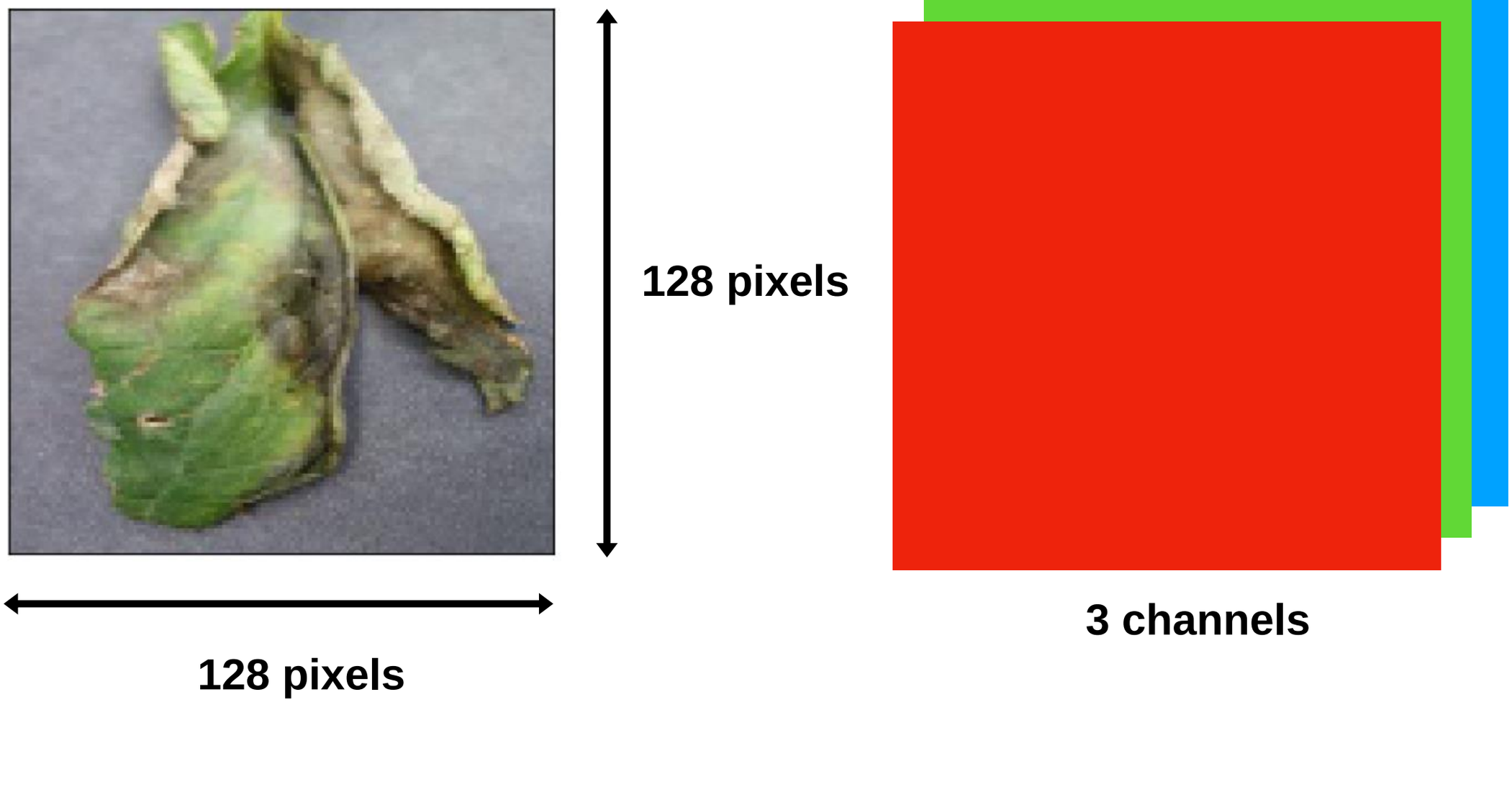


- Many frameworks exist; **TensorFlow**, **CNTK**, **Torch**, **Keras**, **Theano**, **Caffe**, ...

- Tensorflow backend

- Keras R interface

Unpacking the notebook



Unpacking the notebook

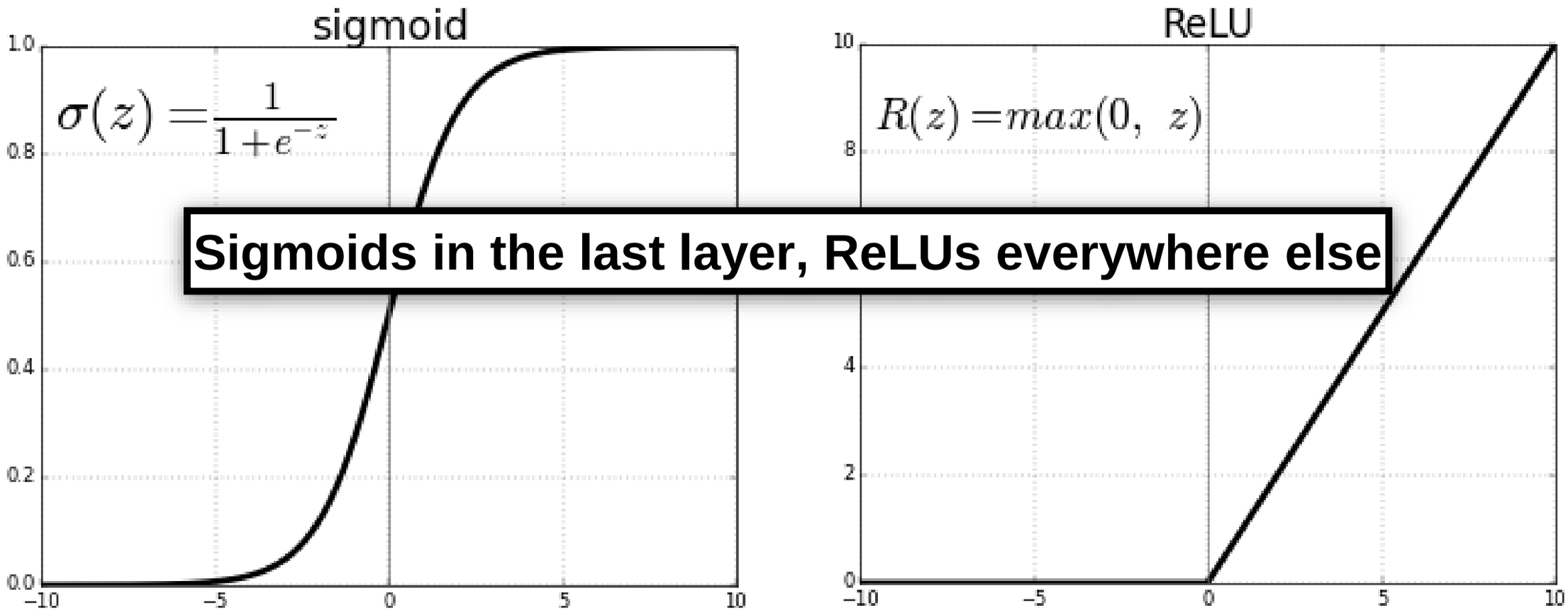
```
from keras.models import Sequential
from keras.layers import Flatten, Dense

model = Sequential()
model.add(Flatten(input_shape=X.shape[1:]))
model.add(Dense(2, activation='softmax'))
model.summary()
```

128 * 128 * 3 = 49.152 pixels / image

Probability distribution over two classes, e.g. [0.3, 0.7]

```
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
flatten_1 (Flatten)          (None, 49152)             0
_________________________________________________________________
dense_1 (Dense)              (None, 2)                 98306
=================================================================
Total params: 98,306
Trainable params: 98,306
Non-trainable params: 0
```

Activation functions



Source: [Activation Functions in Neural Networks]

Unpacking the notebook

```
from keras.optimizers import Adam

model.compile(
    Adam(lr=0.0001),
    loss="categorical_crossentropy",
    metrics=["accuracy"]
)
history = model.fit(X, Y, epochs=25, batch_size=32)
```

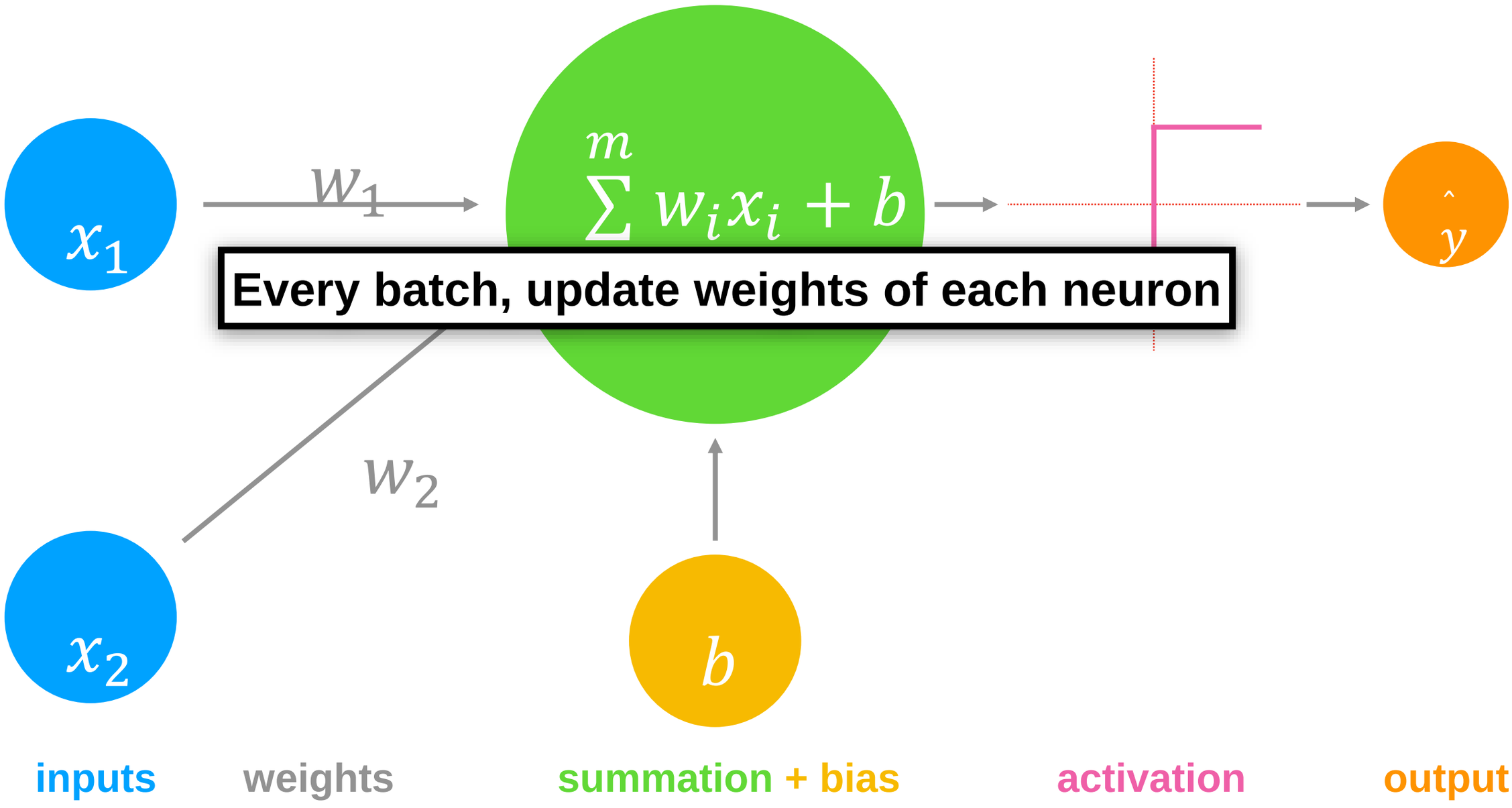
Hyperparameters

```
Epoch 1/25
3500/3500 [==============================] - 1s 306us/step - loss: 0.6972
- acc: 0.6417
```

Hyperparameters

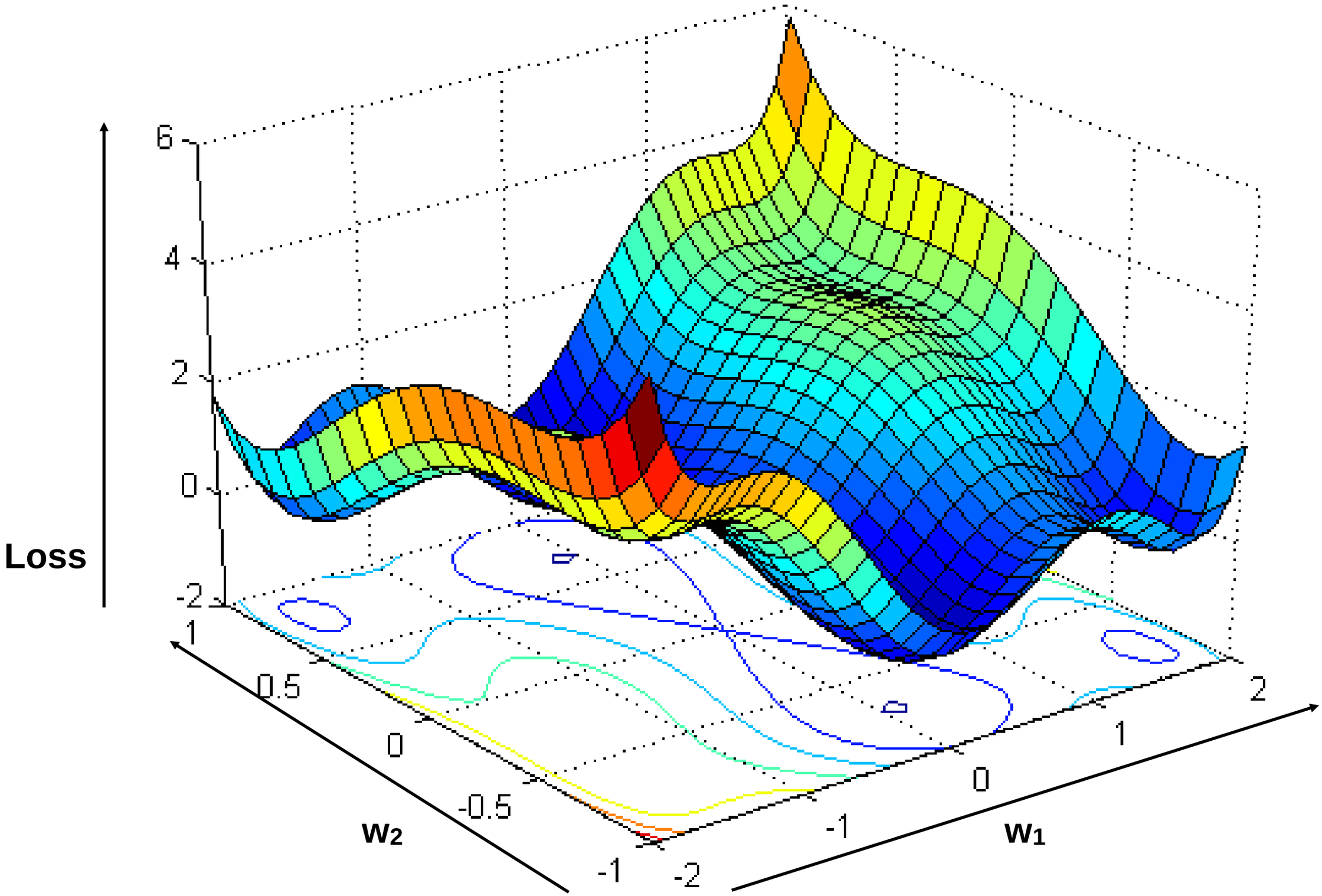
- ‘Ordinary’ parameters: weight and bias parameters
- **Hyperparameters** for network structure and training:
  - Number of layers
  - Number of hidden units
  - Learning rate
  - Batch size

A single neuron



Optimisation

- We are optimising a high-dimensional problem
- Network weights are parameters
- Usually millions/dozens of millions of parameters
- **Loss function** quantifies network performance



Source: [Introduction to loss functions]

Updating weights

(batch) Gradient descent

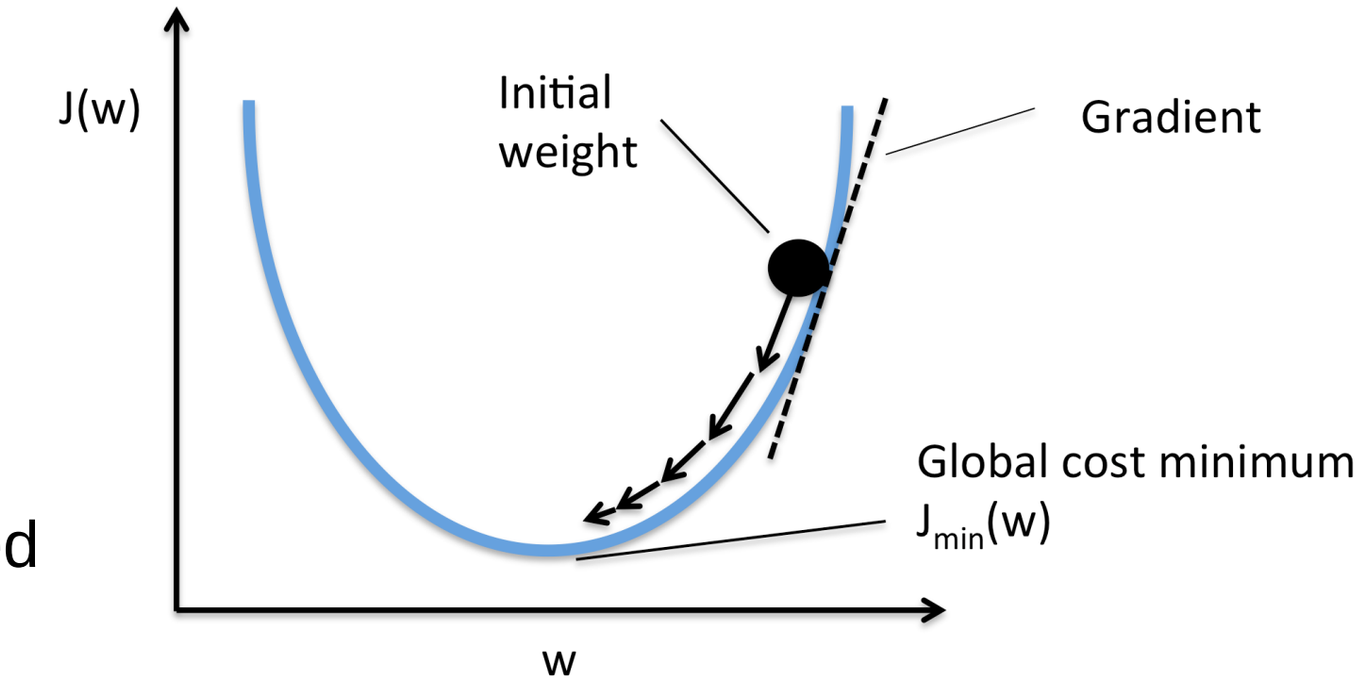
- We apply this procedure a few times, in each iteration we update the weights s.t.

$$w_i := w_i - \mu \frac{\partial J(w)}{\partial w_i}$$

where μ is a value in (0;1] called the **learning rate**

- This algorithm is called **(batch) gradient descent** (GD).

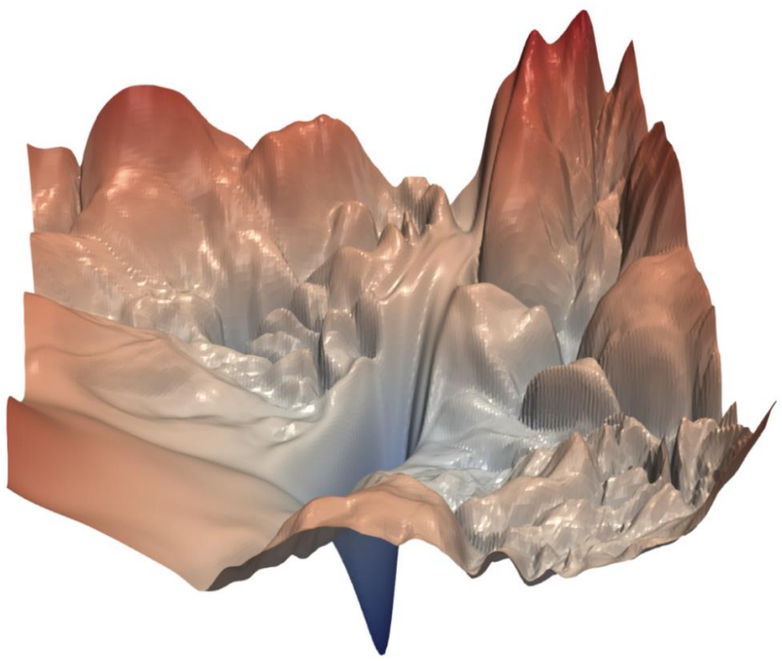
- The loss (and therefore the gradient) is computed over **all elements** in the dataset.

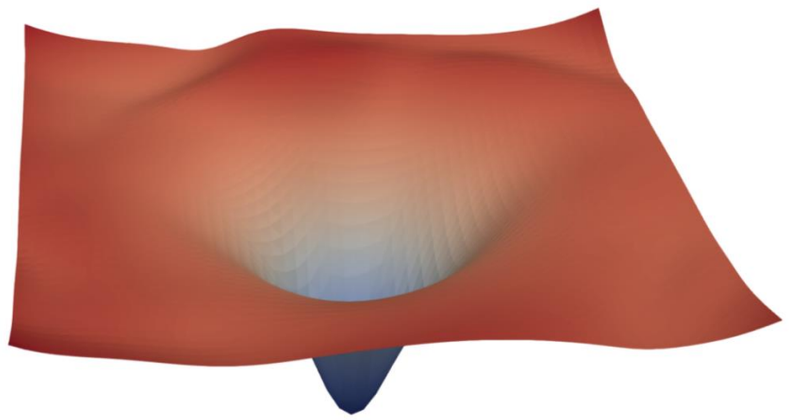


Source: [Gradient optimization]

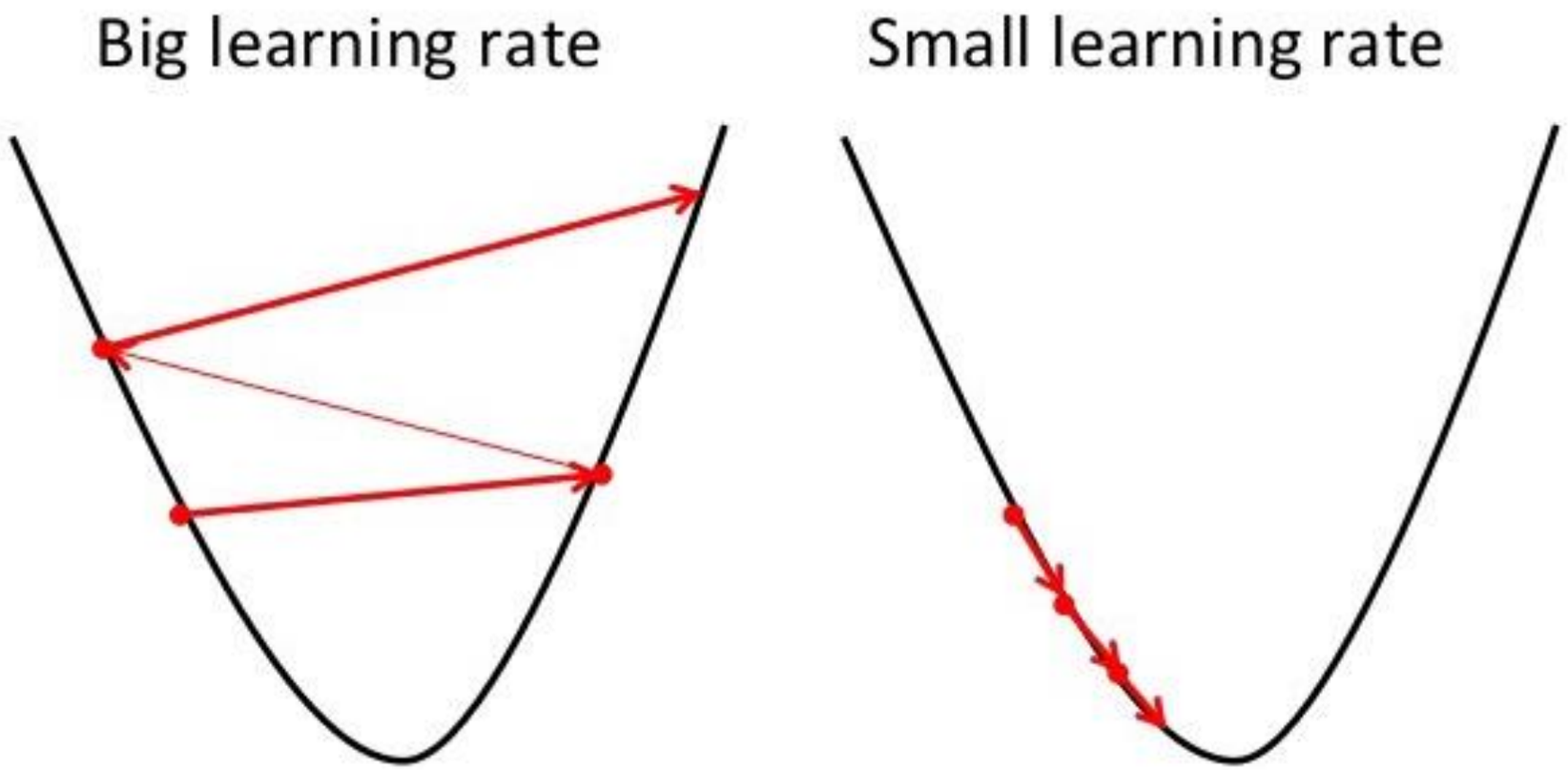
Updating weights

- Batch gradient descent is time-consuming
- Batch gradient descent expects convex loss surfaces
- Use **mini-batch gradient descent** instead
- Batch size = 1 is **stochastic gradient descent**



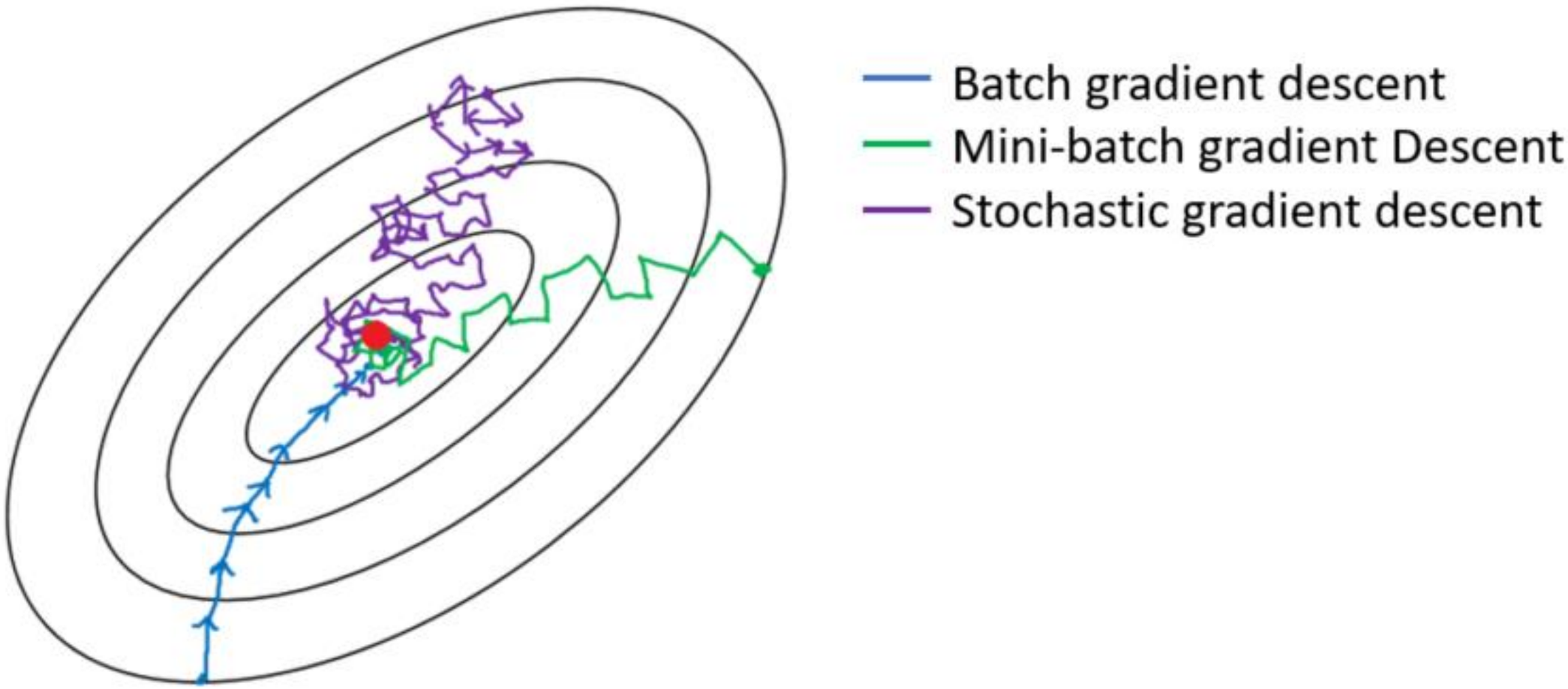


Learning rate



Source: [What are Hyperparameters?]

Batch size

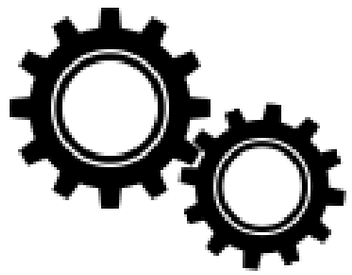


Source: Andrew Ng, deep learning course, Coursera

Training & validation

Training set

Model training



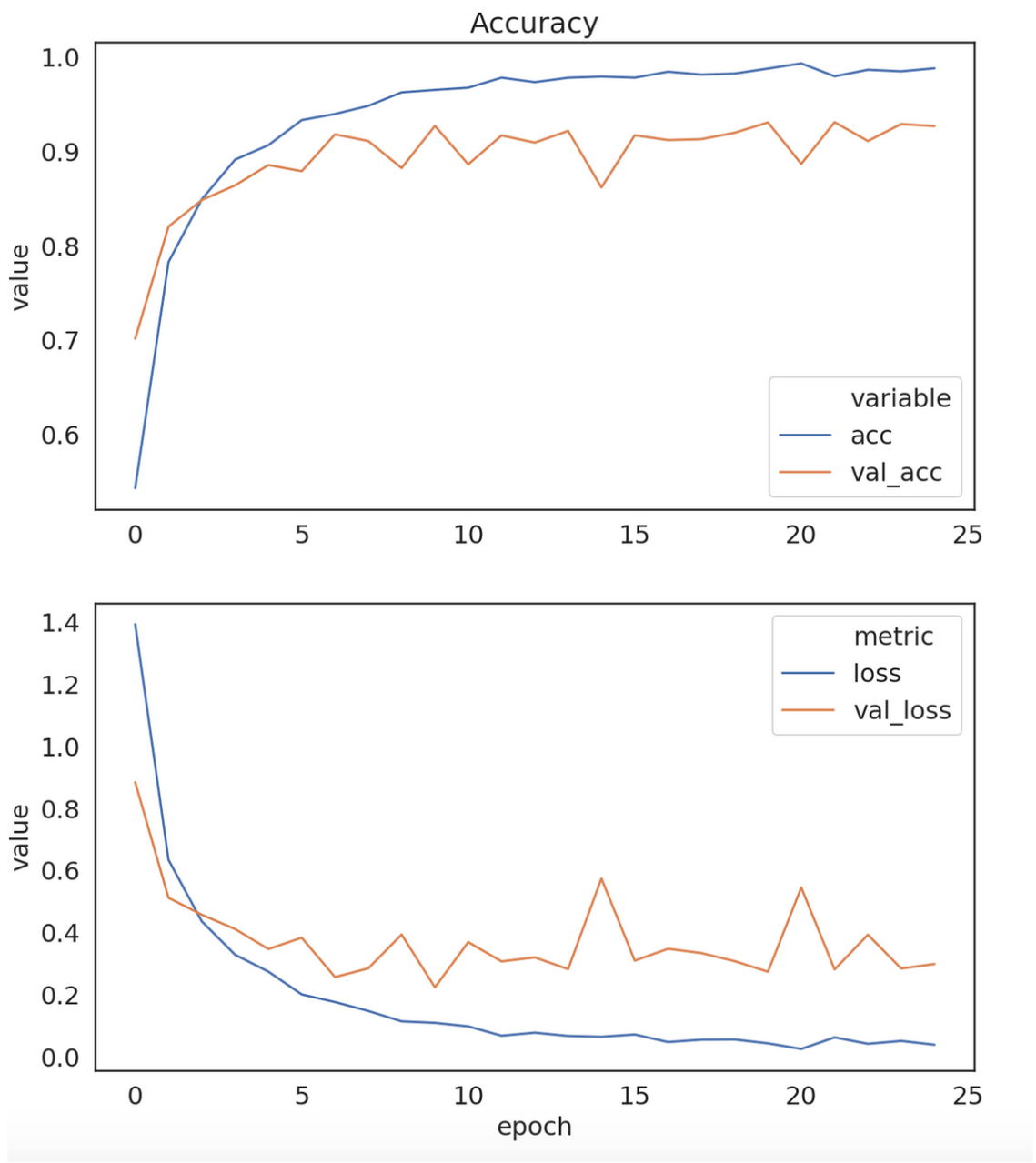
Best model parameters
Weights

Validation set

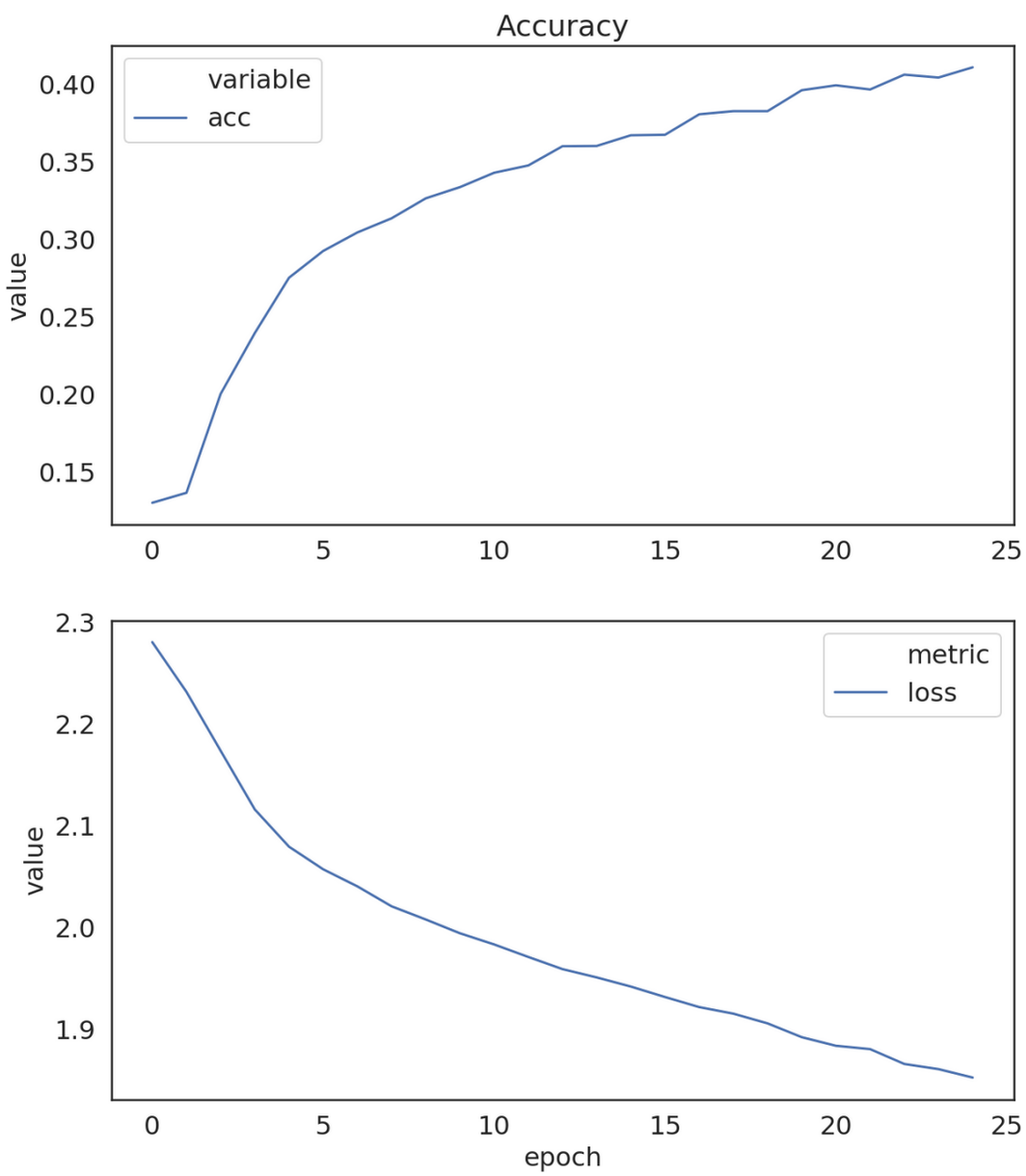
Model selection

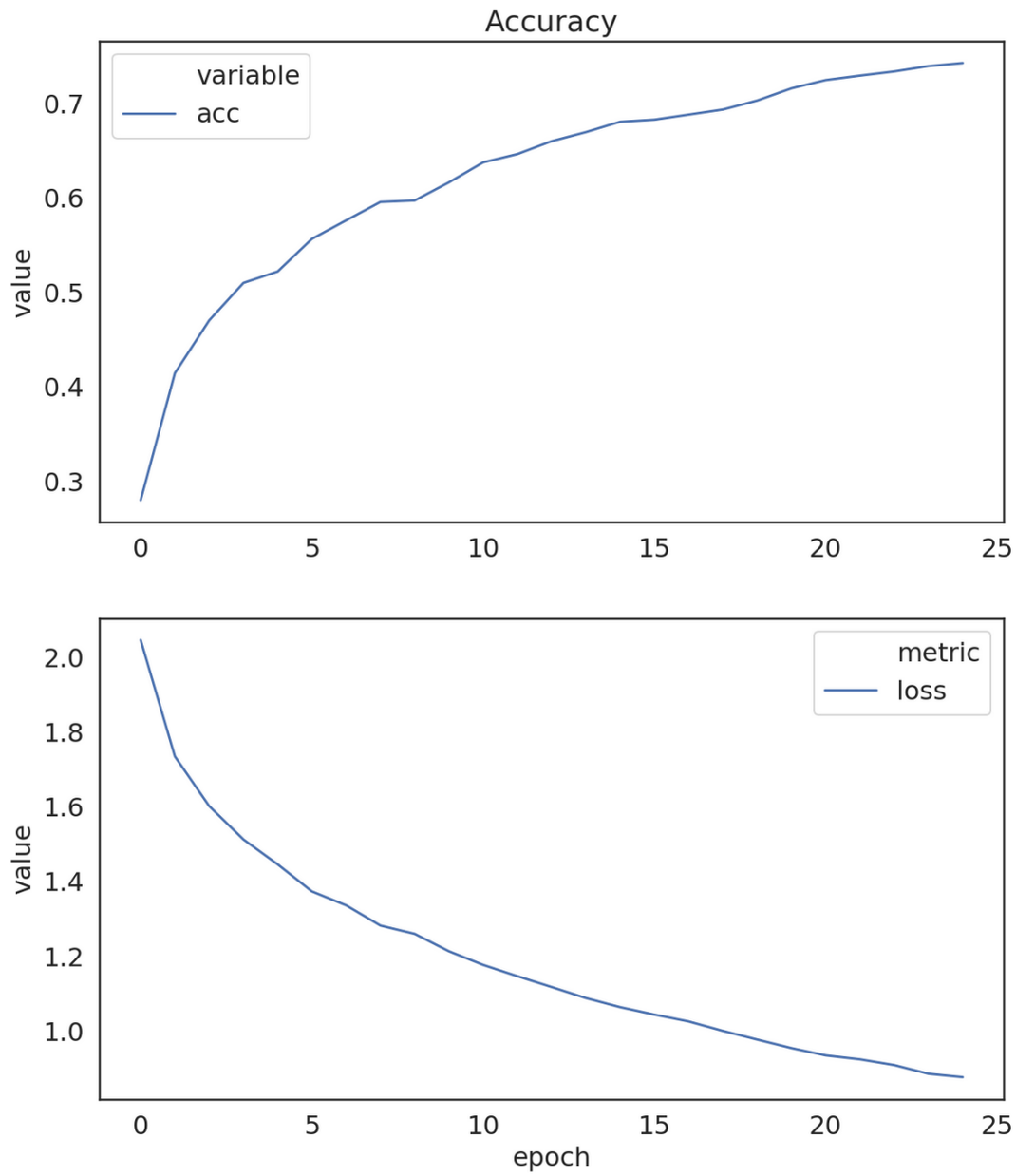
Best hyperparameters
Learning rate
#neurons
#layers

Training & validation



Model capacity

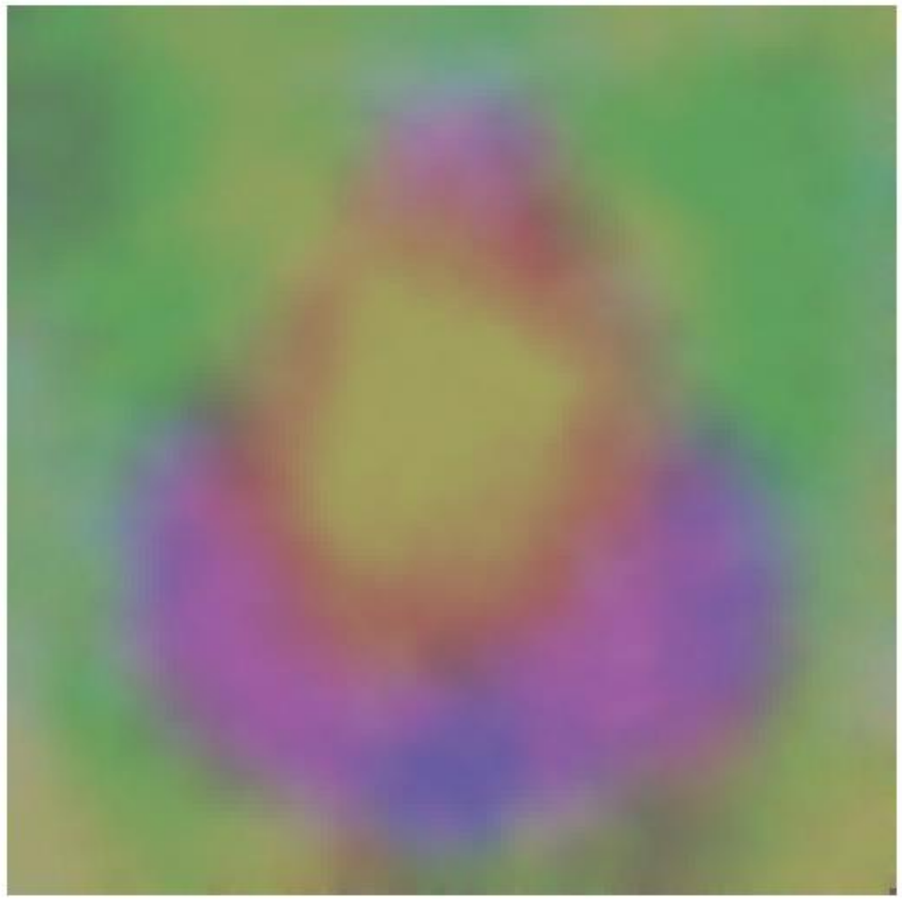




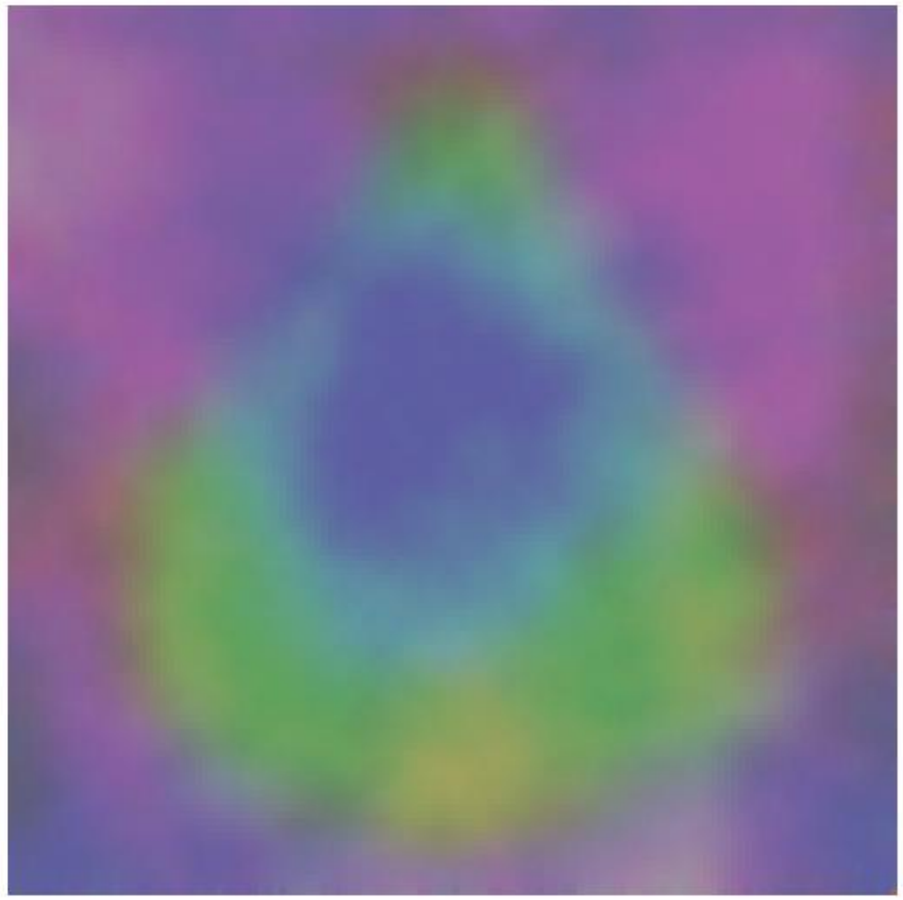
Activations

Each image is a feature detector

diseased

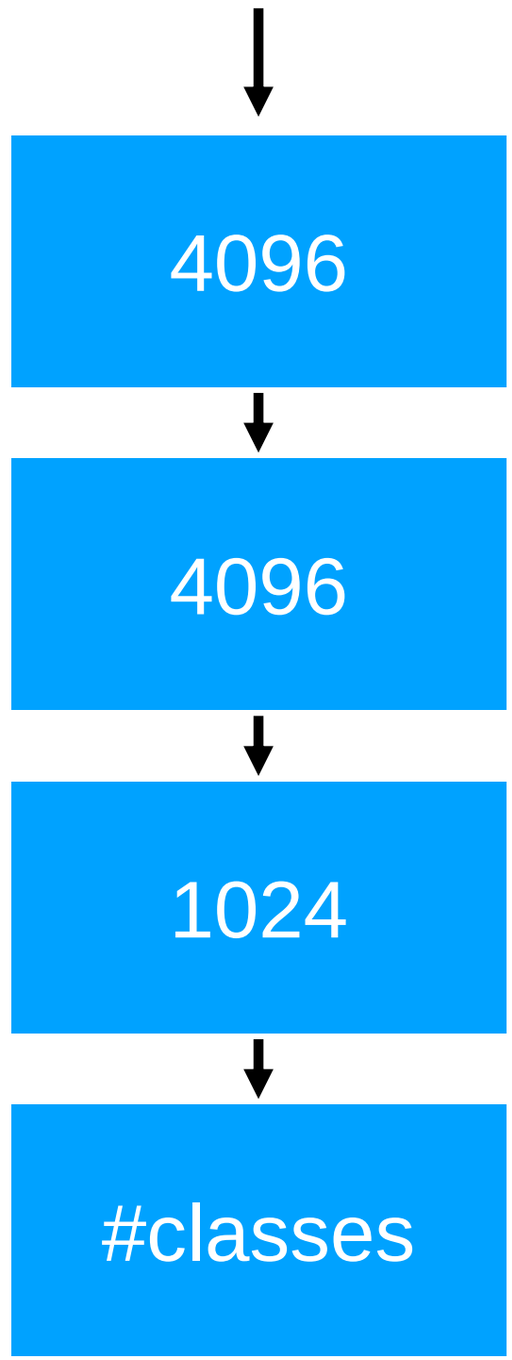


healthy

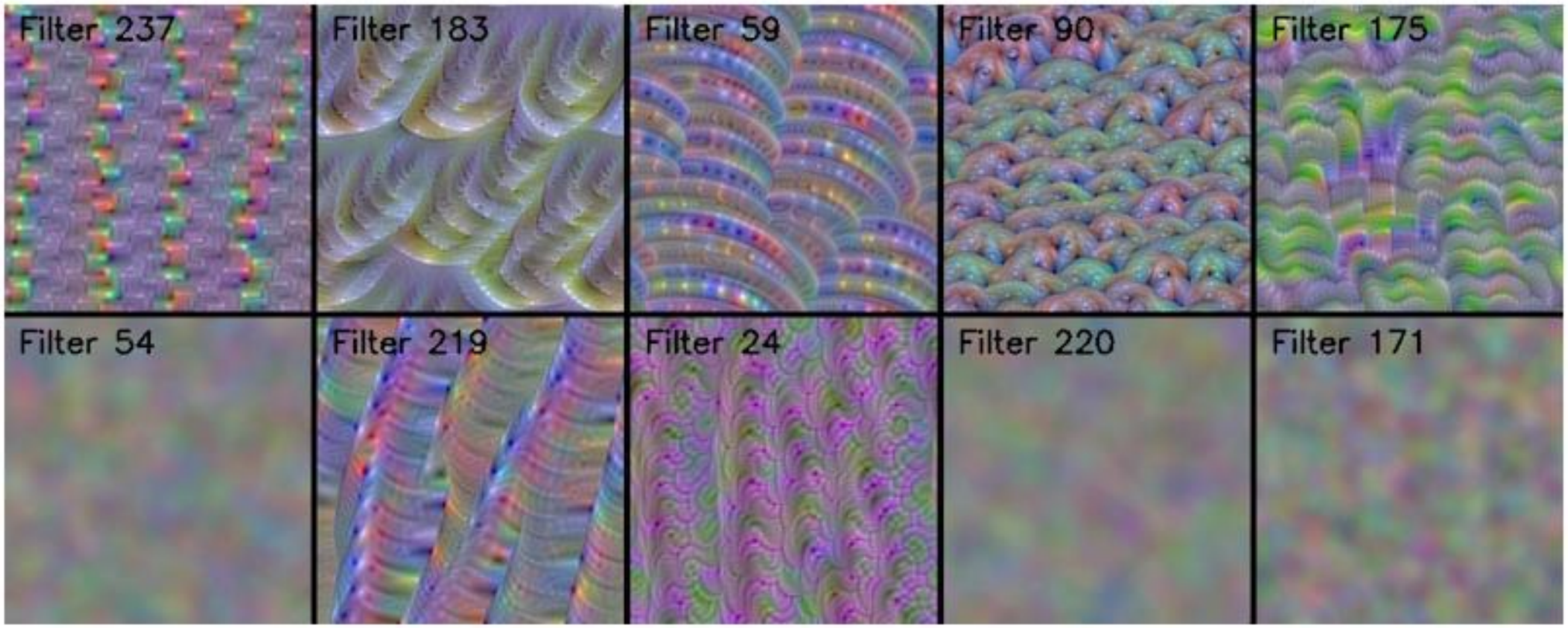


Rules of thumb

- Three hidden layers should be sufficient
- Number of units as multiple of two
- Think of the network as a funnel
- Softmax in last layer
- ReLU everywhere else
- Batch size of 32
- Learning rate dependent on optimiser (0.001)



Activations



Hands-on

Check https://github.com/sara-nl/PRACE-intro-dl

Notebook: 02-hyperparameter-tuning.ipynb

You can work again on https://localhost:5XXX

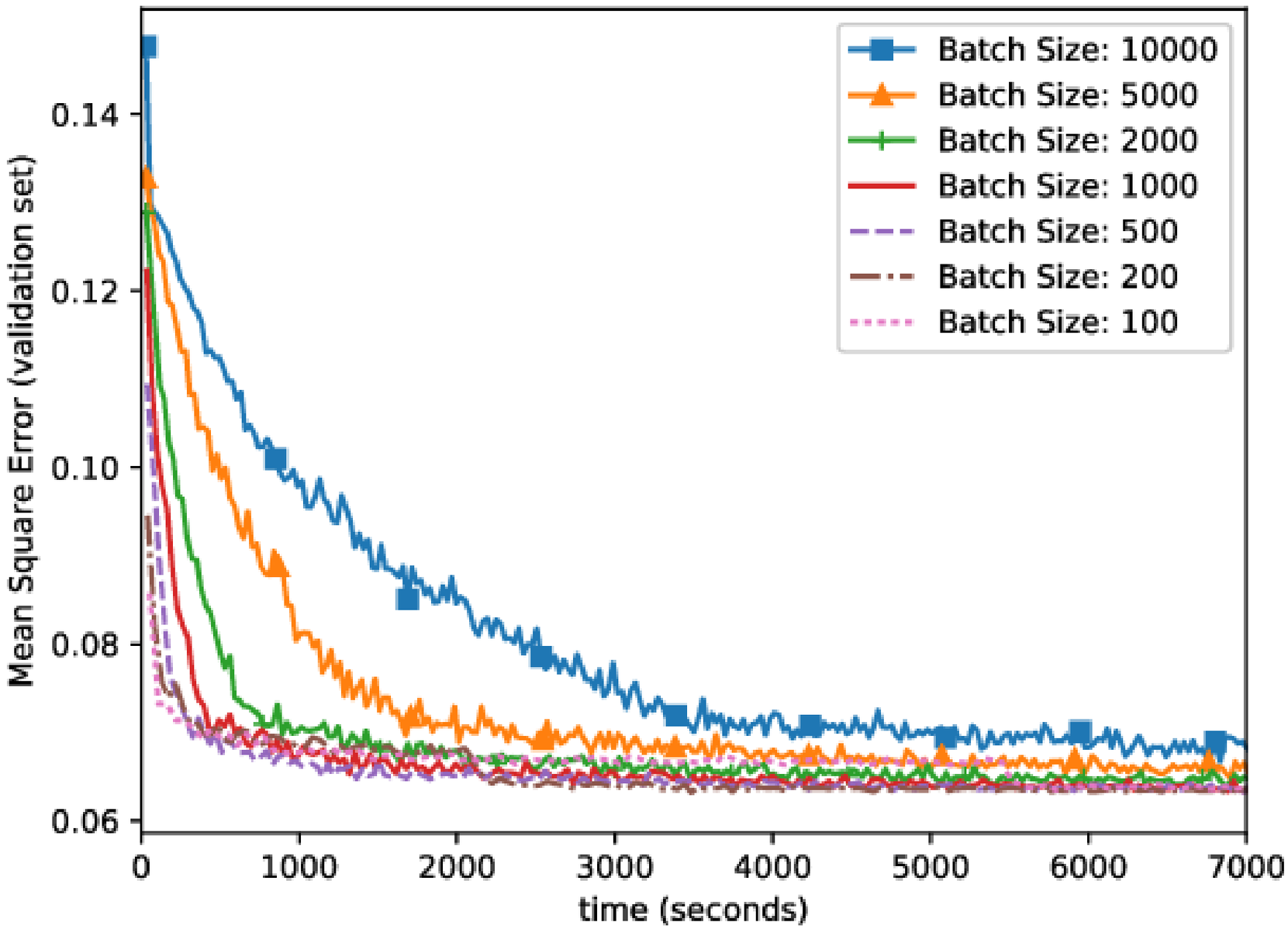
Lunch at 12:00

LUNCH

Return at 13:00

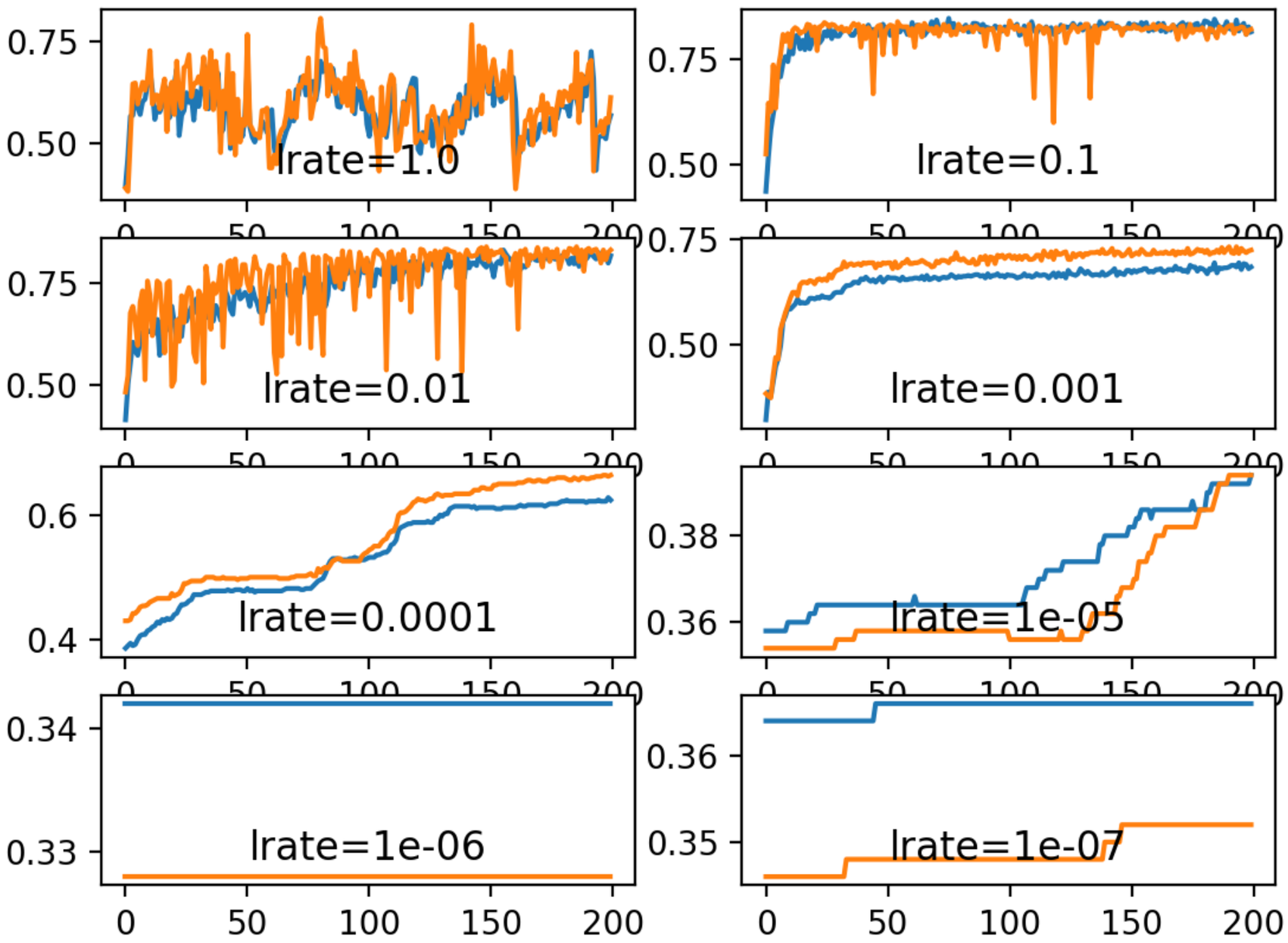
Please sign the attendance sheet!

Recap



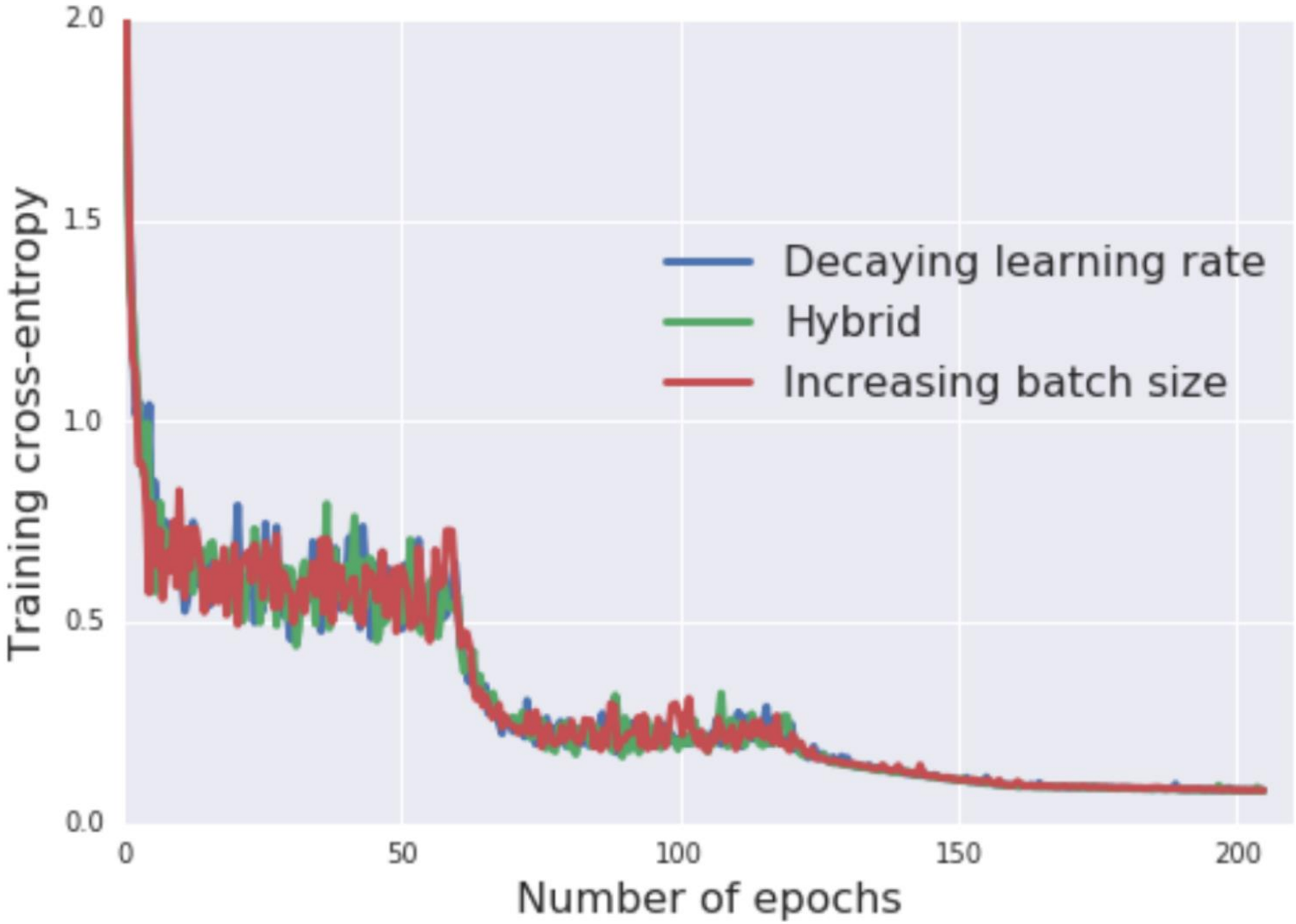
(a) Batch size selection

Learning rates



Source: [Understand the Impact of Learning Rate on Model Performance With Deep Learning Neural Networks]

Convergence is not linear

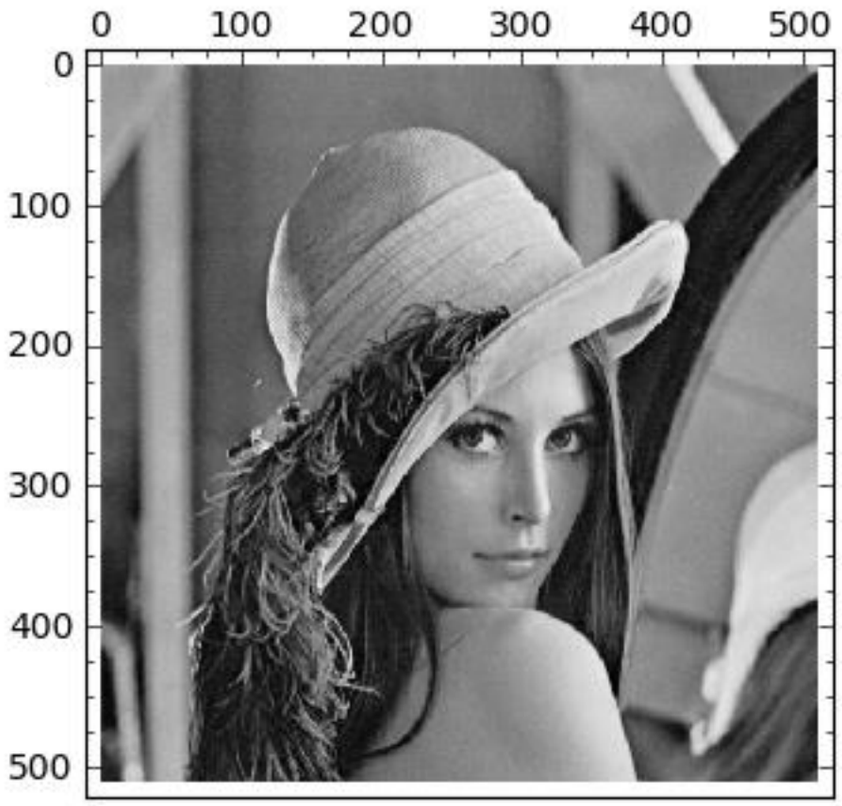


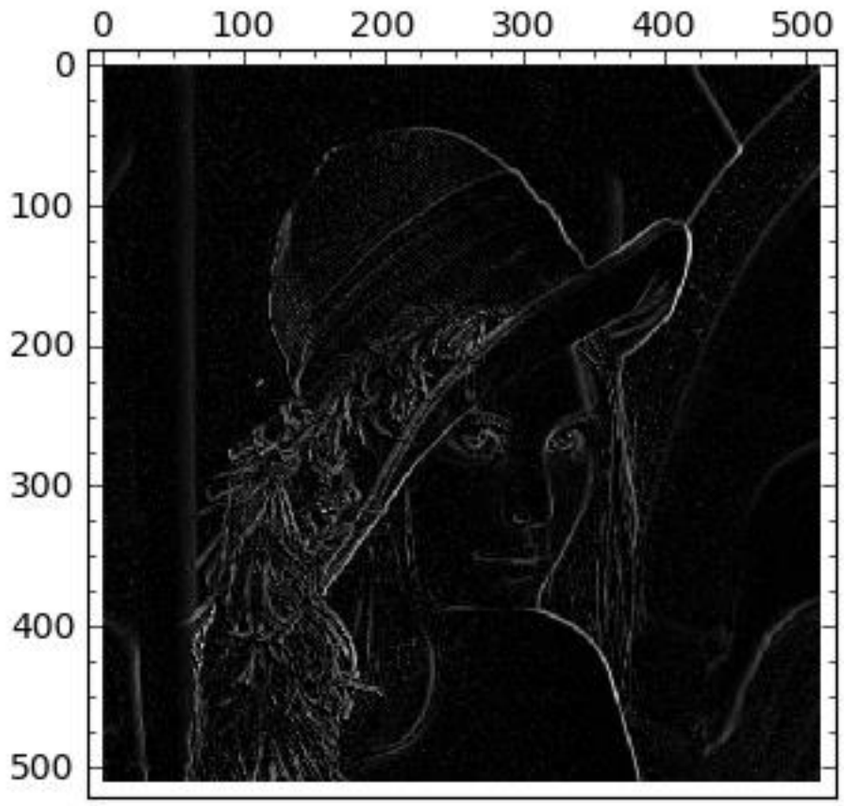
Rules of thumb

- Change one hyperparameter at a time
- Learning rates in orders of magnitude (0.001, 0.0001, etc.)
- Initial phase of exploring hyperparameters
- Hyperparameter optimisation is active area of research
- Convergence is not linear. Be patient!
- **Be patient!**

Convolutions

- Applying a filter to an image.



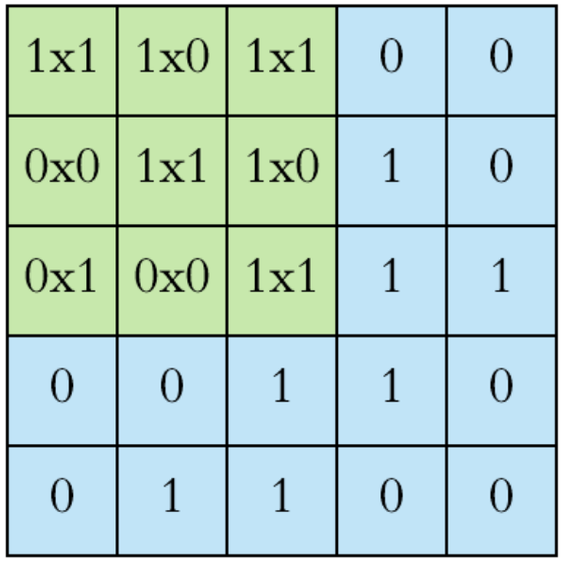


Source: http://gearons.org/2018-02-02-tLSTM/

Convolutions

- We can think of convolutions as small filters on the image.

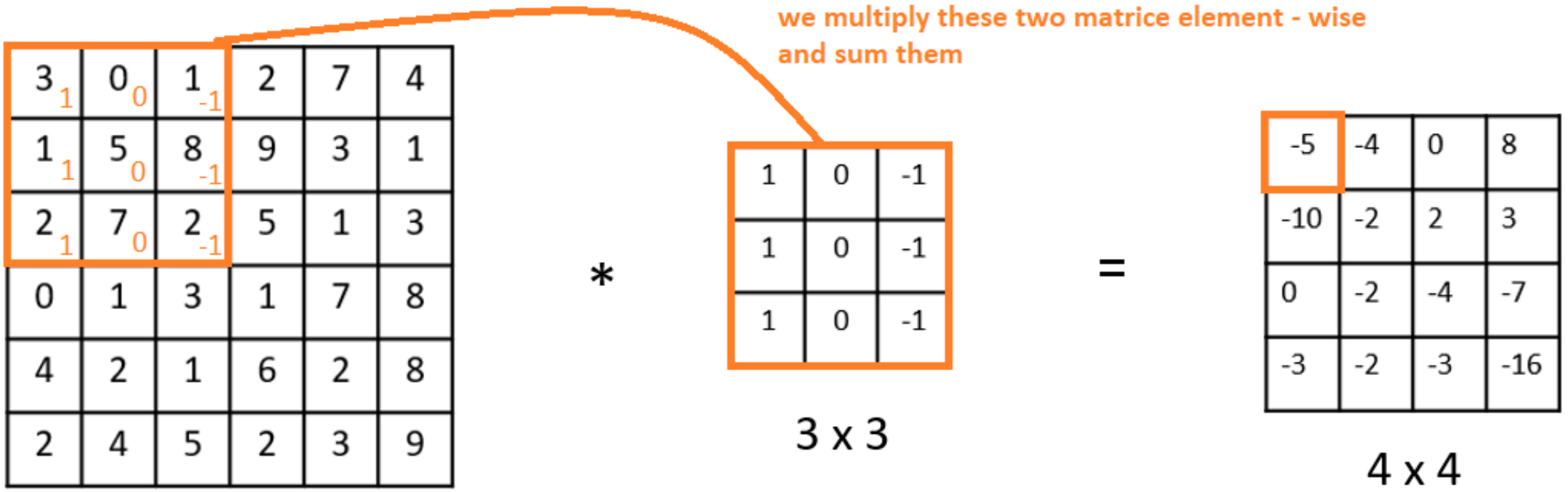
- They process parts of the image and "fire" when they detect the filter pattern.



Source: https://medium.freecodecamp.org/an-intuitive-guide-to-convolutional-neural-networks-260c2de0a050

Convolutions

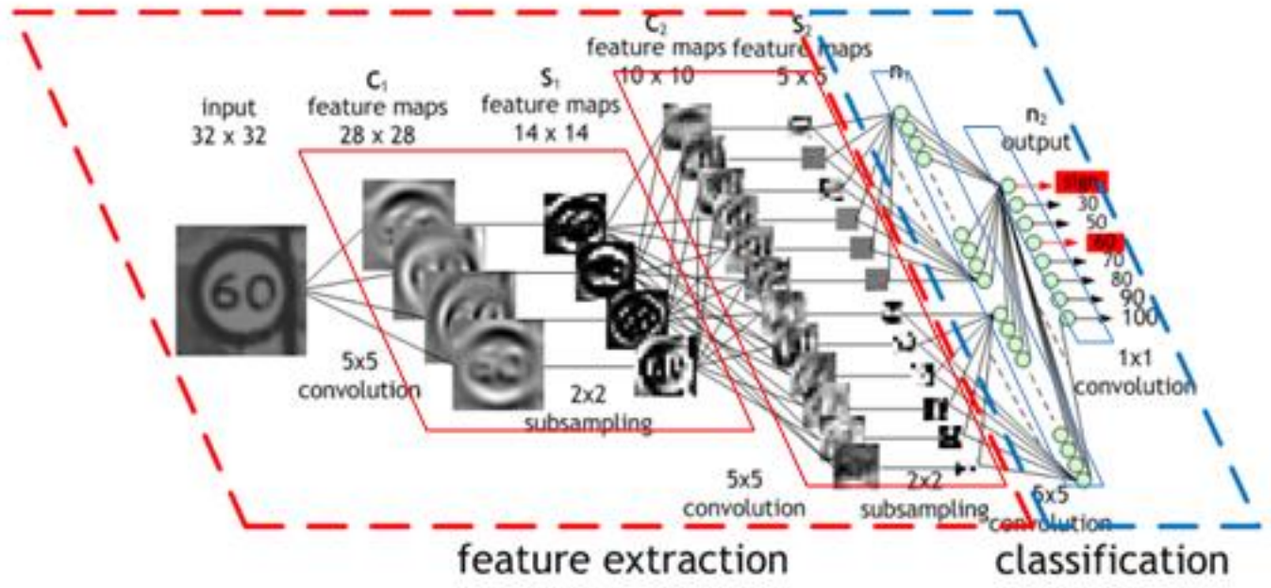
Technicalities



Source: https://developer.nvidia.com/discover/convolutional-neural-network

Convolutions

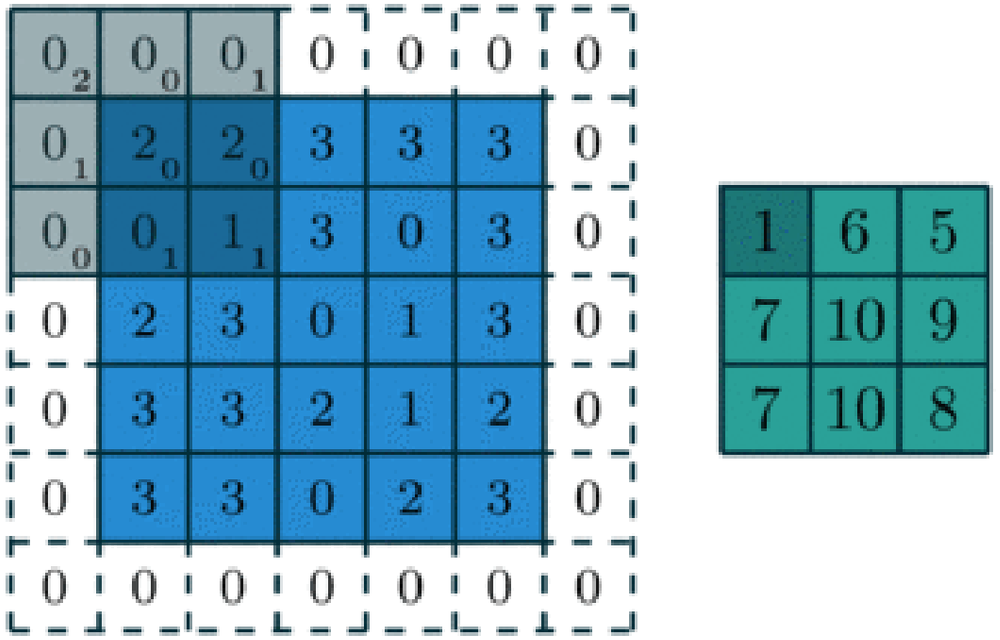
- Stack convolutions
- Create filters from other filters
- Detect more complex patterns



Source: https://developer.nvidia.com/discover/convolutional-neural-network

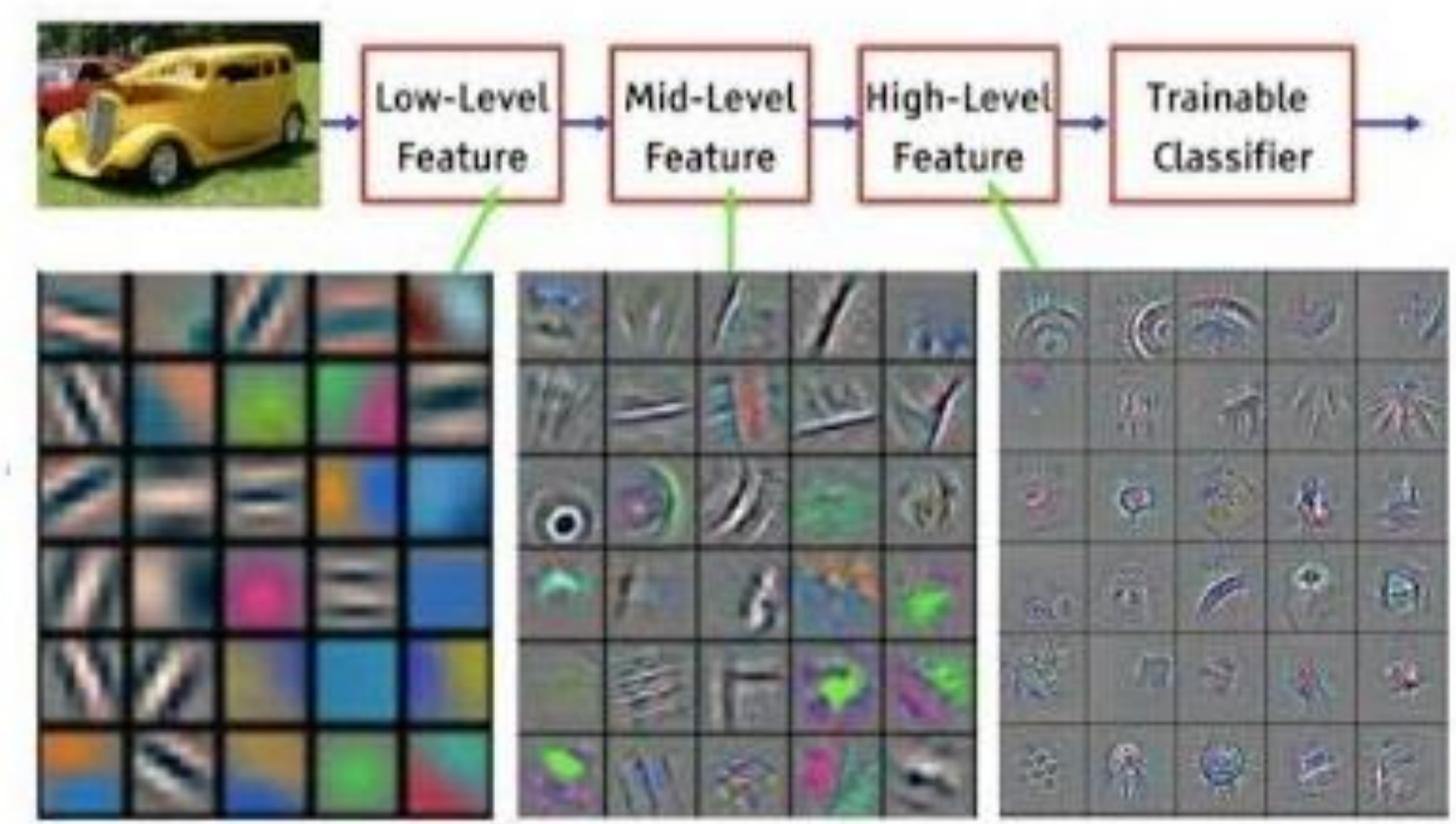
Convolutions

- We apply a **kernel** with dimensions (3, 3).
- Using **stride** = 2.
- **Padding** = 1, to increase output size
- **Same-padding** = Output is same size as input
- Otherwise **valid-padding**.
- Apply activation function to output.
- We try to **learn the filters**! The filters are the parameters/weights.



Source: http://deeplearning.net/software/theano_versions/dev/tutorial/conv_arithmetic.html

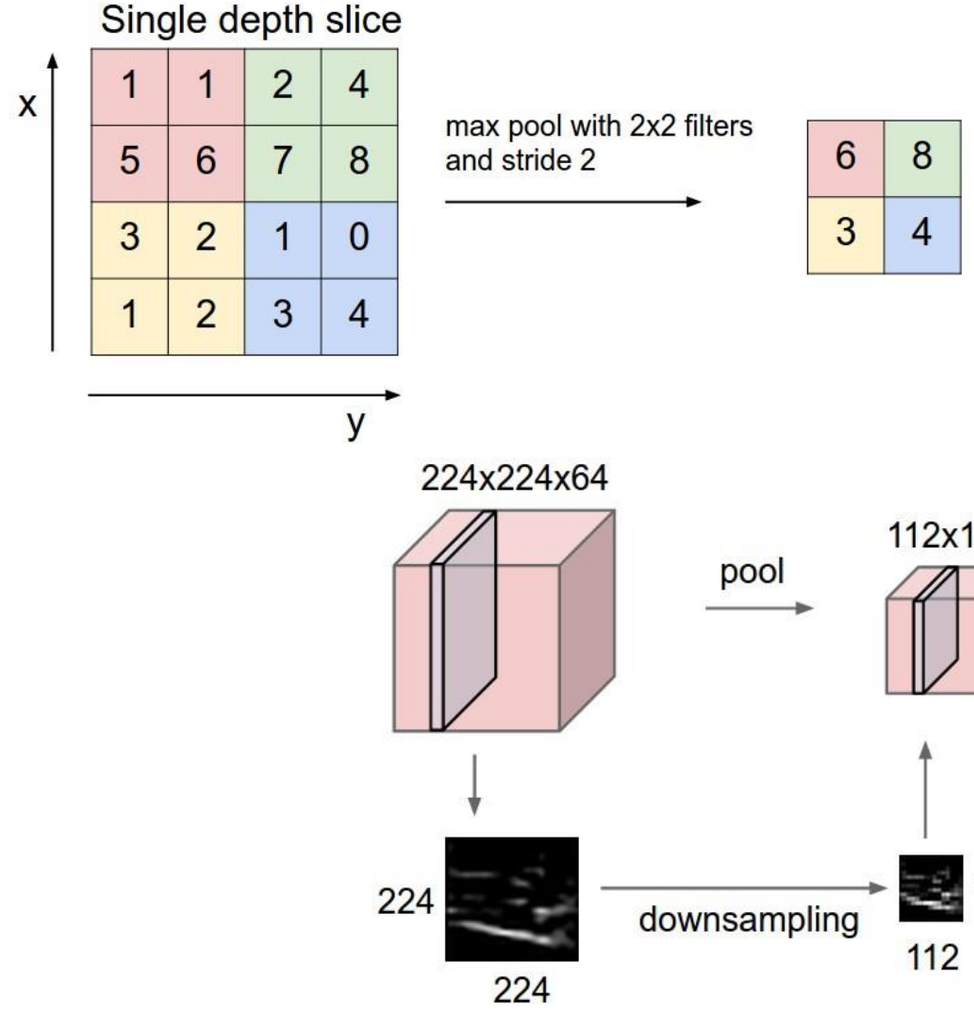
Feature hierarchy



Feature visualization of convolutional net trained on ImageNet from [Zeiler & Fergus 2013]

CNNs

Pooling layers



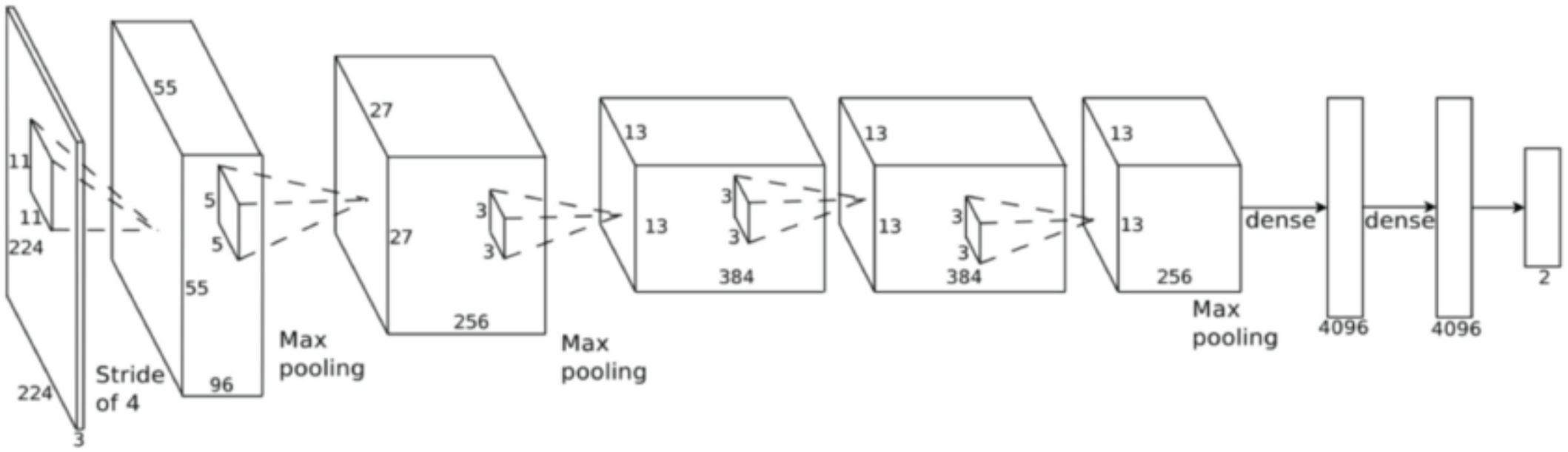
- Our filter maps are sometimes very large, so we make them **smaller using pooling**.
- **Max pooling**, take the max.
- Applied after convolutions

Source: http://deeplearning.net/software/theano_versions/dev/tutorial/conv_arithmetic.html

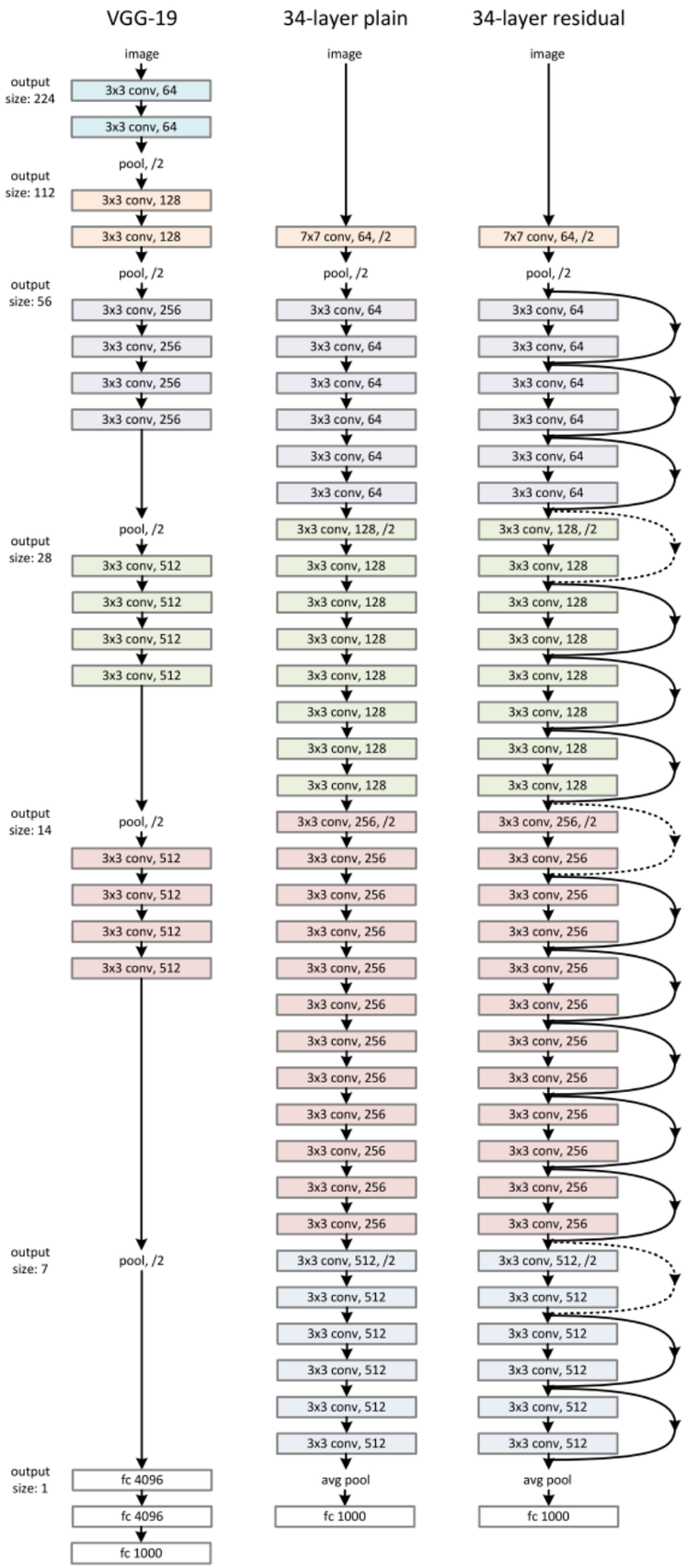
CNNs

Architectures - AlexNet

- By chaining different combinations of them we can create Convolutional Neural Networks (CNNs).



Source: https://www.jeremyjordan.me/convnet-architectures/

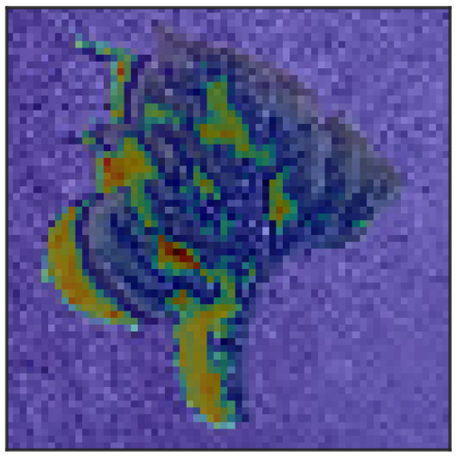
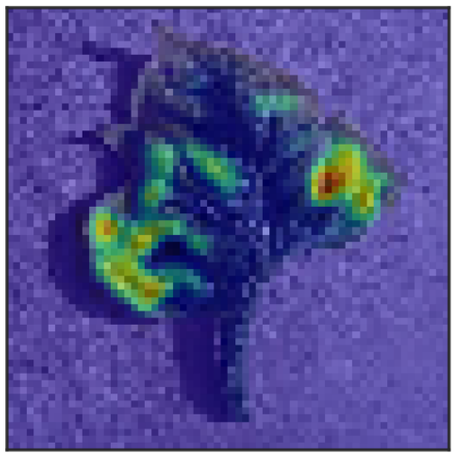
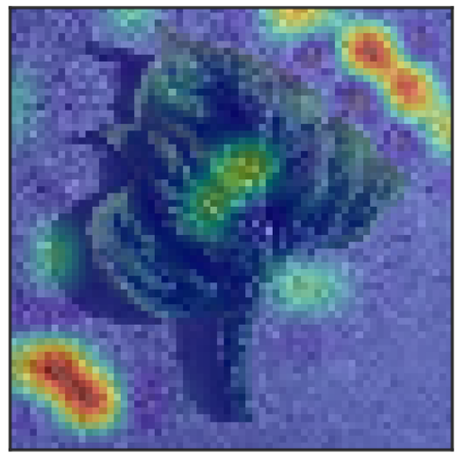
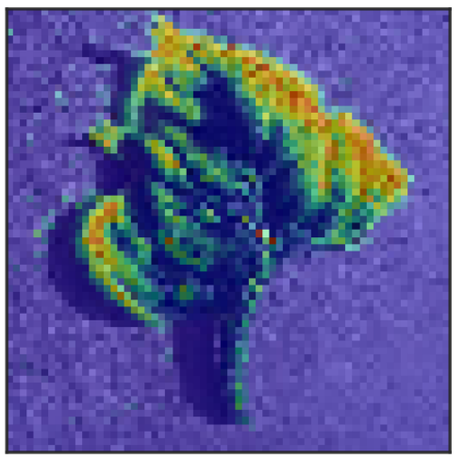
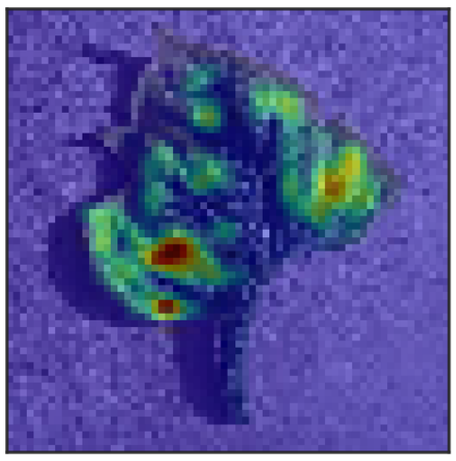


CNNs

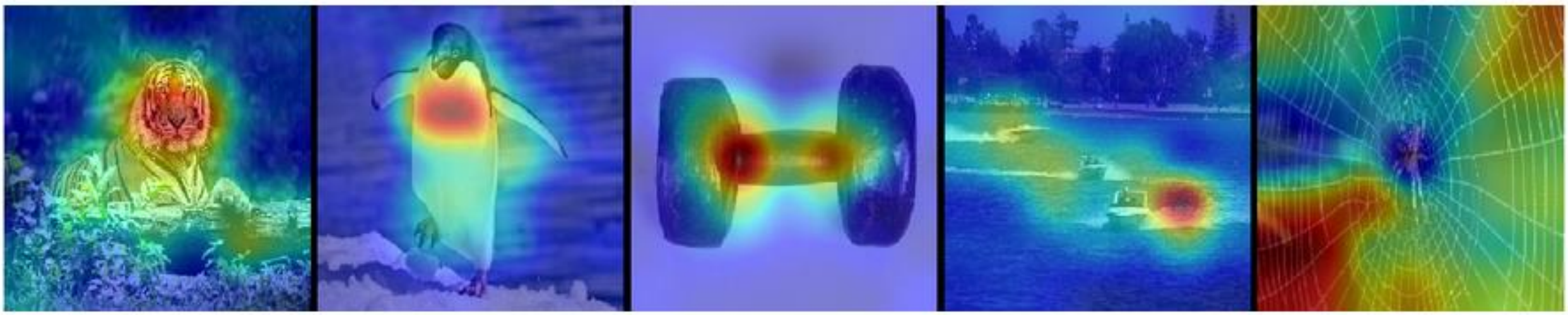
Architectures - ResNet (2015)

Source: https://arxiv.org/abs/1512.03385

Class activation maps

	Conv. layer 1	Conv. layer 2	Conv. layer 3
Healthy			
Diseased			

Class activation maps



Hands-on

Kill your notebooks!

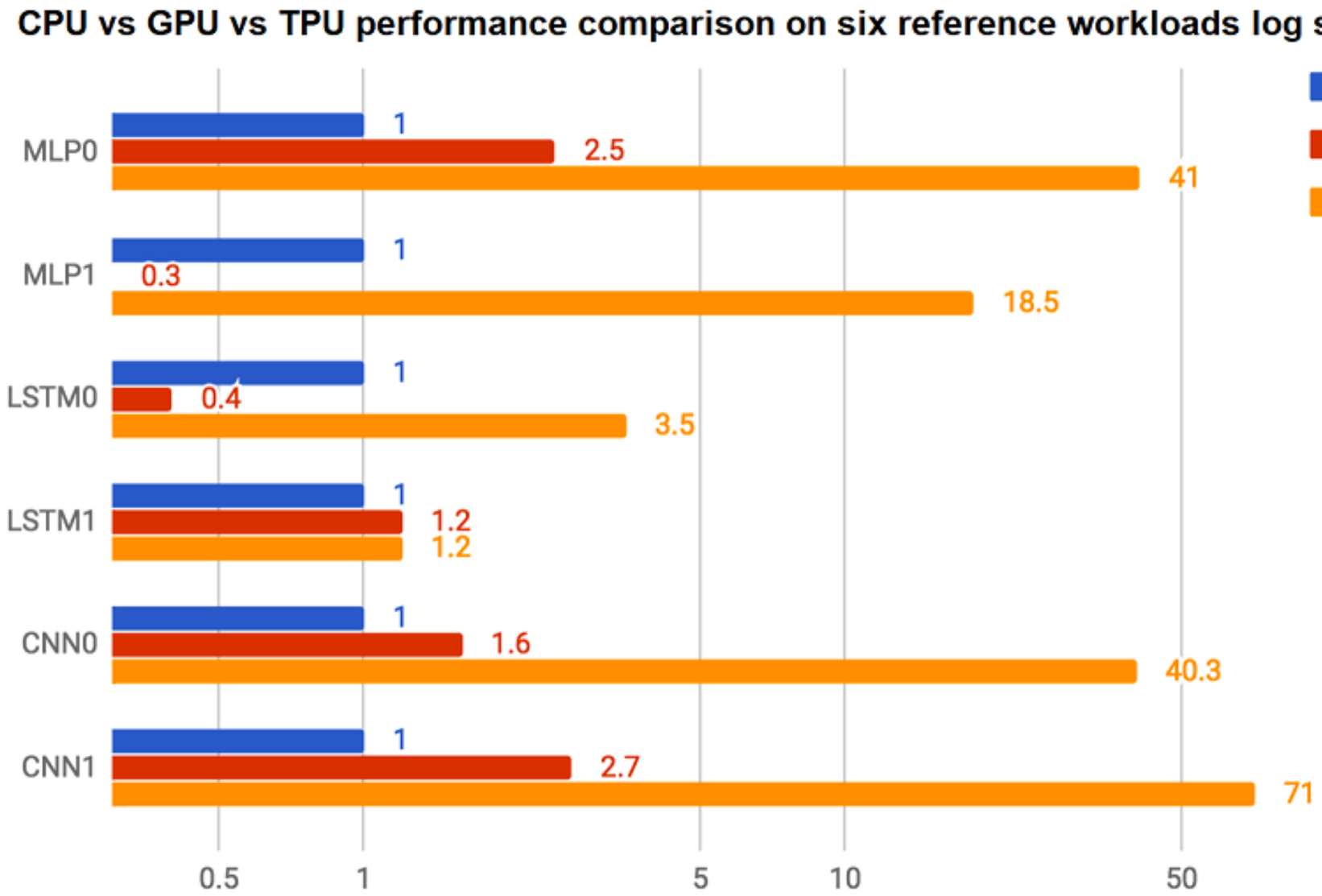
Notebook: 03-your-first-cnn.ipynb

Break at 14:30

Recap

- Initialisation of weights is random
- Filters can be redundant or useless
- Class activation maps are not perfect
- Pixel values are normalised
- Fully-convolutional networks and dense layers

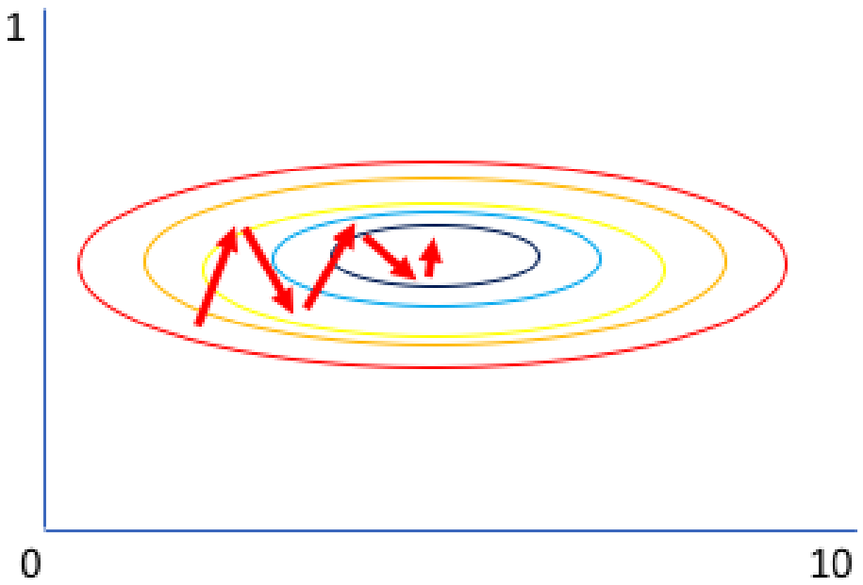
CPUs, GPUs, TPUs



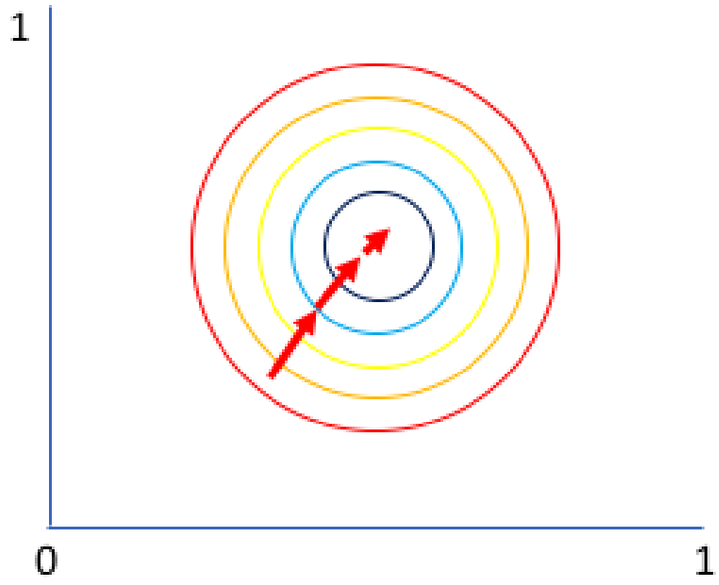
Source: https://www.androidauthority.com/google-powering-ai-816146/

Input normalisation

Why normalize?



Gradient of larger parameter dominates the update



Both parameters can be updated in equal proportions

Source: https://www.jeremyjordan.me/batch-normalization/

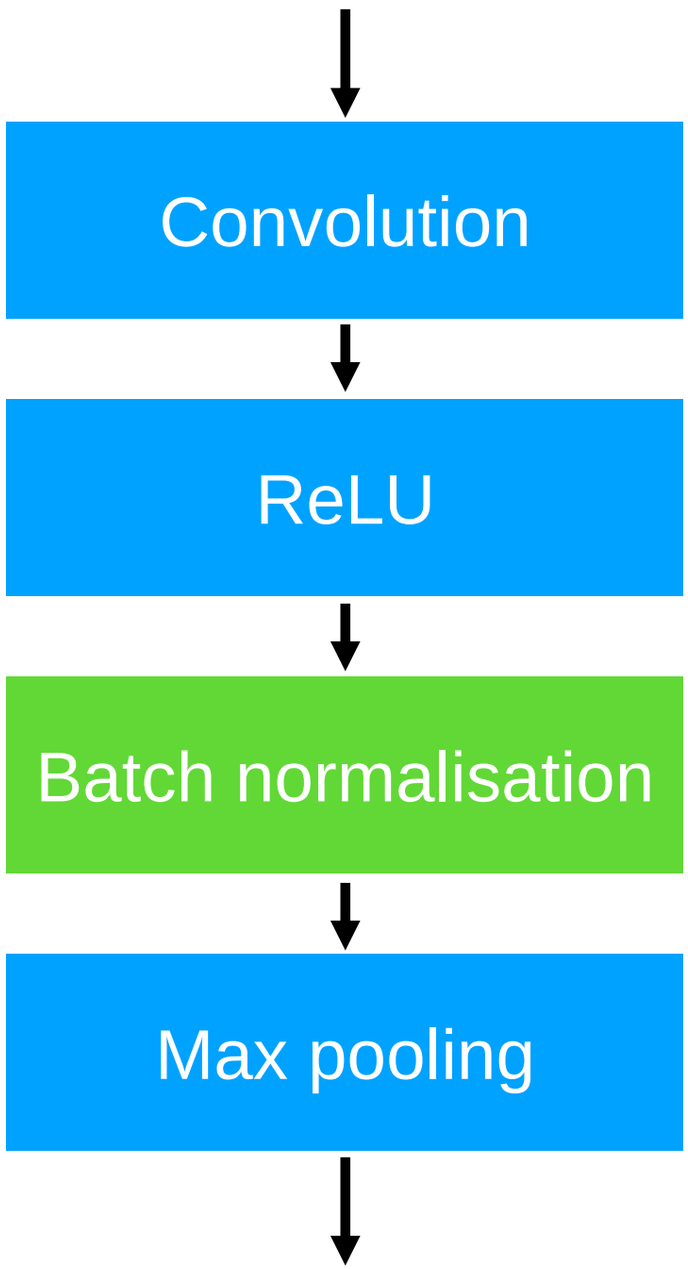
Model improvement

Batch normalisation

- Why only do this normalisation on the input?

- Renormalising in an intermediary layer speeds up learning.

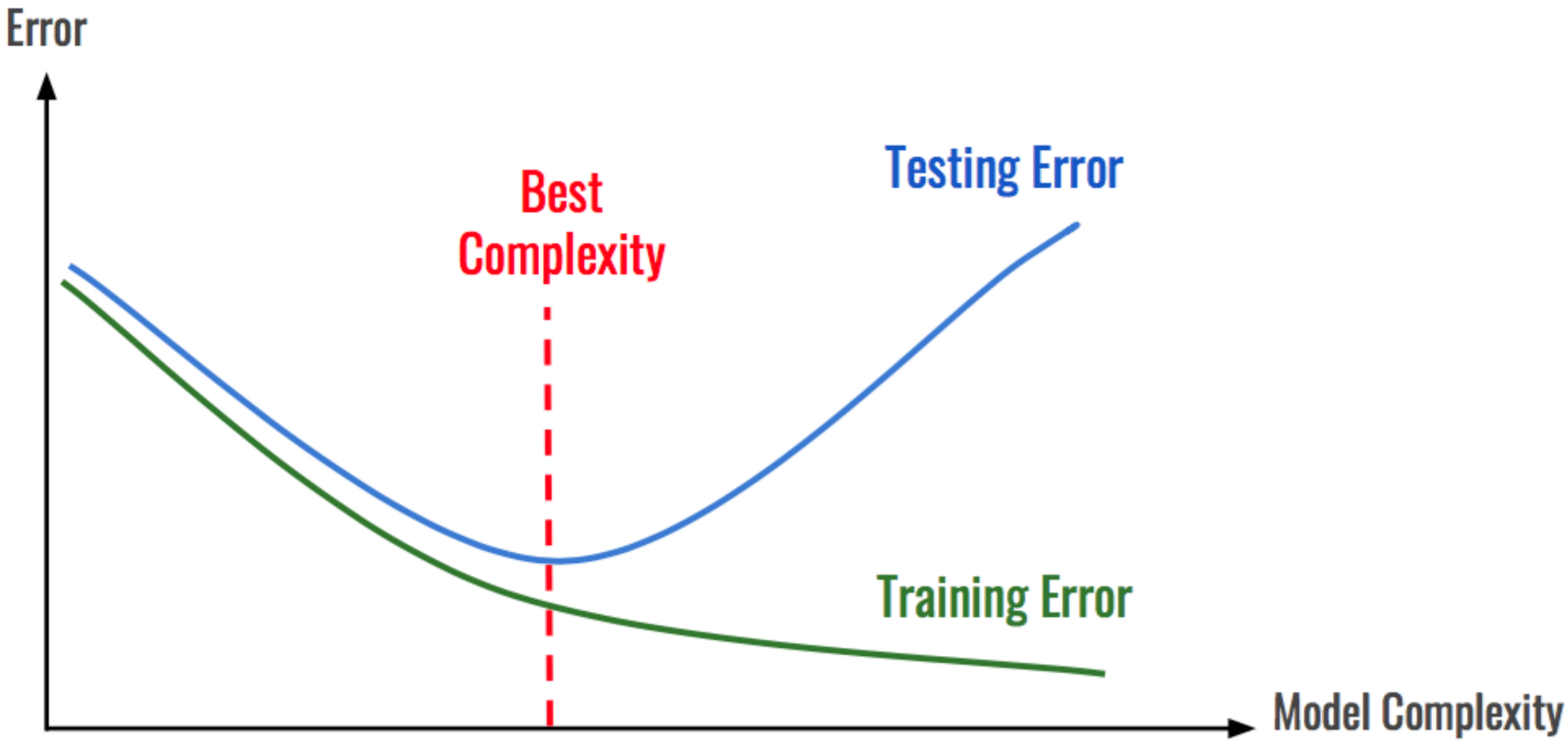
- We compute the mean and variance per batch and uses it to normalise to **0 mean** and **variance 1**.



Batch normalisation

- Adding BN will add more parameters to the model and extra computation.
- BN allow us to more easily train deeper networks.
- BN makes the network more robust to hyperparameter selections.
- BN allows us to train with a higher learning rate.
- We apply BN before the activations.

Controlling overfitting



Source: [Hackernoon]

Regularisation

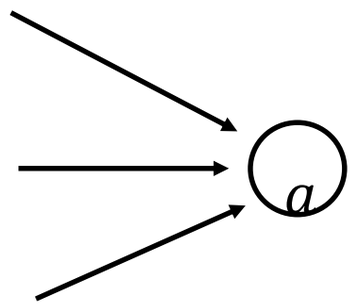
- Controlling the complexity of the model
  - Early stopping
  - Simplifying our network
  - L2 regularisation
  - Dropout

L2 regularisation

- We add a new term to the total loss function.
- This term adds additional loss to the function which takes the value of the weights into account.
- We then optimise this new loss function instead.
- A new **hyperparameter**, λ is added. This is usually a small value and we will need trial and error to find an acceptable value.

L2 regularisation

- Why does L2 regularisation work?



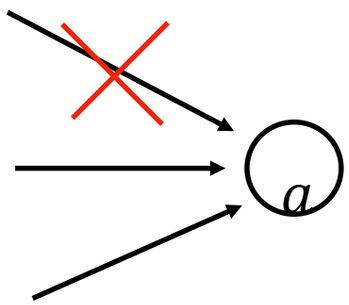
- We add a cost to the weights, thus making a "**more complex**" model **more expensive**.

- If some learnt weight is high (say, 10) it "costs" more than a weight with value 1.

- Thus, our model becomes "simpler" by **forcing the weights down**.

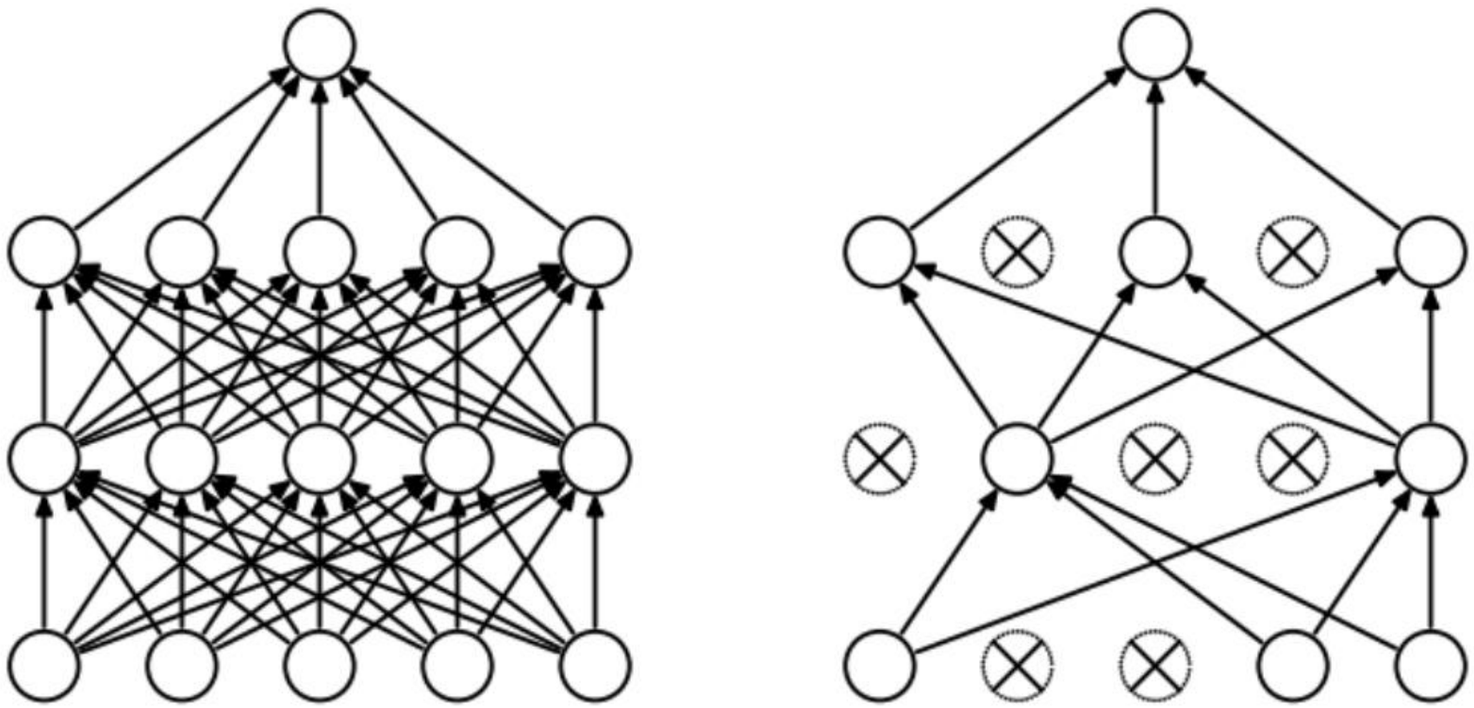
- When some weights are forced to 0, we are effectively "**removing**" **connections**.

Set weight to 0



Dropout

Dropout will **randomly set** the **activations** of neurons **to 0**.



(a) Standard Neural Net

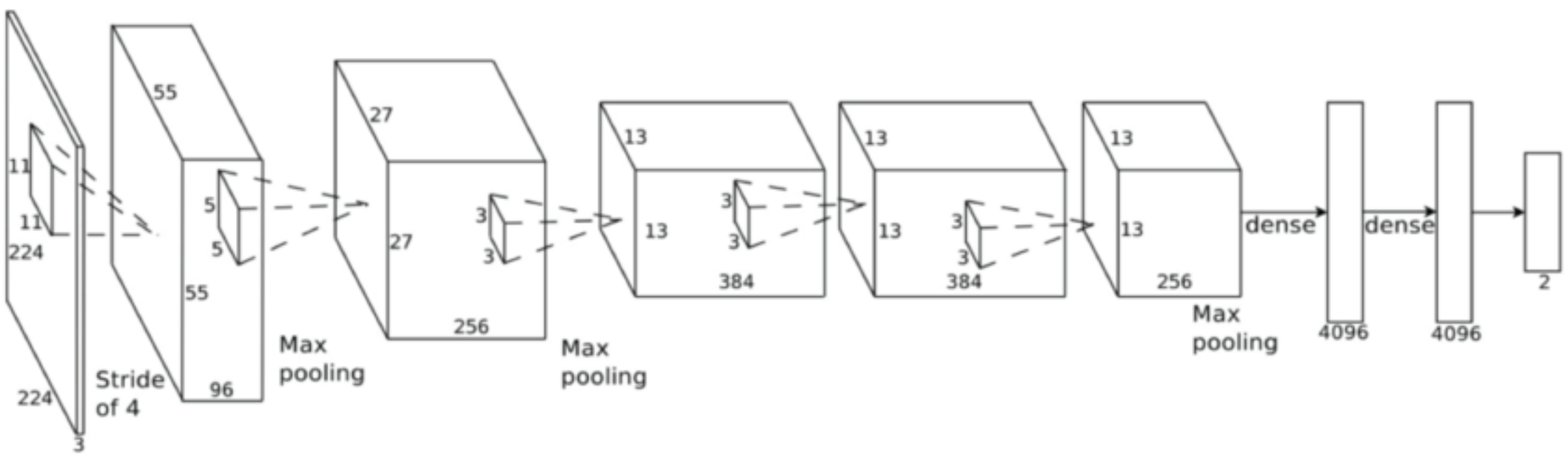
(b) After applying dropout.

Source: [Dropout: A Simple Way to Prevent Neural Networks from Overfitting](), Srivastava et al., 2014

Transfer learning

Pretrained CNNs

- Should we develop CNNs ourselves?
- No, we used them, pre-trained
- This is called **transfer learning**.

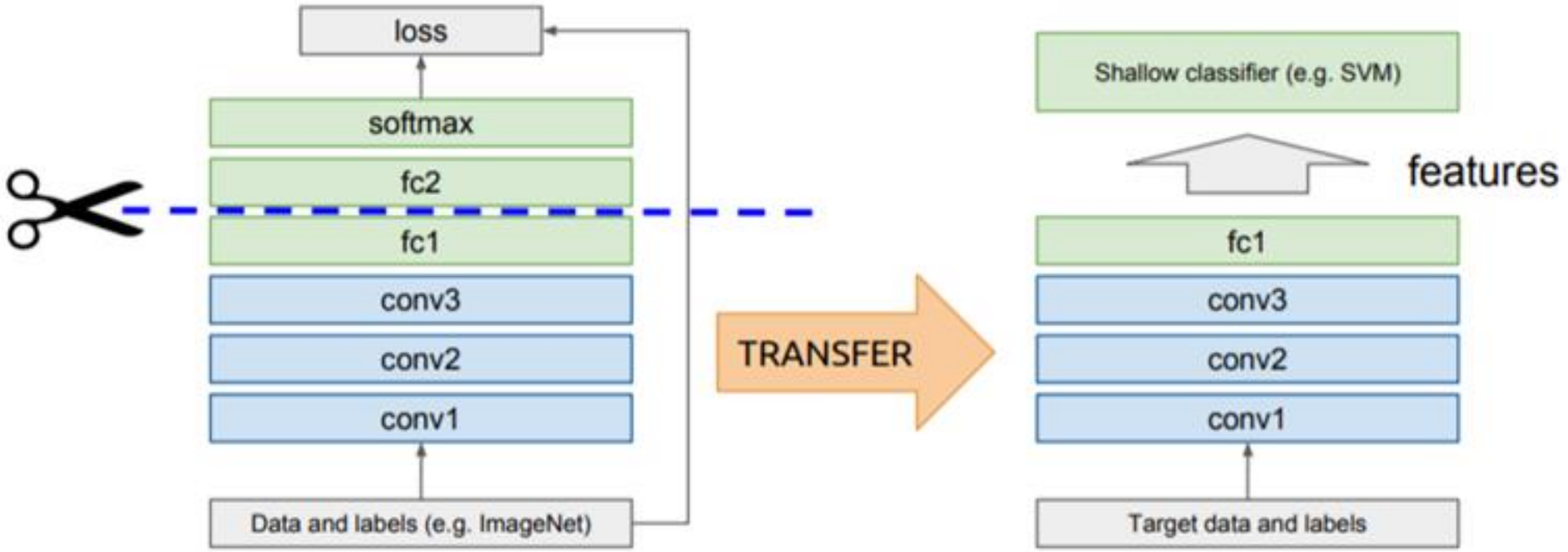


Source: https://www.jeremyjordan.me/convnet-architectures/

Transfer learning

Idea: use outputs of one or more layers of a network trained on a different task as generic feature detectors. Train a new shallow model on these features.

Assumes that $D_S = D_T$

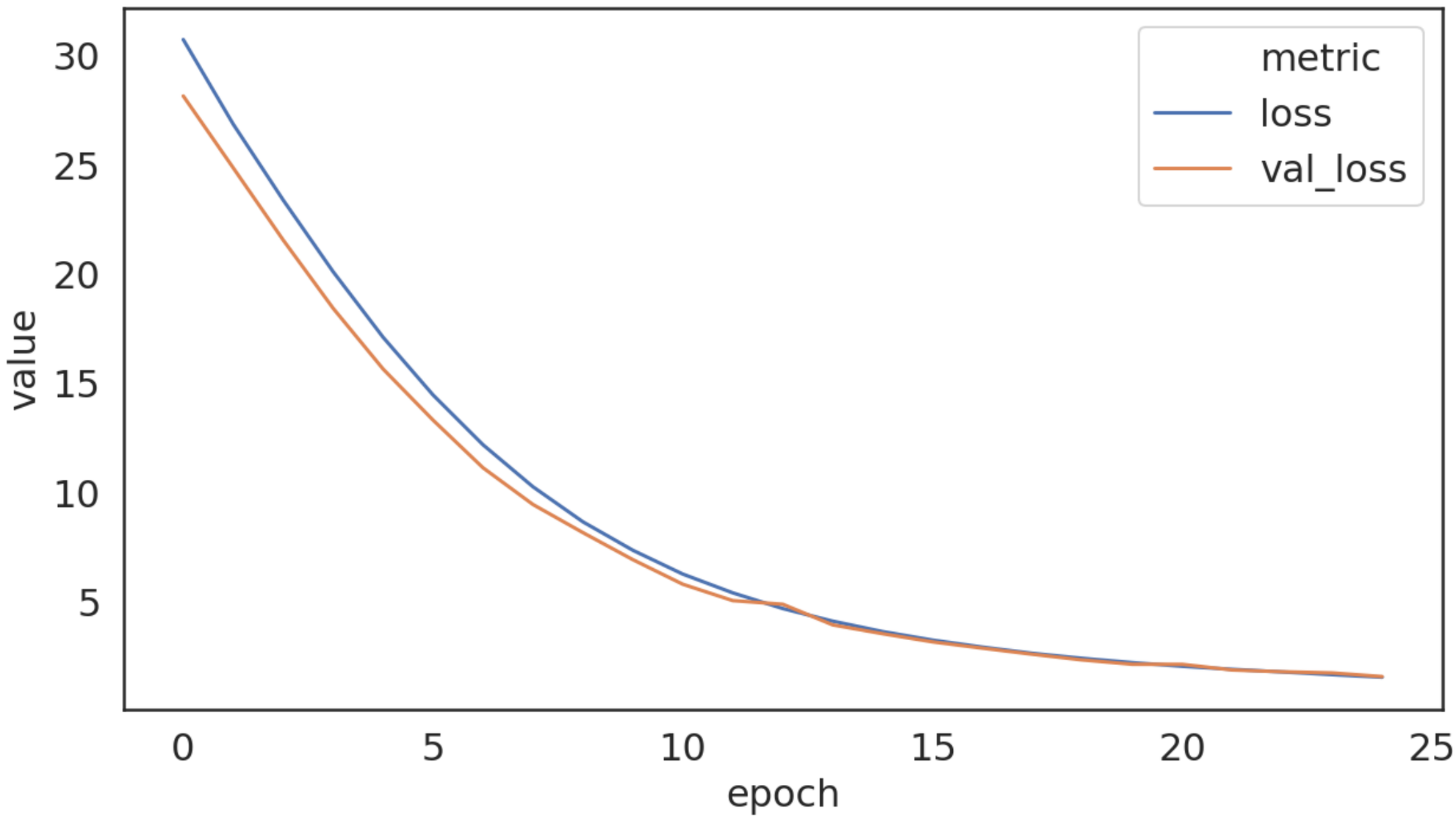


Hands-on

Kill your notebooks!

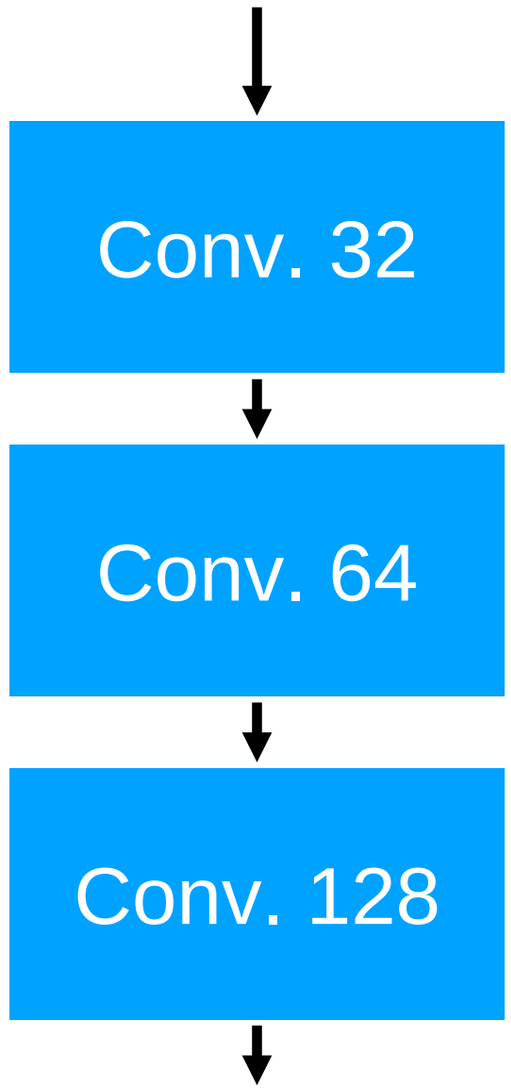
Notebook: 04-improving-neural-networks.ipynb

Recap



Rules of thumb

- Number of filters as multiple of two
- Context with convolution
- Classification with dense networks
- First overfit, then regularise



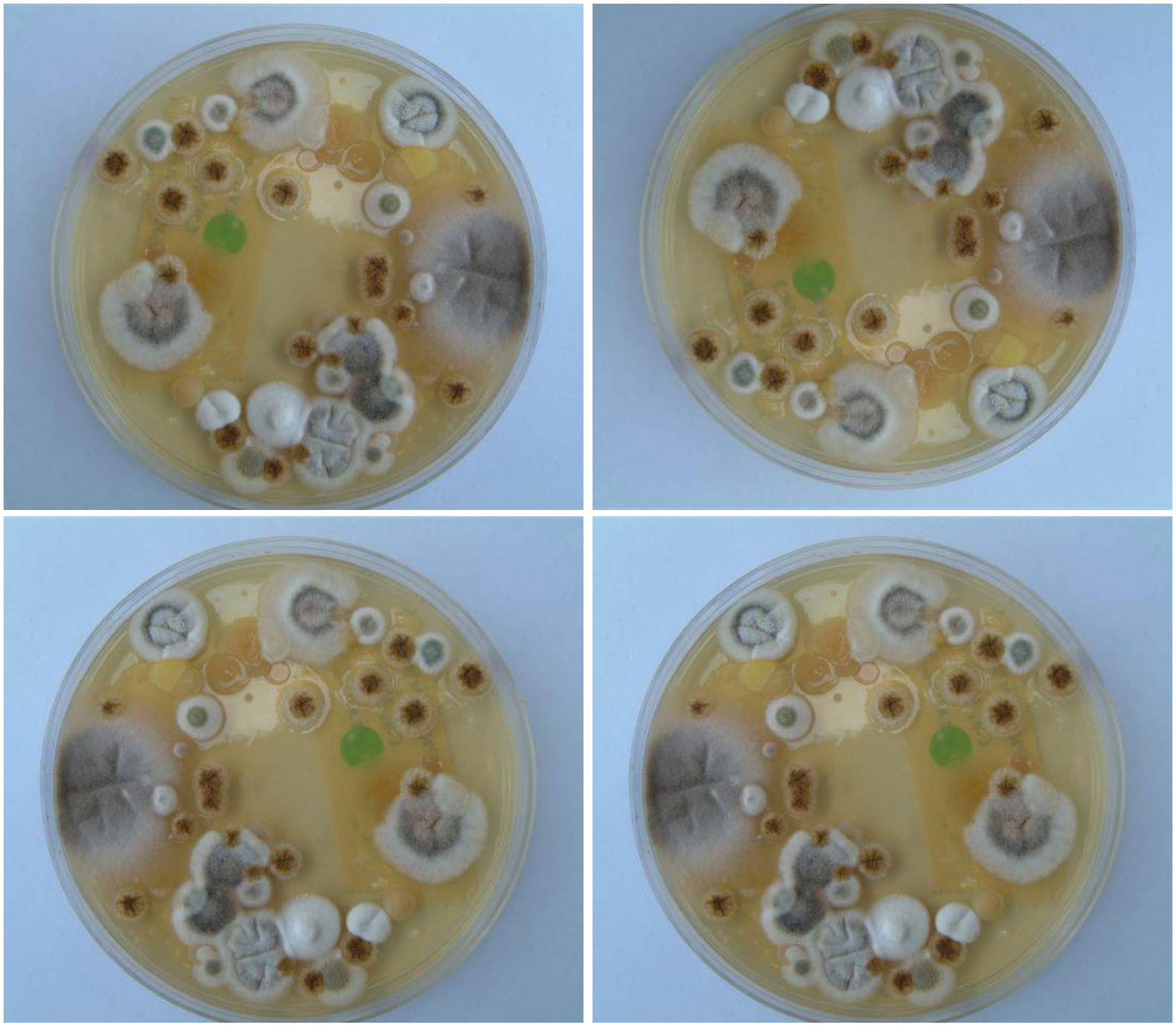
Life science & deep learning

Augmentation for small data sets

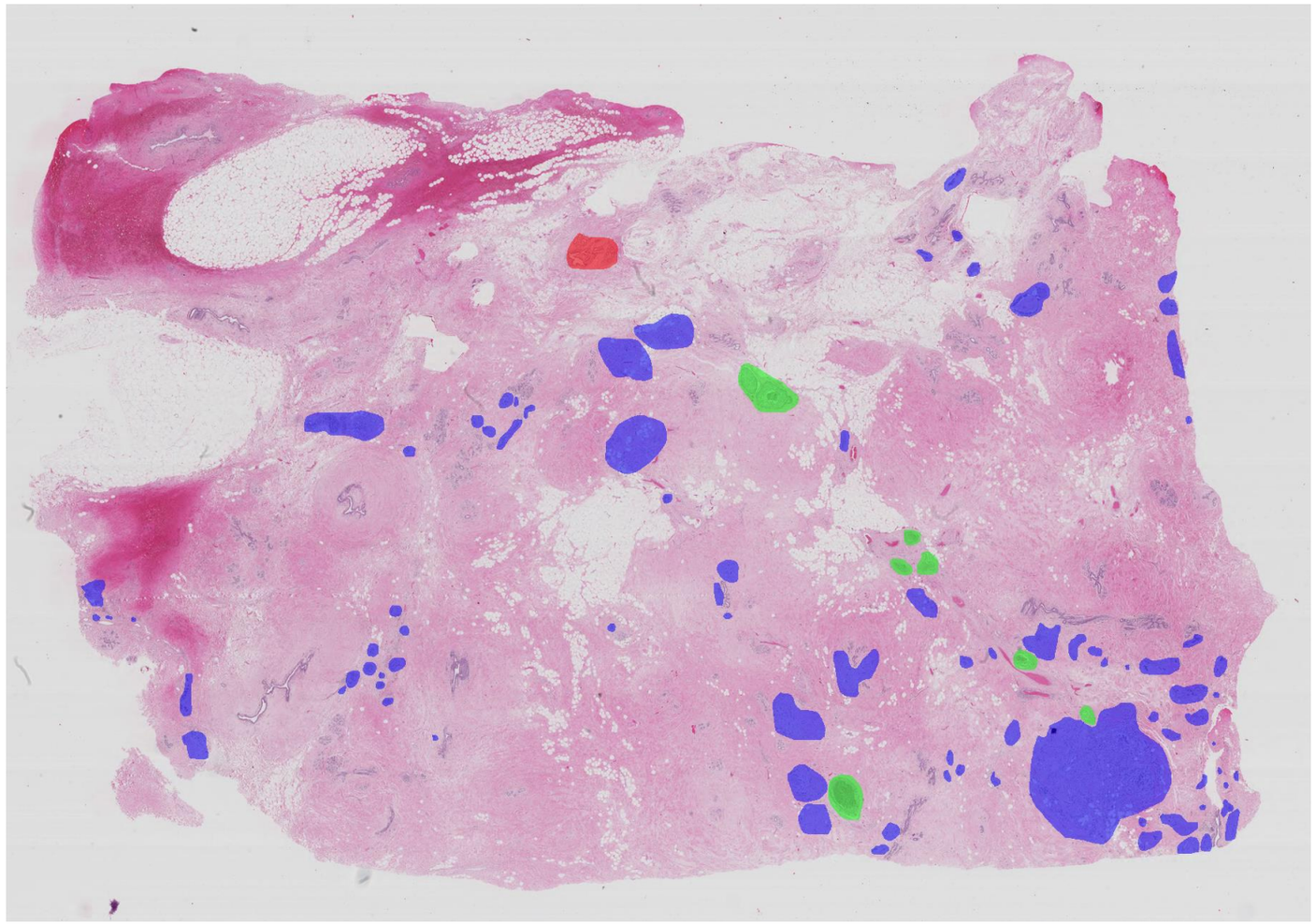
	Original	Positional Augmentation	Color Augmentation
Base			

Source: [Data Augmentation with Masks]

Augmentation



Large images

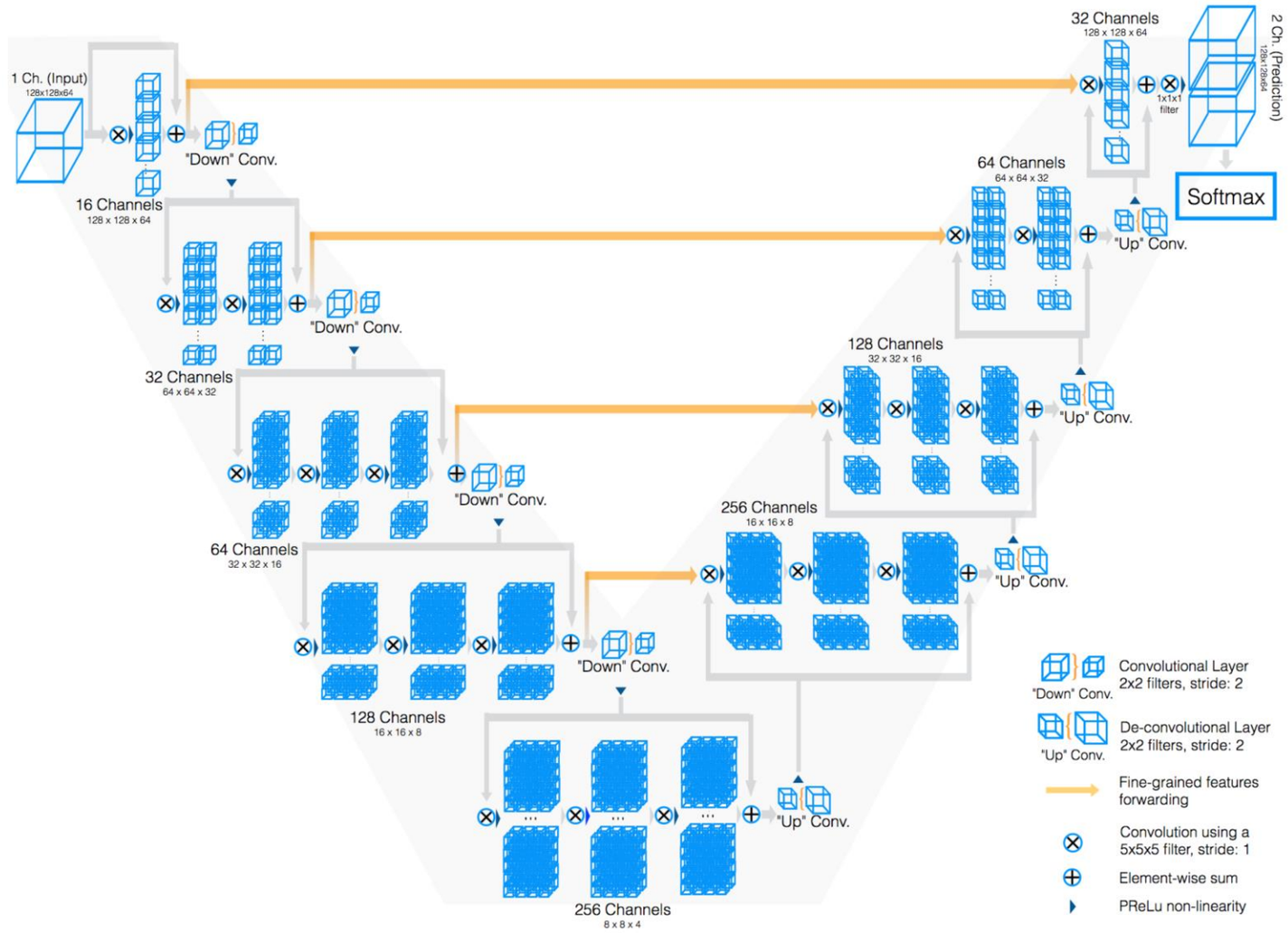


42113 x 62625 pixels

Source: [BACH Grand Challenge]

Life science & deep learning

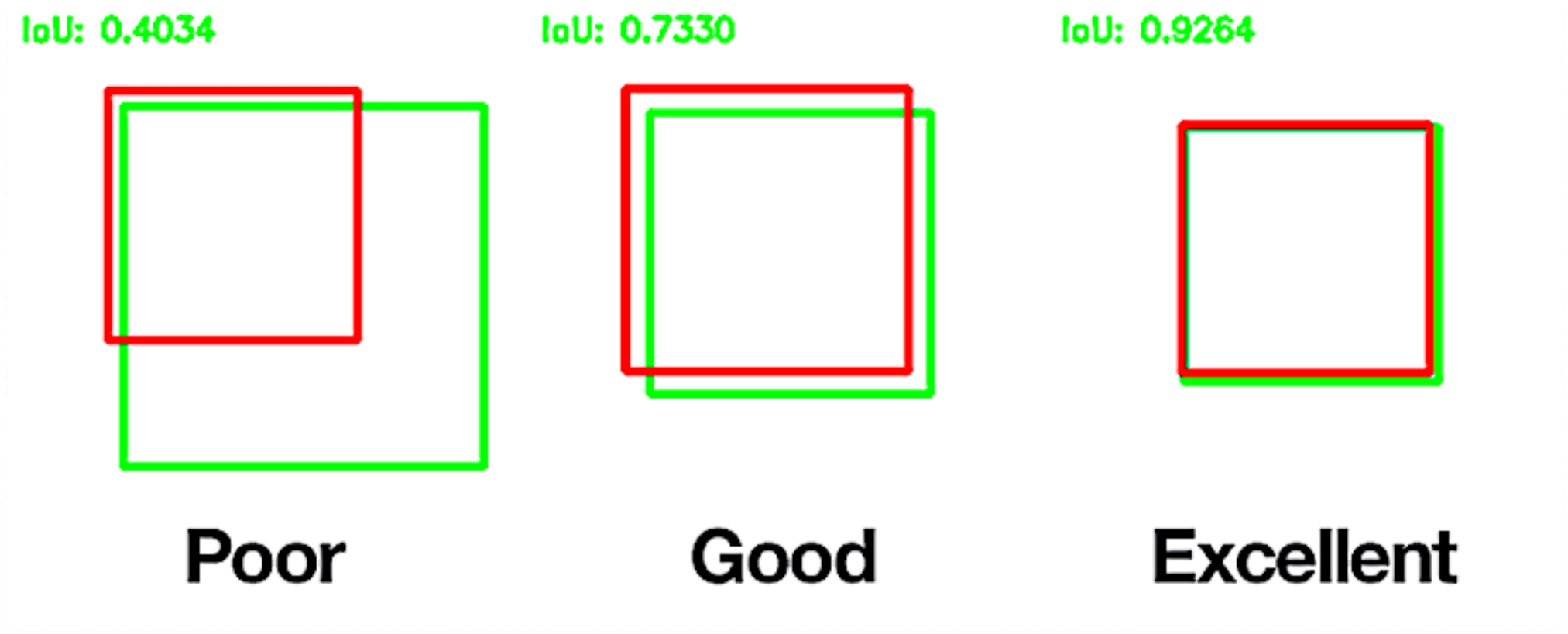
Large (volumetric) images



Source: [V-Net: Fully Convolutional Neural Networks forVolumetric Medical Image Segmentation]

Life science & deep learning

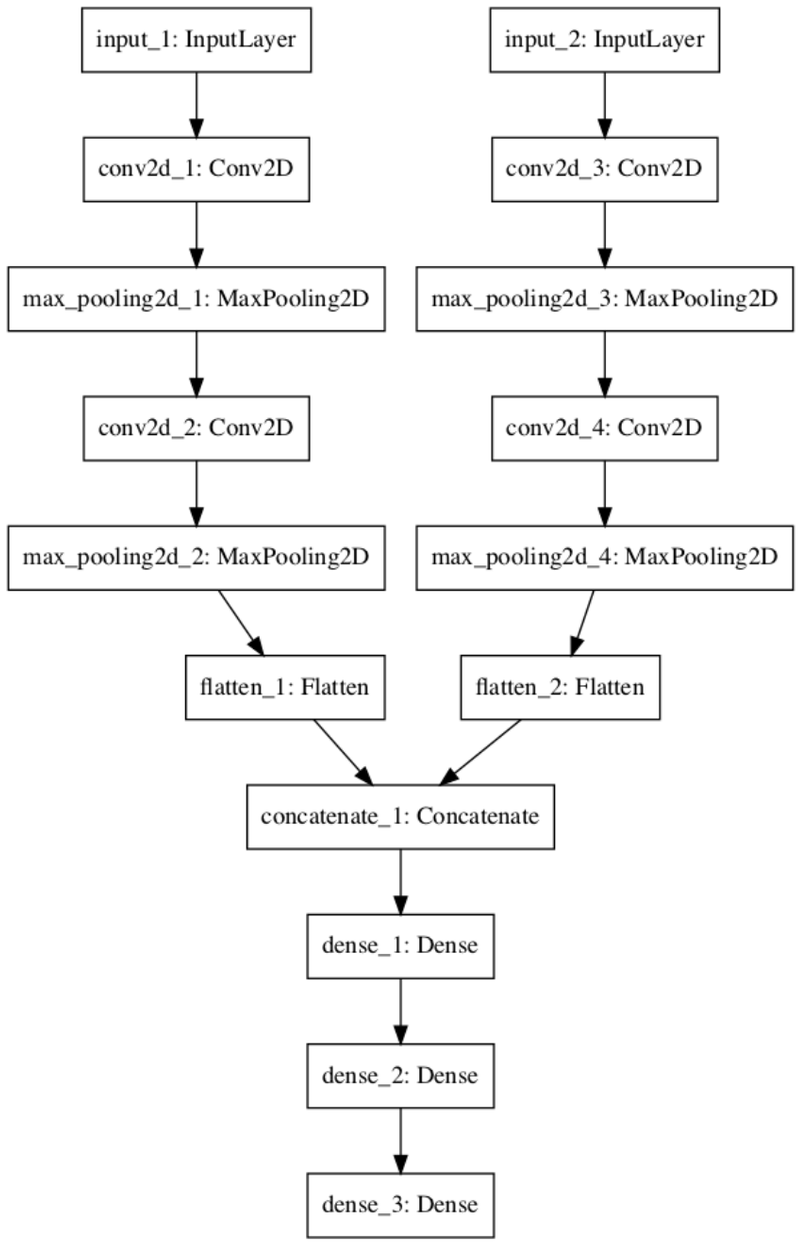
Custom metrics or optimisation



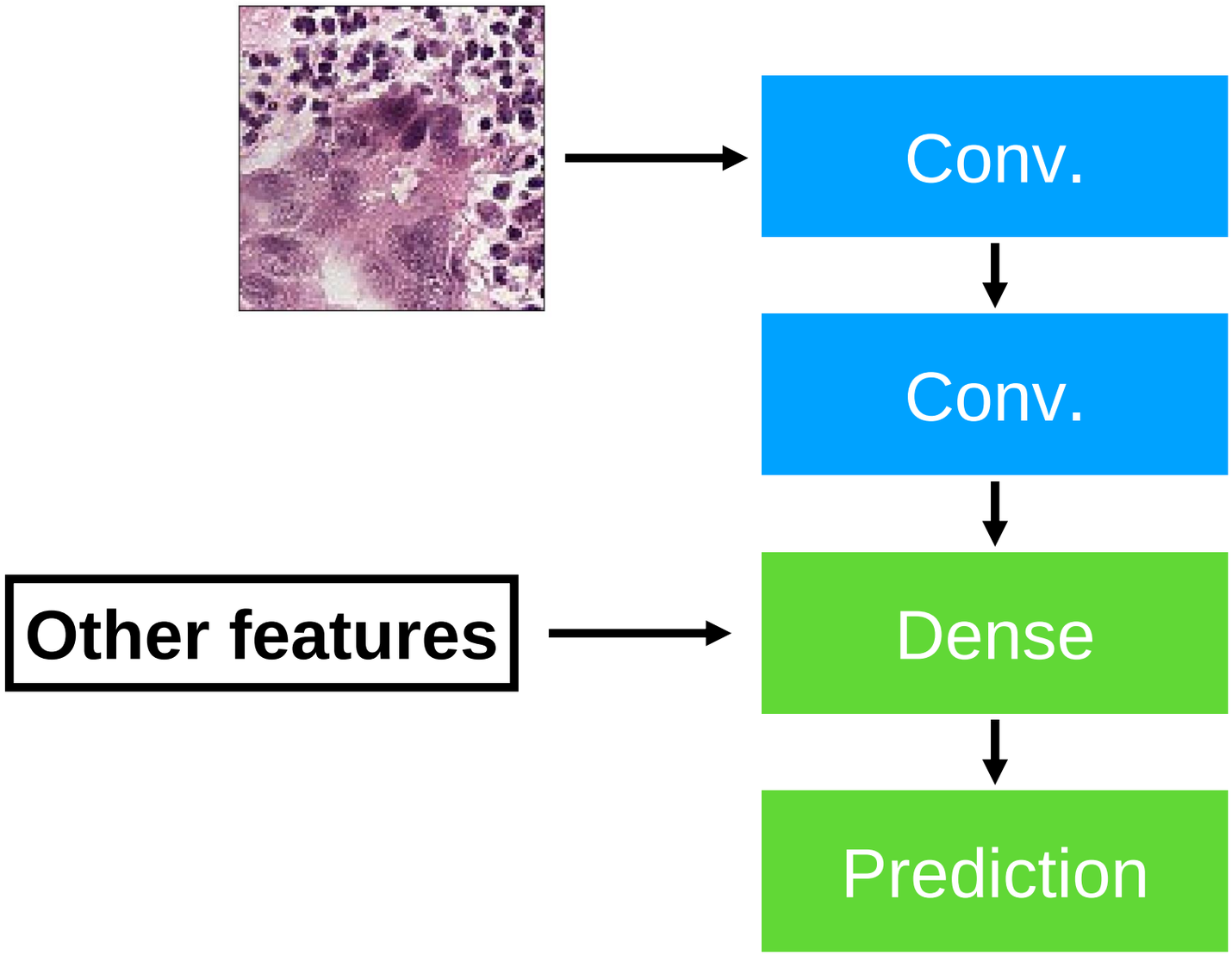
Source: [Deep Learning in Medical Imaging V]

Domain-specificity

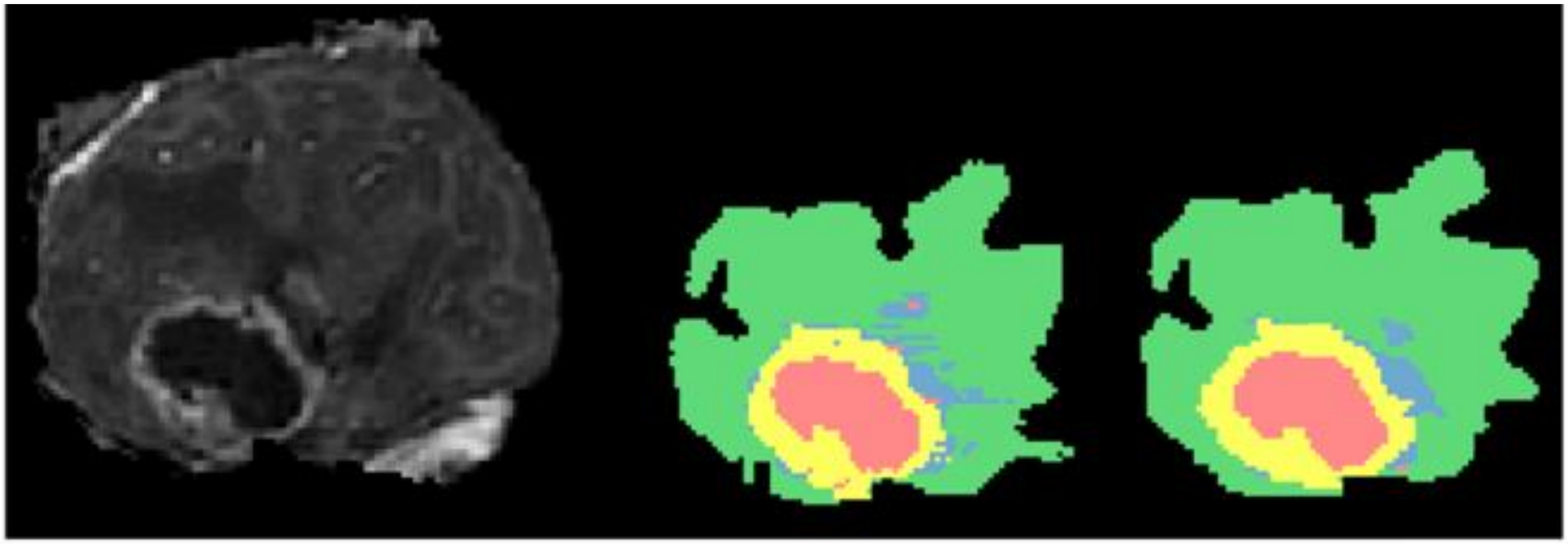
- Combining data
- Application of domain knowledge
- ‘Domain-specific’ normalisation



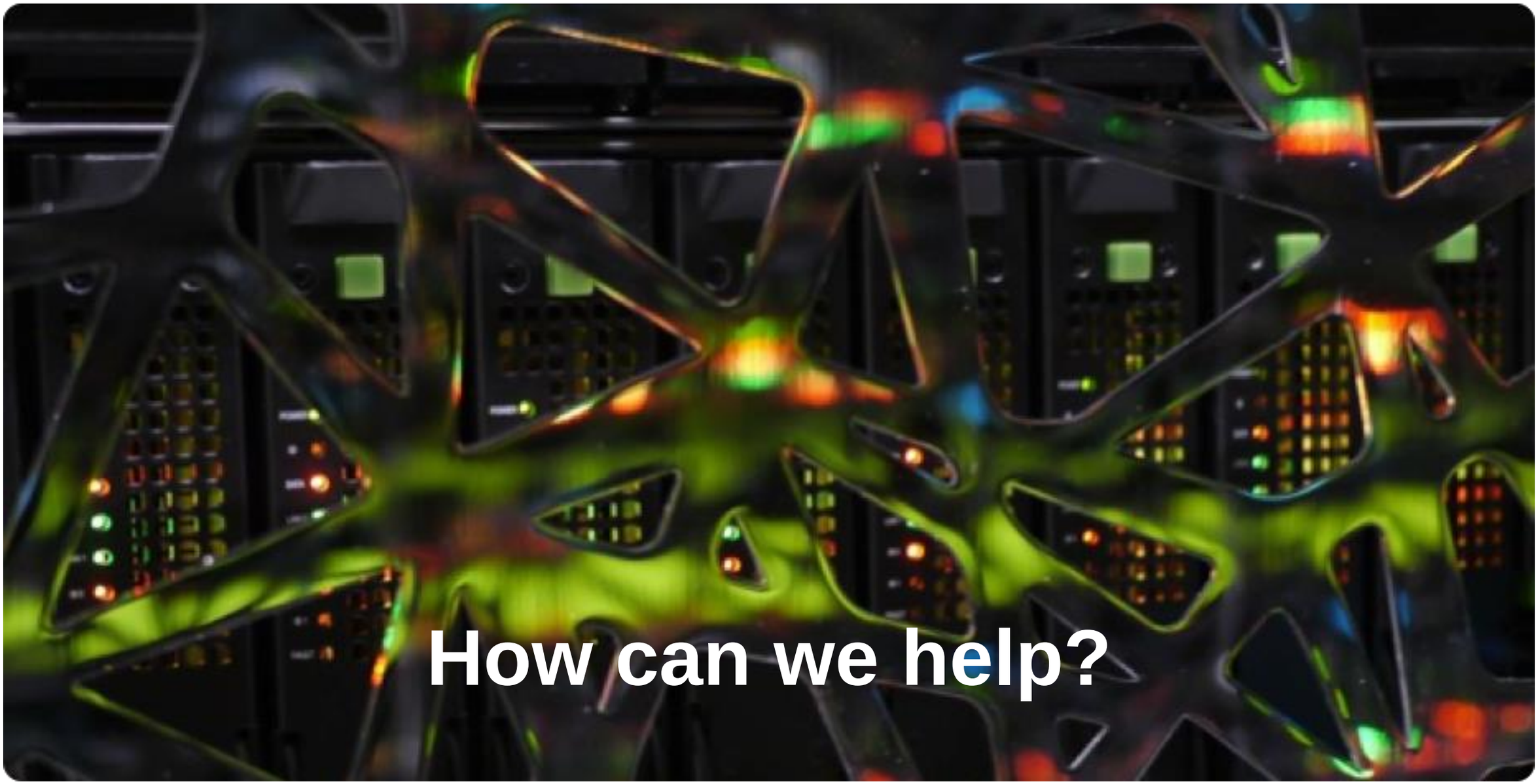
Combining data

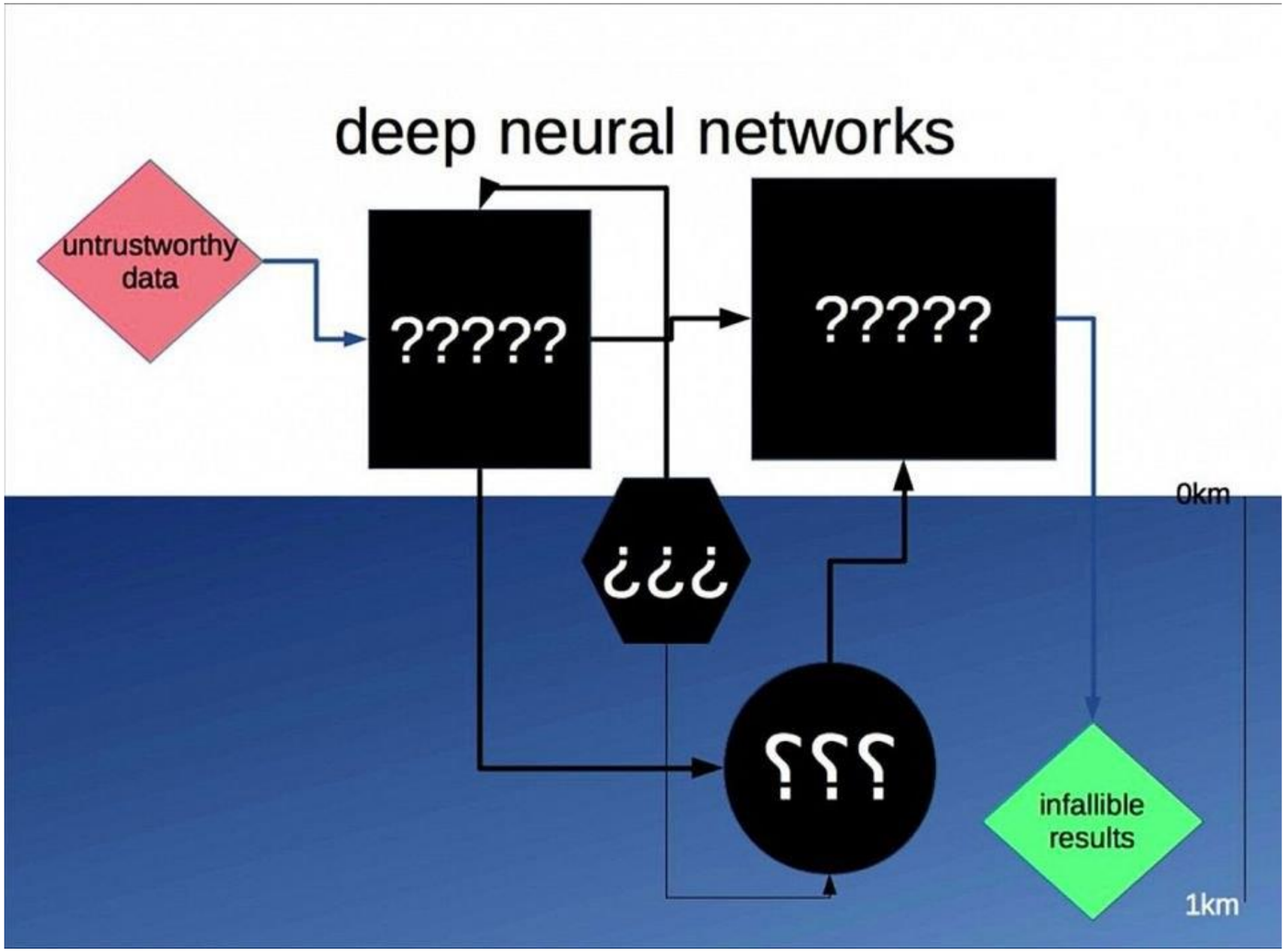


Interpretability



Consultancy





helpdesk@surfsara.nl