PROGRAMMING IN PYTHON II

Neural Network Implementation: Inference

Michael Widrich
Institute for Machine Learning

JOHANNES KEPLER
UNIVERSITY LINZ

Institute for
Machine Learning

Outline

MOTIVATION

Motivation

- In order to design our neural networks efficiently, we would like to have
  - modular structure of layers and building blocks
  - consistent interfaces between modules
  - free combination of modules (not only sequential but also tree-like structures)
  - automated optimization of computations
  - automated deployment to CPU, GPU, or other dedicated hardware
  - automated computation of gradients for training

Motivation

- In order to design our neural networks efficiently, we would like to have
  - modular structure of layers and building blocks
  - consistent interfaces between modules
  - free combination of modules (not only sequential but also tree-like structures)
  - automated optimization of computations
  - automated deployment to CPU, GPU, or other dedicated hardware
  - automated computation of gradients for training

→ PyTorch provides these features!

PYTORCH FOR BUILDING NEURAL NETWORKS

torch.nn.Module

- torch.nn.Module is the base class for all neural network modules
- All custom networks/layers/modules should be derived from this class
- Can contain and utilize other modules
- Automated registration of trainable parameters and parameters in submodules
  - For now we will treat this as magic, later we will learn how it actually works

torch.nn.Module: Usage

- torch.nn.Module usage is simple:
  1. Create class that inherits from torch.nn.Module
  2. Define your `.forward()` method
  3. Define your `.init()` method
  4. Create an instance of your class and apply it to input

torch.nn.Module: Details

- The `.forward()` method will be executed when your class instance is applied to an input
- Using PyTorch (sub)module instances as module attributes will register the submodule automatically
- Using PyTorch parameter instances as module attributes will register the parameter automatically
  - `torch.nn.Parameter` will create trainable tensors, e.g. for NN weights
- PyTorch modules behave a lot like PyTorch tensors
  - Can be sent to devices using `.to(device=...)`
  - Can be converted to datatype using `.to(dtype=...)`

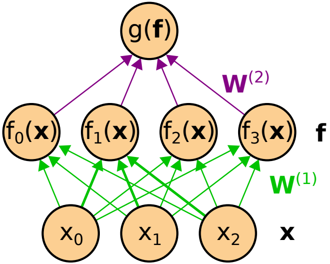
Predifined PyTorch modules

- Many predefined PyTorch modules exist
- Sometimes include additional optimization
  - E.g. PyTorch LSTM with specialized CUDA support but less flexible design
- Should be preferred over custom modules unless special functionality is desired

QUICK GUIDE: DESIGNING YOUR NEURAL NETWORK

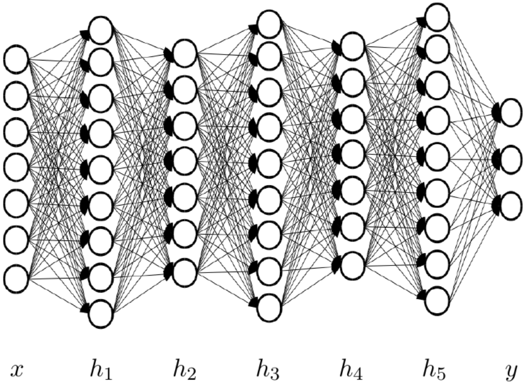
NN types: FFNN (1)

- Fully-connected feed-forward NN (FFNN):
  - High complexity, high number of weights
  - Not utilizing order in feature vectors
  - Multi-dimensional inputs are typically flattened (reshaped to flat vector as input)



NN types: FFNN (2)

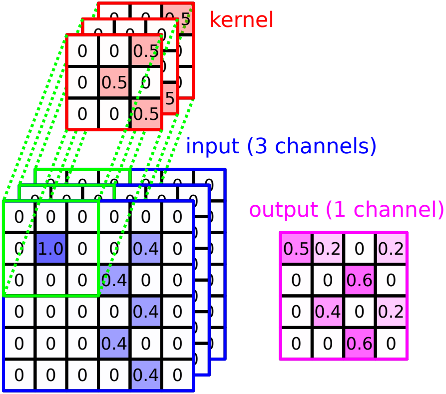
- Layers in deep FFNN



$$y = f\left(h_5(h_4(h_3(h_2(h_1(\mathbf{x}; \mathbf{W}_1); \mathbf{W}_2); \mathbf{W}_3); \mathbf{W}_4); \mathbf{W}_5); \mathbf{W}_6 \right)$$

NN types: CNN (1)

- Convolutional NN (CNN):
  - Weight kernels are slided along (=convolved) an input tensor



NN types: CNN (2)

- Convolutional NN (CNN):
  - 1D CNNs: Kernels convolved over one dimension (e.g. time dimension in a time-series)
  - 2D CNNs: Kernels convolved over 2 dimensions (e.g. spatial dimensions in image)
  - nD CNNs: Possible but uncommon at the moment (expensive/lacking optimization)
  - Less complexity, fixed kernel size to incorporate information about adjacent features
  - Depth of network increases field of vision
  - Typically employ pooling operations to pool adjacent features (e.g. max-pooling)
  - Outputs sometimes flattend and then fed into FFNN or max-pooled to 1D feature vector

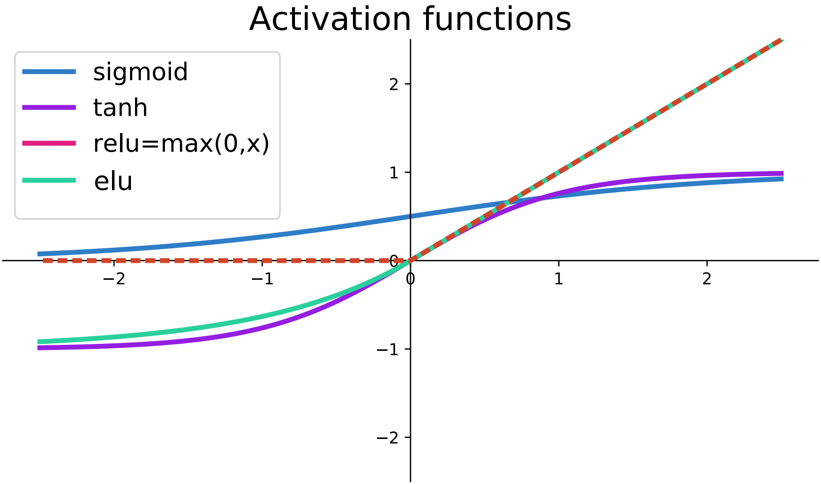
NN types: RNN

- Recurrent NN (RNN):
  - NN applied to a list of inputs, using the same weights for each input
  - NN has access to output/hidden state from previous input (=recurrent)
  - Turing complete (but need to be trained somehow)
  - 1D: Sequence (=list of feature vectors) as input
  - nD: Multidimensional RNN variants for matrices or tree-like structure
  - Most popular, since no vanishing gradient: LSTM
  - Alternative to RNNs: Transformer NNs

Common activation functions

- Pay attention to recommended weight initialization and input normalization for the specific activation functions
- Scaled Exponential Linear Unit (SELU)
  - Self-normalizing properties benefit learning and design
  - Common for FFNN but also successes in CNN
- Recified Linear Unit (ReLU)
  - Very common in CNNs
  - Units can “die” once they get stuck in 0-activation (=no gradients)
- Sigmoid activation function
  - Common in (older) NNs
  - Introduce vanishing gradients
  - Outputs in range $[0, 1]$

Common activation functions



PYTHON II PROJECT

Python II Project: NN Design

- We deal with image data $\rightarrow$CNN is a natural choice
- Hyperparameters (see Unit 07): Number of kernels, size of kernels, pooling operations, activation function, skip connections, and number of layers
- Additional data can be fed to CNN by creating a new feature channel (see Assignment 2)
- CNN could be combined with FFNN but probably not necessary
- SELU or ReLU activation functions are good candidates

FURTHER READING

Further reading

- ÖAW AI summer school slide-set: `https://github.com/ml-jku/oeaw_ai_summer_school`
- Courses and lecture materials in AI-study (Hands-on AI, Machine Learning: Supervised Techniques, LSTM and Recurrent Neural Nets, . . .)
- *Pattern Recognition and Machine Learning* (C. Bishop)
- *Dive into Deep Learning* (A. Zhang, Z. Lipton, M. Li, A. Smola): `https://d2l.ai/`
- `https://pytorch.org/tutorials/index.html`
- `https://pytorch.org/tutorials/beginner/blitz/neural_networks_tutorial.html`