Deep learning introduction

netherlands eScience center

netherlands eScience center

ChatGPT

https://poe.com/

netherlands eScience center

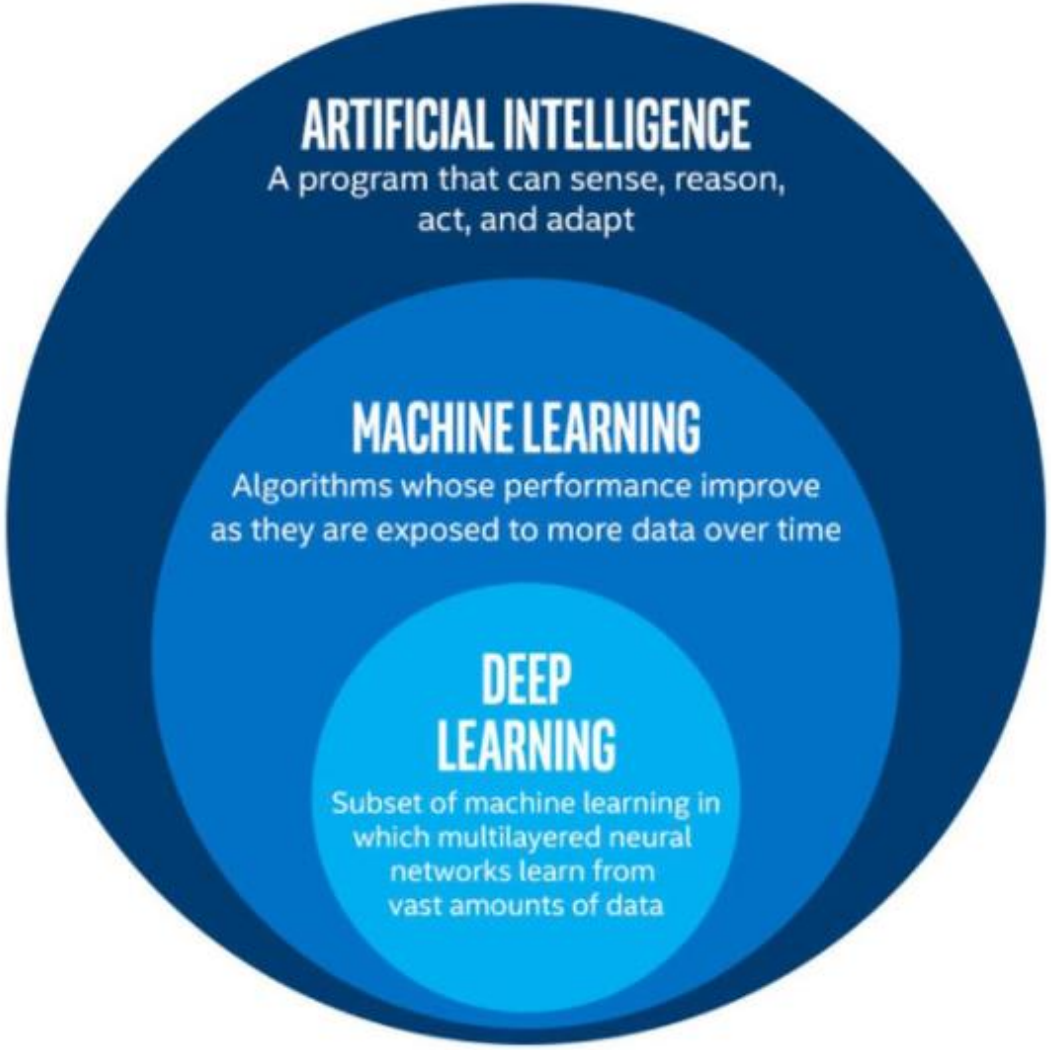
Rationale

Provide you with just enough intuition about deep neural networks to start implementing them.

Then learn by doing.

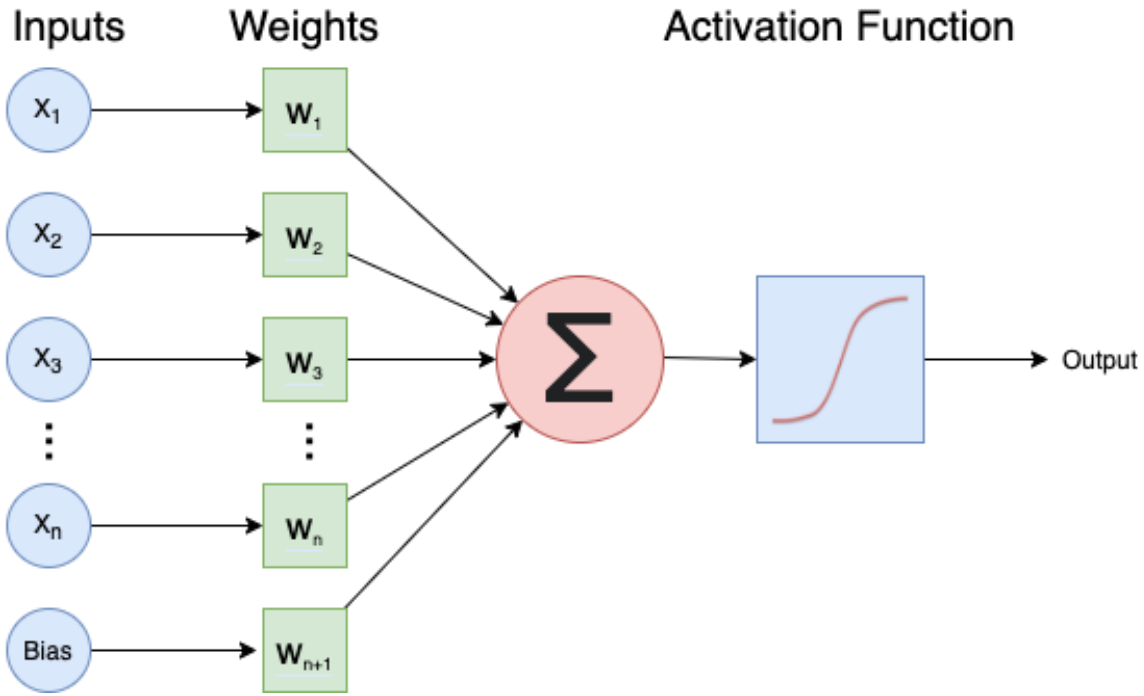
netherlands eScience center

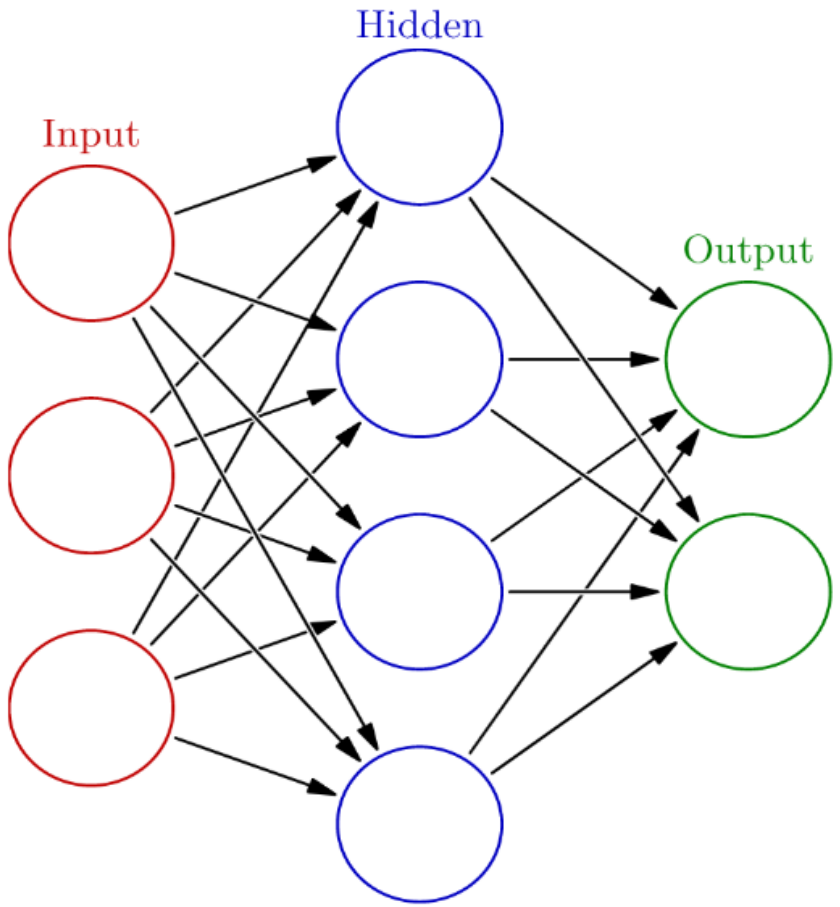
AI Landscape



netherlands eScience center

Neural network





netherlands eScience center

Networks as a team of detectives

- Each neuron has a certain expertise, focusing on particilar patterns in the evidence (the input data)
- Together they make a decision on who is guilty.

netherlands eScience center

GPT-4 explaining what neurons do in GPT

Bills et al. (2023) trained GPT-4 to give explanations of what neurons in another GPT-4 network do:

https://openaipublic.blob.core.windows.net/neuron-explainer/paper/index.html#sec-intro

netherlands eScience center

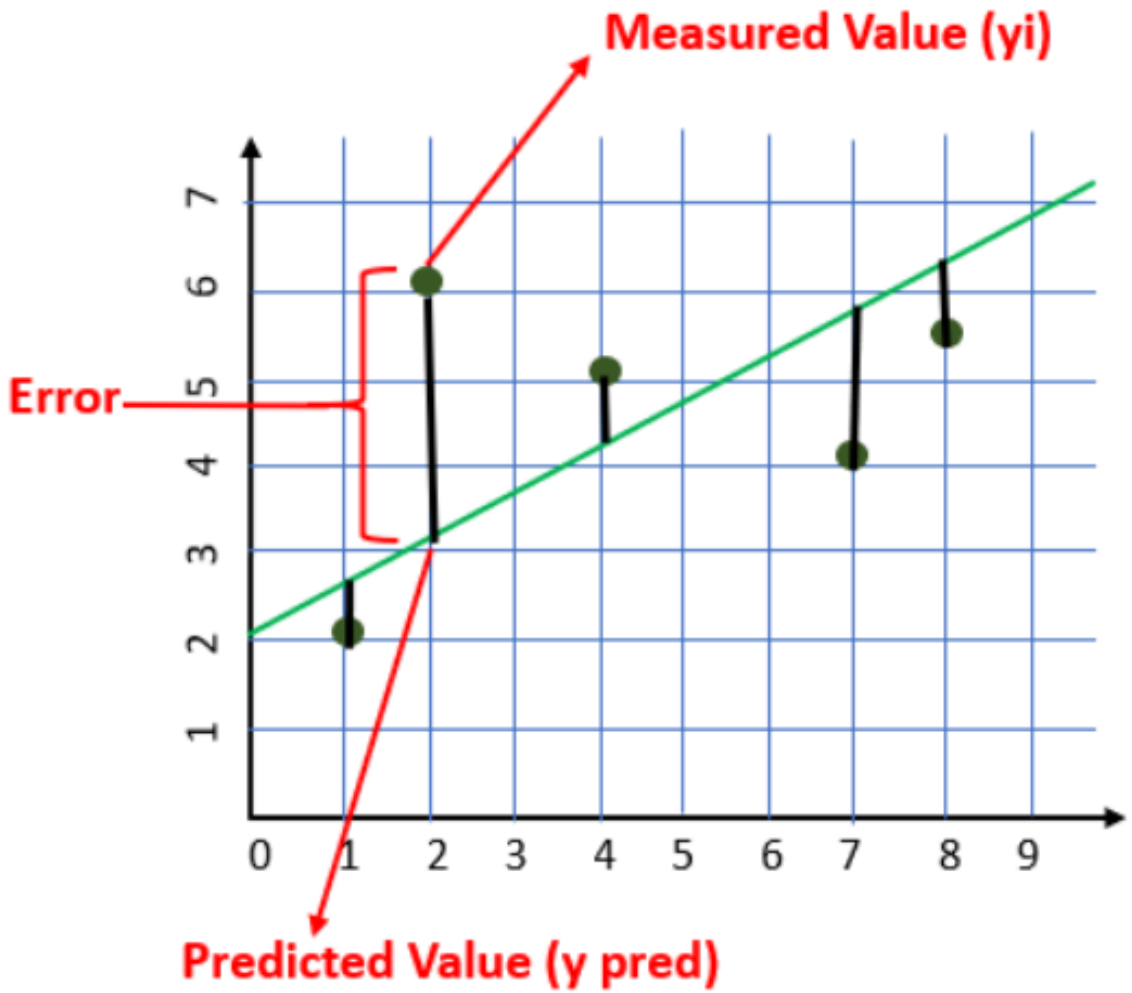
Calculate the output for one neuron

Suppose we have

- Input: X = (0, 0.5, 1)
- Weights: W = (-1, -0.5, 0.5)
- Bias: b = 1
- Activation function *relu*: `f(x) = max(x, 0)`

What is the output of the neuron?

Note: You can use whatever you like: brain only, pen&paper, Python, Excel…


Measured Value (yi)
Error
Predicted Value (y pred)
0
1
2
3
4
5
6
7
8
9
1
2
3
4
5
6
7

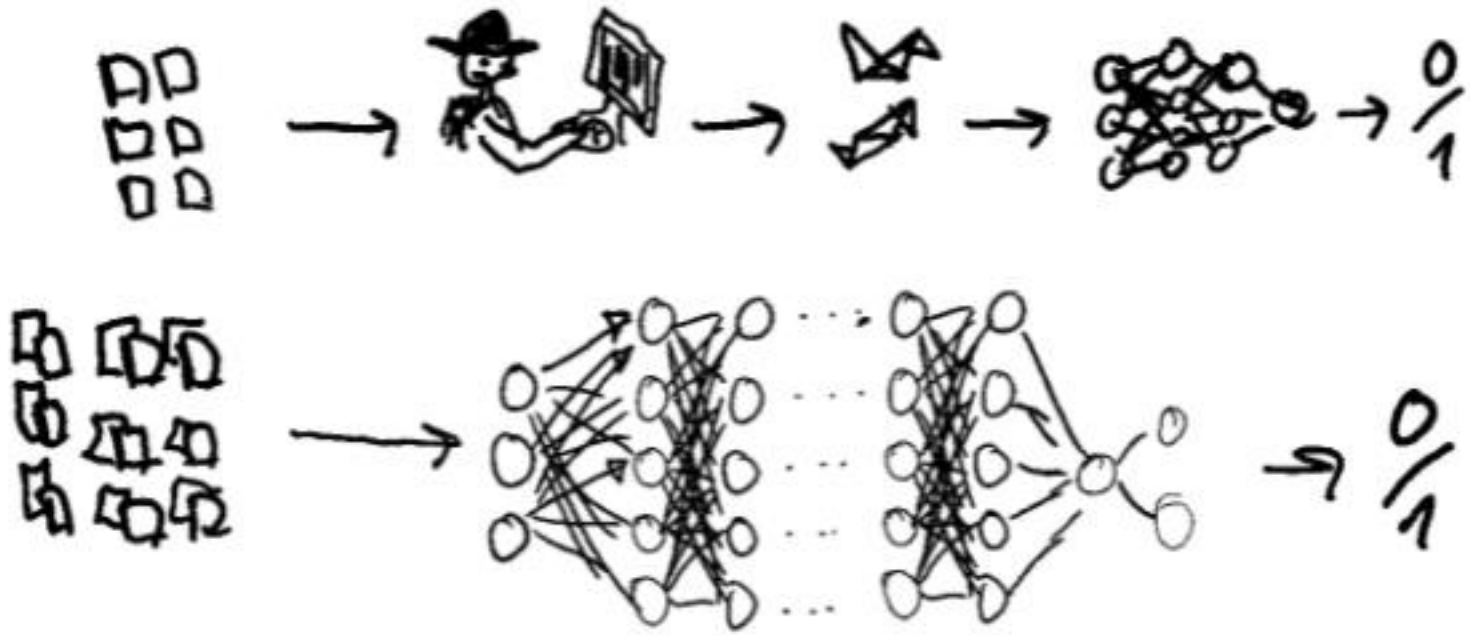
netherlands eScience center

Why deep neural networks? Intuition.

- No hidden layer, simple dataset
- No hidden layer, complex dataset
- Hidden layer, complex dataset

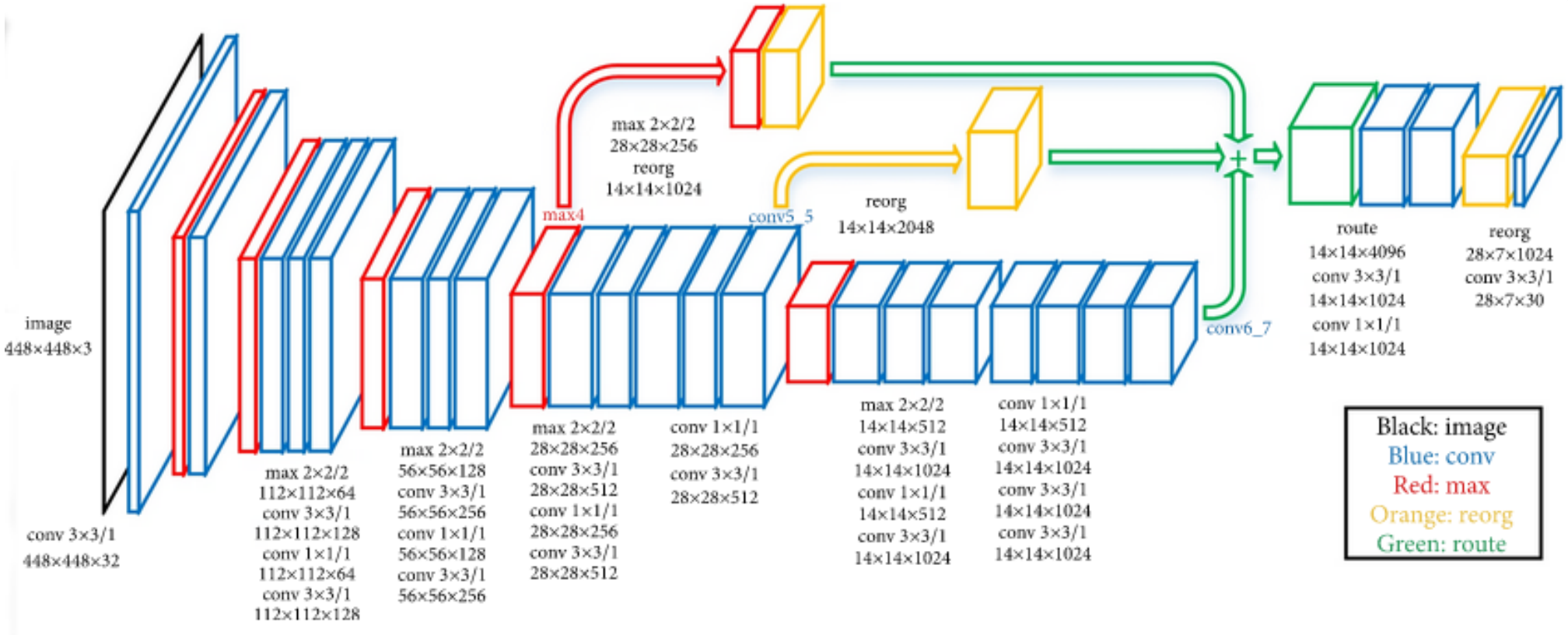
netherlands eScience center

Deep vs shallow neural networks



netherlands eScience center

Example deep network



From https://www.kaggle.com/keras/resnet50

DNN: What is it good for?

What sort of problems can deep learning solve?

- Pattern/object recognition

DOG

CAT

leisergu, CC BY 2.0 <https://creativecommons.org/licenses/by/2.0>, via Wikimedia Commons

DNN: What is it good for?

What sort of problems can deep learning solve?

- Segmenting images (or any data)

B.Palac, CC BY-SA 4.0 <https://creativecommons.org/licenses/by-sa/4.0>, via Wikimedia Commons

DNN: What is it good for?

What sort of problems can deep learning solve?

- Translating between one set of data and another, for example natural language translation.

https://blazepress.com/2014/10/36-of-the-funniest-translation-fails-ever/

DNN: What is it good for?

What sort of problems can deep learning solve?

- Generating new data that looks similar to the training data, often used to create synthetic datasets, art or even “deepfake” videos.

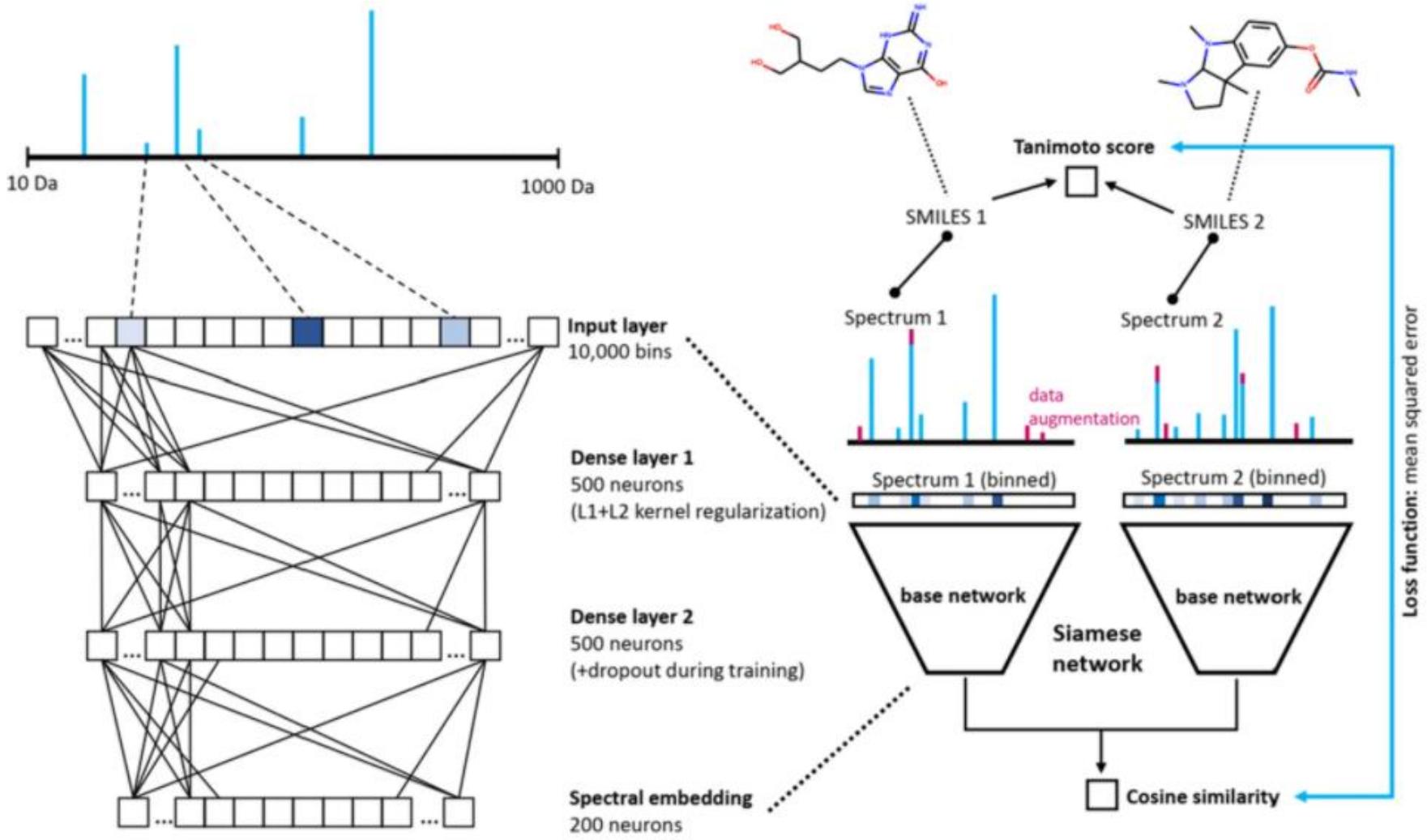
Datascientist55, CC BY-SA 4.0 <https://creativecommons.org/licenses/by-sa/4.0>, via Wikimedia Commons
https://en.wikipedia.org/wiki/StyleGAN

netherlands eScience center

What are examples that you have of deep learning applied to research?

netherlands eScience center

Example of Deep Learning applied to Research: MS2DeepScore: a novel deep learning similarity measure to compare tandem mass spectra



DNN: What is it good for?

What sort of problems deep learning *cannot* solve?

- Where only small amounts of training data is available.
- Tasks requiring an explanation of how the answer was arrived at.
- Being asked to classify things which are nothing like their training data.

netherlands eScience center

Deep Learning Problems Exercise

Which of the following would you apply Deep Learning to?

1. Recognising whether or not a picture contains a bird.
2. Calculating the median and interquartile range of a dataset.
3. Identifying MRI images of a rare disease when only one or two example images available for training.
4. Identifying people in pictures after being trained only on cats and dogs.
5. Translating English into French.

netherlands eScience center

Deep learning workflow

1. Formulate/outline the problem
2. Identify inputs and outputs
3. Prepare data
4. Choose a pre-trained model or build a new architecture from scratch
5. Choose a loss function and optimizer
6. Train the model
7. Perform a Prediction
8. Measure Performance
9. Tune hyperparameters
10. Share model

netherlands eScience center

Deep learning workflow exercise

Think about a problem you'd like to use Deep Learning to solve. As a group, pick 1 problem.

1. What do you want a Deep Learning system to be able to tell you?
2. What data inputs and outputs will you have?
3. Do you think you'll need to train the network or will a pre-trained network be suitable?
4. What data do you have to train with? What preparation will your data need? Consider both the data you are going to predict/classify from and the data you'll use to train the network.

Discuss your answers in your breakout group. Write them (concisely) down in the collaborative document.

Deep Learning Frameworks

- Tensorflow
  - Google
  - General Tensor Network Caculations
- PyTorch
  - Facebook
  - Very Fast
- Keras
  - Designed for Ease of Use
  - On top of Tensorflow
  - Good Documentation
- And many others (Theano, Caffe, etc.)

What we are using

- Keras – Deep Learning Framework
- Sklearn – Machine Learning Framework
- Seaborn – Visualization Library

netherlands eScience center

What have we learned?

- What deep learning is
- How neural networks work
- When to apply deep learning
- Applying deep learning with the ‘deep learning workflow’

netherlands eScience center

You are pioneers

netherlands eScience center

Check versions

```
from tensorflow import keras
print(keras.__version__)

import seaborn as sns
print(sns.__version__)

import sklearn
print(sklearn.__version__)
```

netherlands eScience center

Next steps

- Practice!
  - For example try a Kaggle competition: https://www.kaggle.com/competitions
- Read/watch blogs and videos
  - For example: 2-minute papers
- Fast.ai course: making neural nets uncool again
  - https://course.fast.ai/
- Try a quick and dirty approach first, then optimize
- Get acces to a GPU
  - If experiments take seconds instead of 20 minutes, you can iterate over hypothesis -> experiment -> conclusion much much quicker