B. Basics of ANNs

1. Introduction to various models, especially artificial Neural Networks
2. Plenary session 3
3. Configurations of artificial neural networks
4. Train the ANN

(B1) Introduction to artificial Neural Networks

- An artificial neural network (ANN) is an AI system that mimics the structure of the human brain
- It is one of the most popular approaches to ML
- An artificial neural network is considered as ‘black box model’
- It captures patterns by using simple algorithms

Why a model?

- Both **white** models and **black box** models do exist
- Both have their advantages and disadvantages

NB: ***Any*** model is a (simpler) representation of reality

White models

White models are based on first principles, laws of nature

Advantages

- the ability to incorporate the scientist's view of the process into the model,
- the capacity to describe the internal dynamics of the process, and
- the capability to explain the behaviour of the process.

White models

Disadvantages

- the high *costs* of model development,
- the *bias* that they may have because of the model developer's choices, and
- the *limitations* in including the details due to *lack of information* about specific model properties.

As details are added to the model, it may become too complex and too large to run the model on the computer within an acceptable amount of time.

Why use an ANN?

- White models take a lot of programming time, by programmers
- White models are sensitive to programming errors, by programmers
- White models are prone to errors in parameters (physical/chemical...), by users/programmers/unknown
- The white model computation time may be too long for the application

Instead, the ANN provides us with a

- Fast alternative to programming with code to represent laws of nature

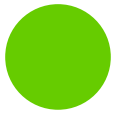
(B2) Plenary session 3 – Let’s play!

Let’s play! Analysis

(B3) Configurations of artificial neural networks

Network elements

Input node

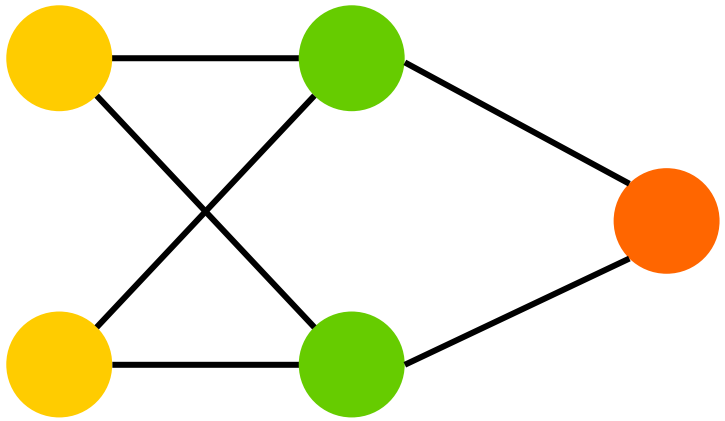


Hidden node

Output node

Connector

Simple ANN



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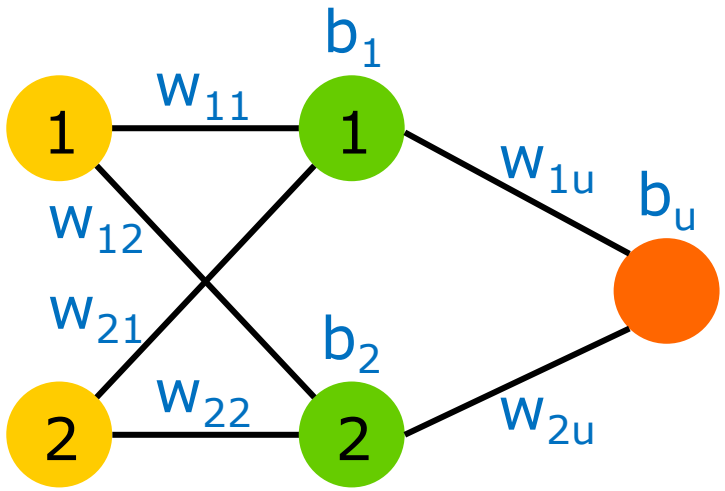
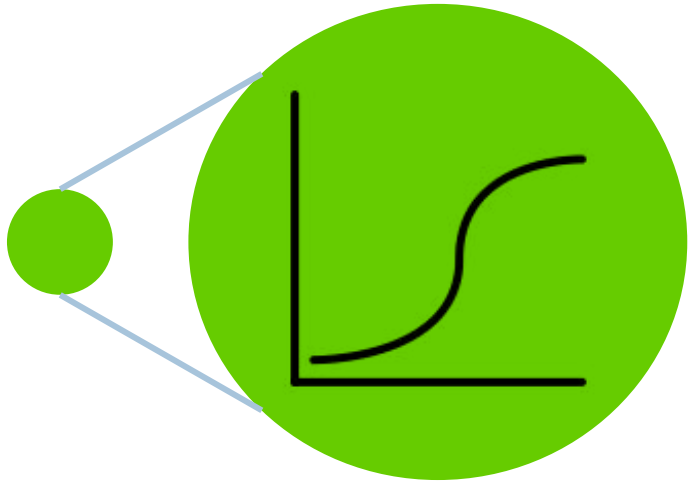
Simple ANN





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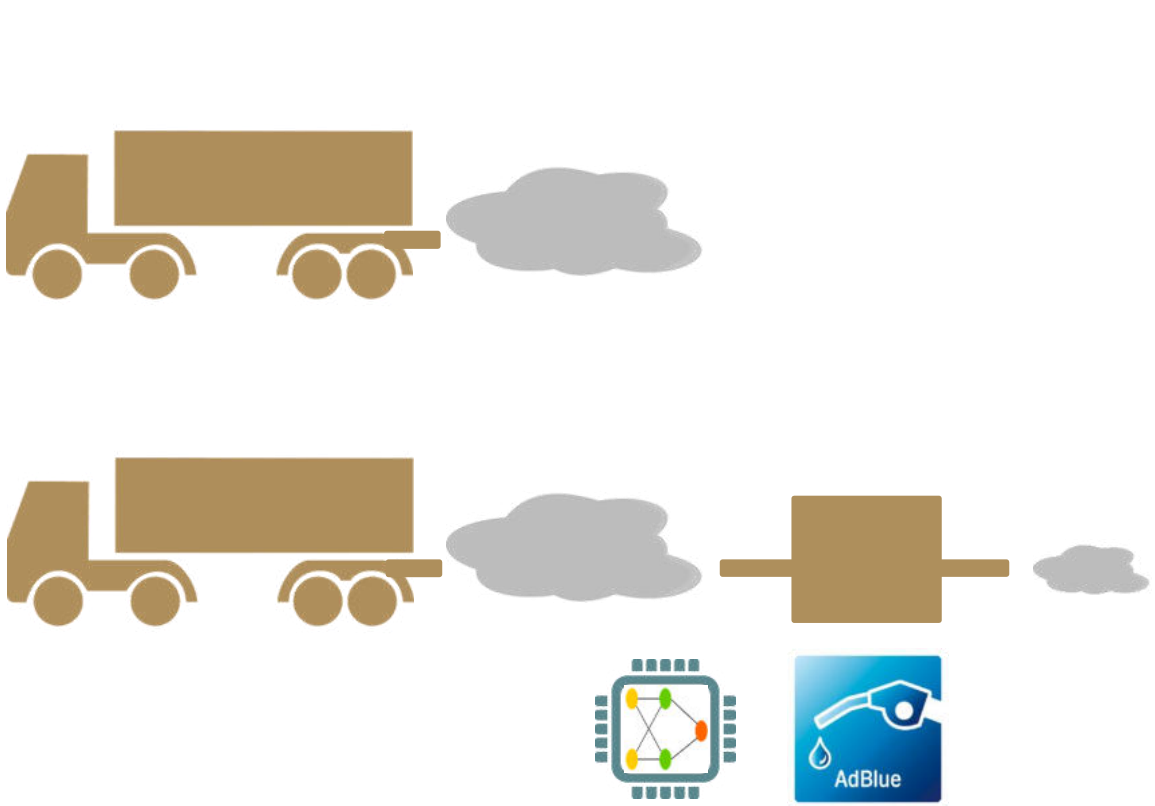
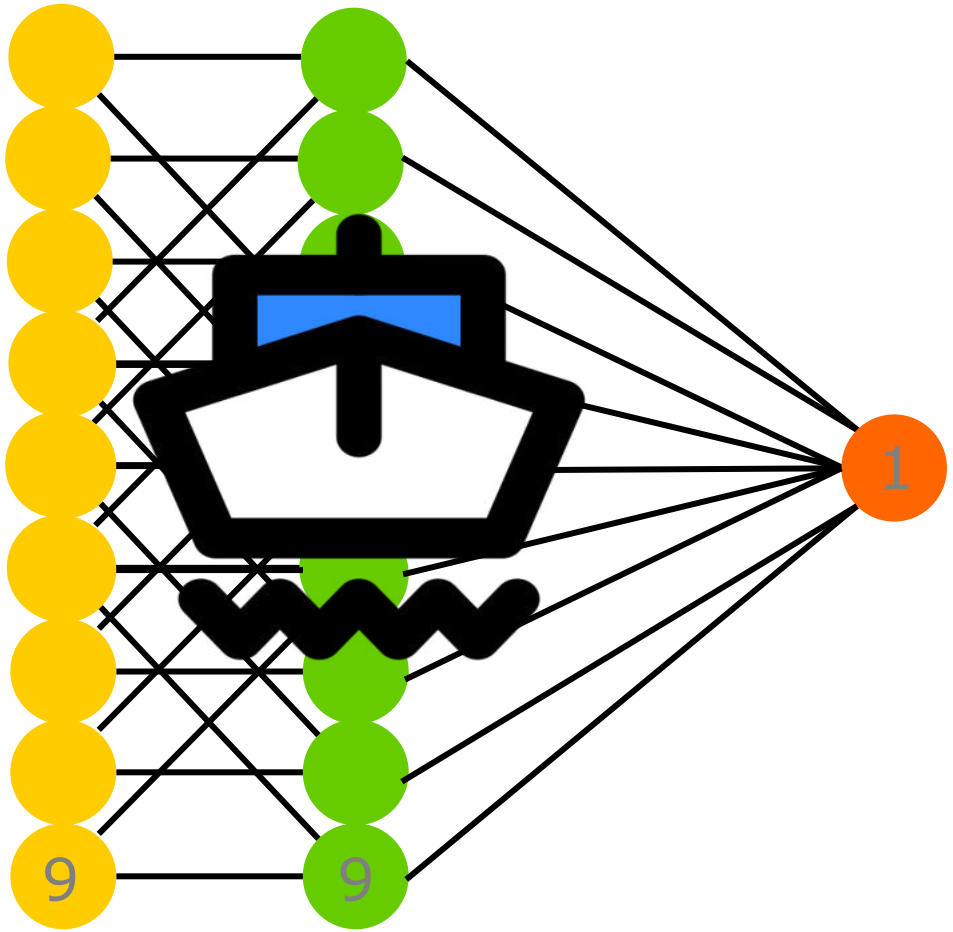
Purpose of the ANN – prediction of NOx emissions (1996-2000)



ANN for NOx emission prediction (steady state engine, 1998)



Diesel generating set (steady-state)
9 inputs, **1 HL with 9 nodes**, 1 output

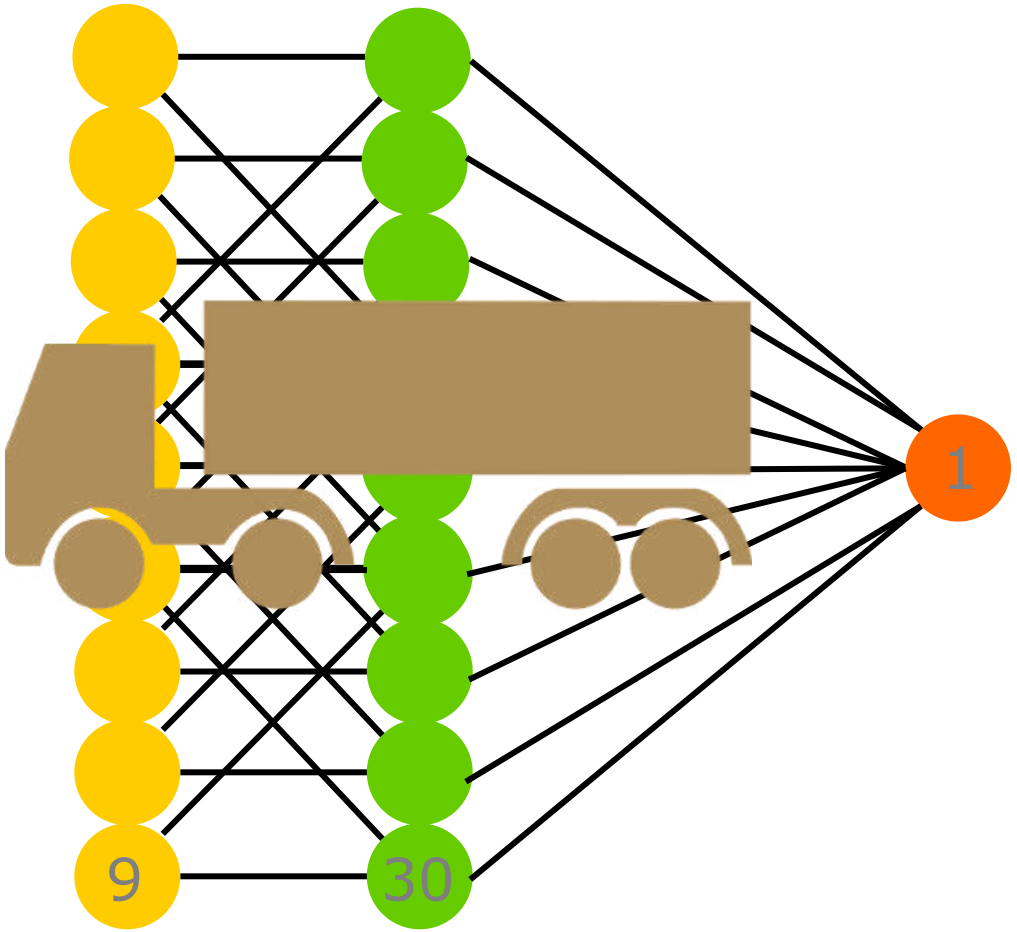
47,000 lines of NOx emission data
Including all relevant parameter values

100 parameters to be finetuned

Inputs: T(t), P(t), H(t), L(t,t-2,t-5,t-8,t-11,t-14)

The error of the output node was reduced by reducing the Mean Square Error

ANN for NOx emission prediction (transient engine, 1999)



Diesel truck (dynamic/transient)
9 inputs, **1 HL with 30 nodes**, 1 output

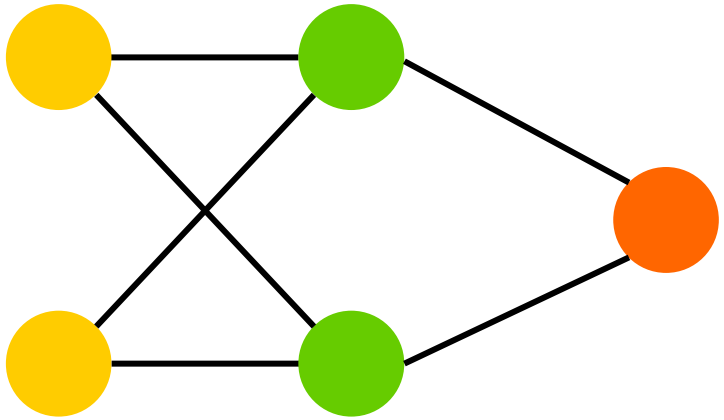
1800 lines of NOx emission data
Including all relevant parameter values

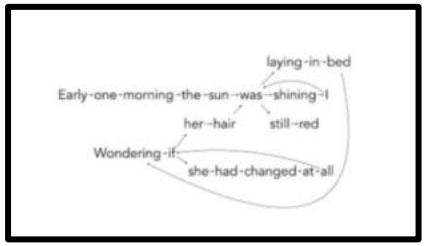
310 parameters to be finetuned

Inputs: T(t), P(t,t-1,t-2), R(t-1,t-2,t-3), N(t,t-1)

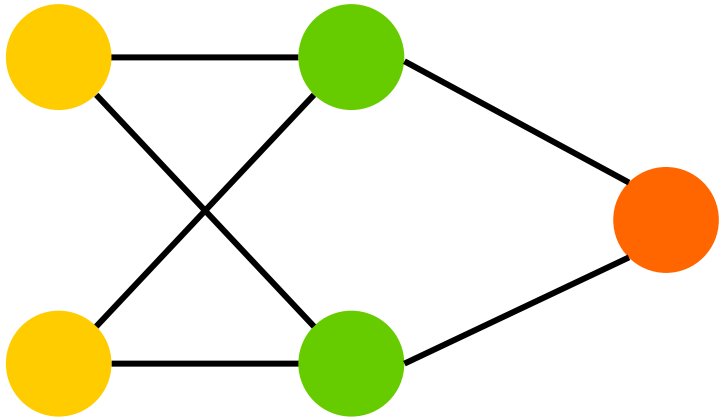
Again, the error of the output node was reduced by reducing the Mean Square Error

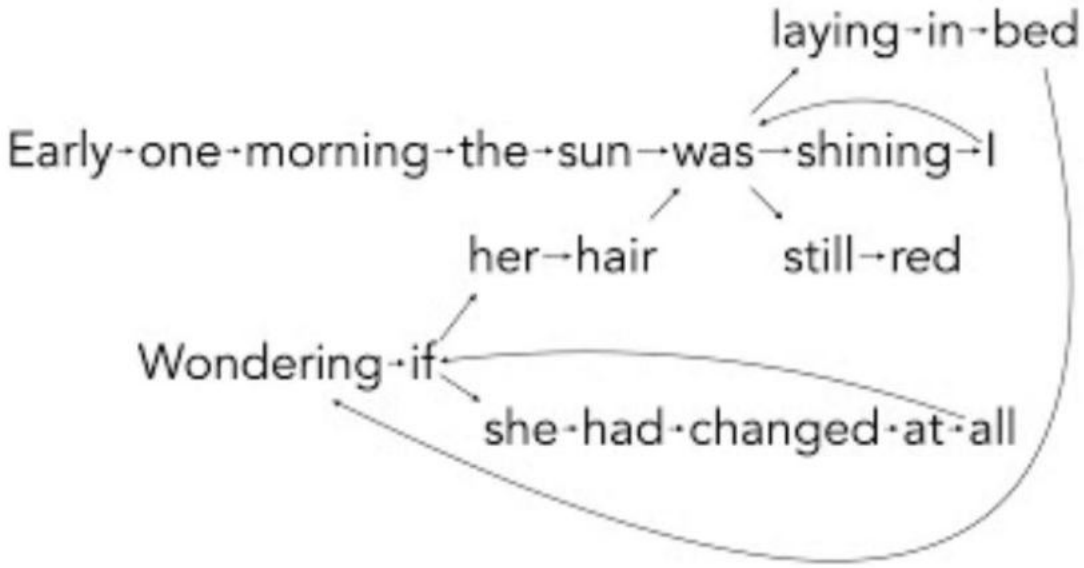
Training a neural network – MSE minimisation



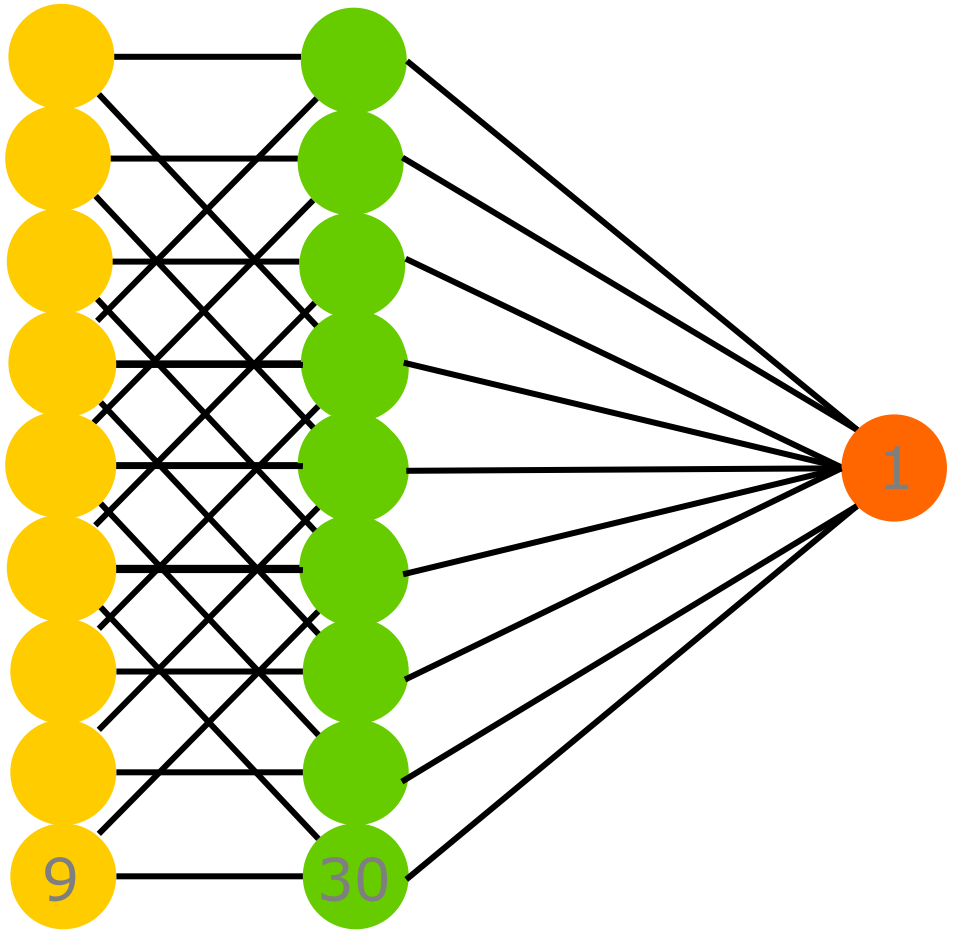


Training a neural network – MSE minimisation





ANN for NOx emission prediction

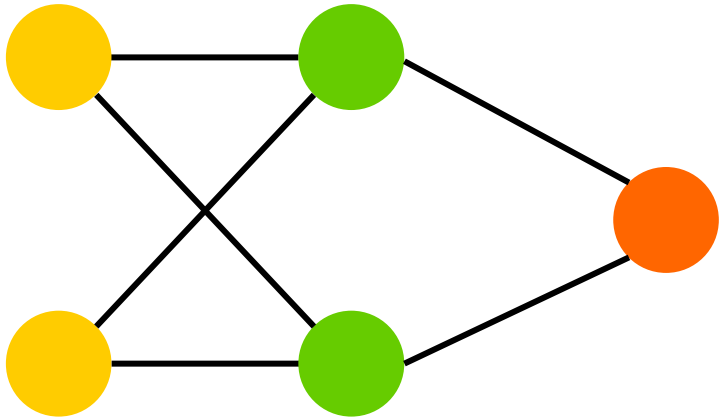


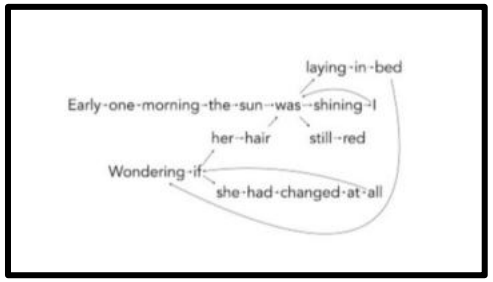
The trained ANN could calculate the NOx emission within 0.2 ms (AD 2000)

The white model

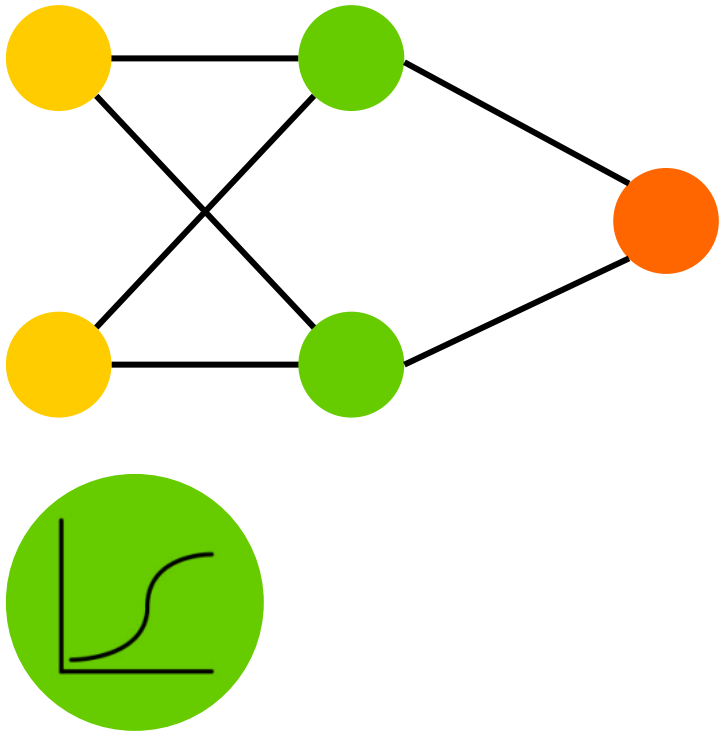
- takes 10 s – 120 hours depending on the complexity of the model;
- describes steady state conditions;
- cannot be exactly programmed as the full burning process in the diesel combustion engine is unknown.

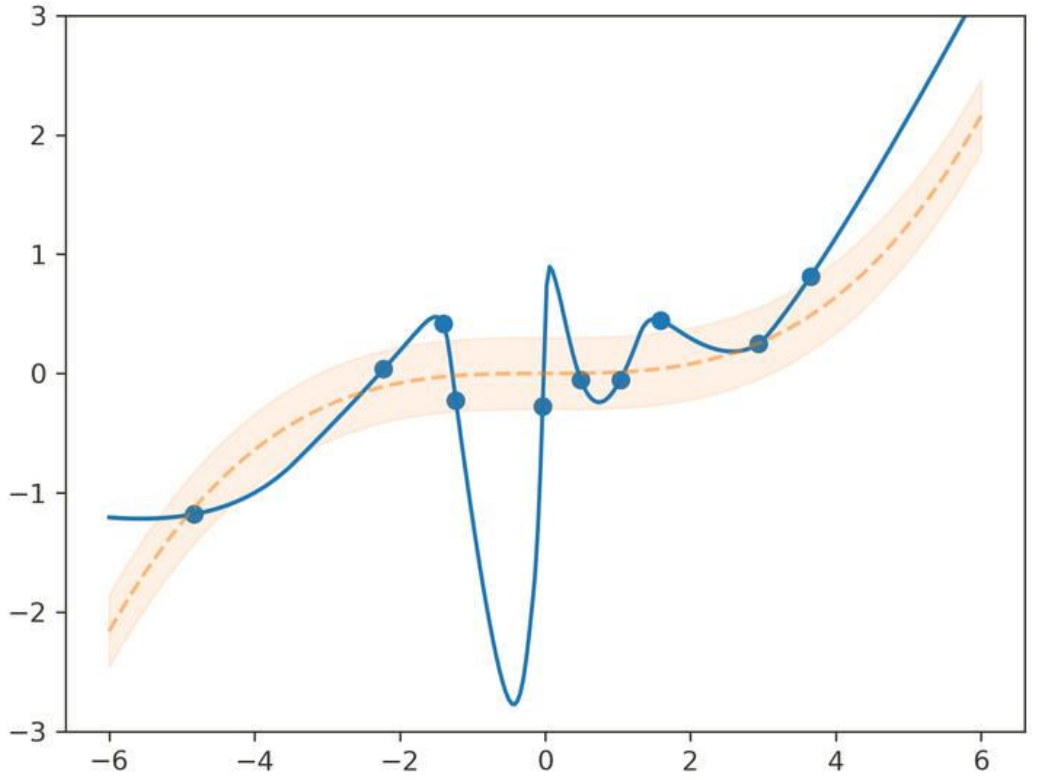
Training a neural network – **Under**fitting





Training a neural network – **Over**fitting





Train the aNN: What ‘steps’ does it involve?

- Collect raw data
- Clean raw data, normalize
- Extract features: identify what inputs are relevant
- Set the activation function, set the number of hidden layers, hidden nodes
- Provide processed data to a machine
- Train the machine based on the processed data
- Test (evaluate) the trained model
- Apply the trained model in an actual situation

The trained ANNs originate from 1996-2000!

- ANNs to train and test were not commercially available at the time
- A colleague specialized in ANNs programming provided the customized software. I could modify the neural network to my heart's content and use my own NOx emission data to train and test
- Training and testing took months

- ANN Training / testing in ~2002
  - No (cor)relation between input - output

Main take-aways messages (part B)

- Neural networks can mimic patterns, are fast and relatively cheap
- Even a small ANN contains quite some parameters, ‘settings’
- The more parameters are present, the more training data is required
  - Thus, training ANNs takes time; all parameters need to be tuned

    All data have to be calculated until the desired output is generated
- ***After training*** all parameters are fixed; basically a simple sum remains
  - Because of the simple calculation (sum), the calculation just takes a matter of milliseconds