Practicalities of Neural Nets

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Lecture 07.2 (v2.0.0)

Implementing Neural Networks

- Implementations are best though of in two classes.
- **Simple networks** have a restricted architecture and can be deployed "out of the box" as a Machine Learning tool.
  - Examples include sklearn.linear_model.Perceptron, R's neutralnet packages, etc
  - Often either shallow or very simple hidden layer structure
- **Deep networks** require a complex specification of architecture and significant computational optimisation, so are very large (and mercifully, open source) endeavours
  - This is the focus here.

Deep NN Implementations

- There are two main libraries for deep neural networks:
- **TensorFlow**, developed by Google Brain.
  - Well documented
  - Easier to use
  - Industry standard
  - Tensorboard visualisation is useful
- **PyTorch**, developed by Facebook.
  - Newer, less support
  - Dynamical coding paradigm: graph can remodel in the light of the data
  - Debugging is easier? As the code is compiled at runtime, like native python

Using implementations

- Tensorflow is a low-level language. You can interact with it through abstraction layers which allows very simple implementations.
  - Keras is very widely used and makes accessing TensorFlow very easy.
  - PyTorch is already conceptually a "high level" implementation.
- Keras can use various **backends** (implementations):
  - TensorFlow
  - MXNet
  - Theano is a pure python library for a wide class of array computation, not just Neural Networks. It was forked into Aesara...
  - Microsoft Cognitive Toolkit, but this is no longer in active development.
- See Tensorflow or keras?

Practical advice

- Explore recommendations. e.g. Practical Advice for Building Deep Neural Networks:
- As a starting point:
  - Use the "adam" optimizer
  - Use a ReLU activation function
  - Remember not to use an activation function for the output layer (except for classification, when use a sigmoid)
  - Add bias to every layer (shouldn't have to worry about this in keras)
  - Whiten (normalize) your input data (we'll see this in the workshop)
- **Don't believe me.** Get other opinions, and try things yourself.

Debugging

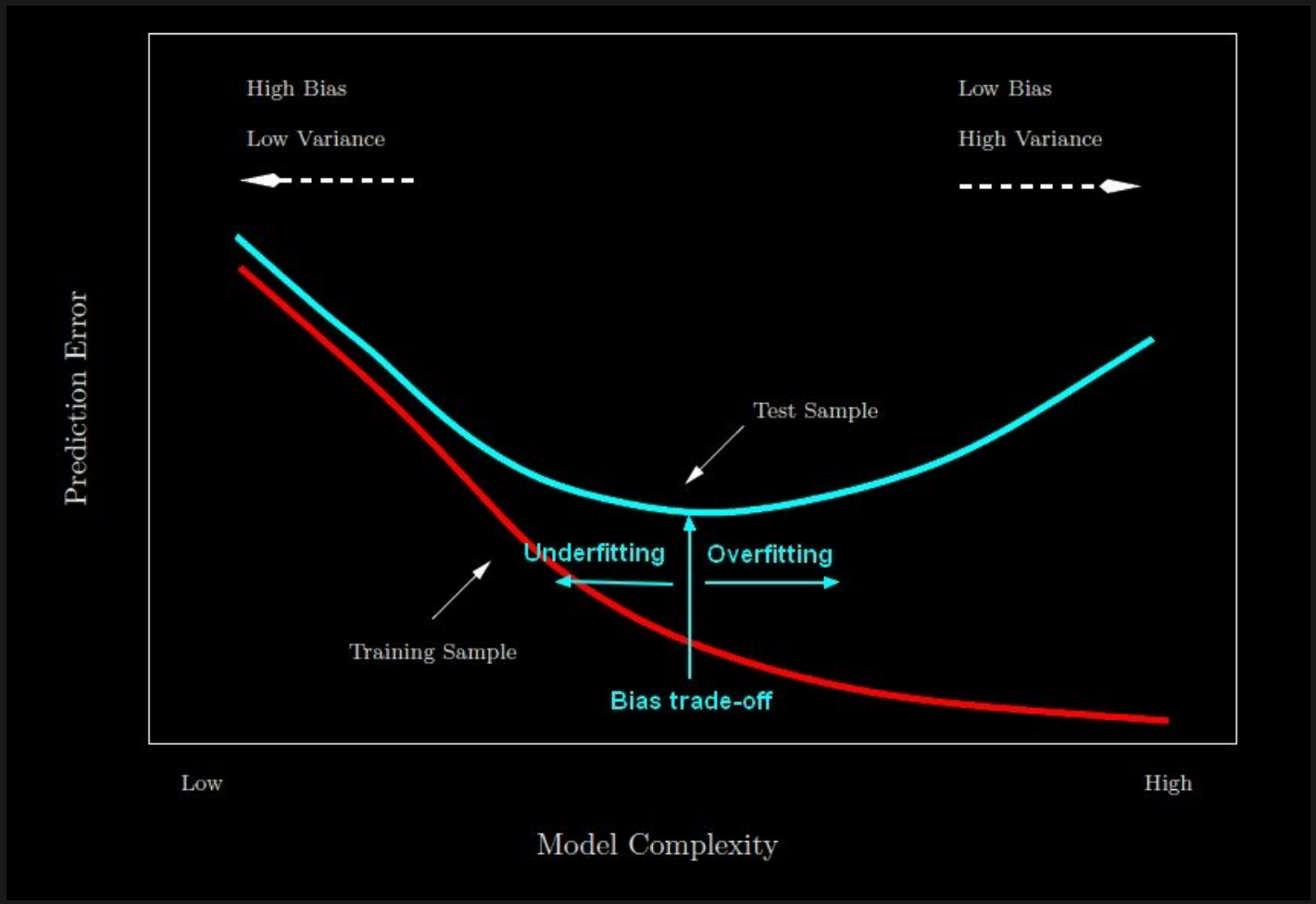
- Check the **input data**. . .
- For many tasks:
  - **OVERFIT**. "Accuracy should be essentially 100% or 99.99%". If it isn't, the network isn't flexible enough, or learning correctly.
- Change the learning rate
- Decrease mini-batch size
- Remove batch normalization (this exposes NA values)
- Reconsider the architecture
- PLOT your results! training loss by epoch is a natural plot

Additional notes on learning

- Learning a Neural Network is still non-trivial. Start with this advice[1]
  - **Second order methods** are often used later in the fitting process, closer to the global optima.
  - **Hyperparameters** matter. Some optimisers, e.g. Adam, can tune them semi-automatically. Standard ones require **manual tuning** for e.g. step size.
- There is nothing here to prevent **overfitting**!

[1] Bengio 2012 Practical Recommendations for Gradient-Based Training of Deep Architectures

Learning rates



- **not** specific to neural networks
- But particularly important due to NN flexibility

Hints on overfitting

- Many optimizers include options for these tricks and more:
- **Penalize** large weights:
  - Ridge (L2) penalisation: $L = L_0 + \lambda \sum_{i,j} |W_{ij}|^2$
  - Lasso (L1) penalisation: $L = L_0 + \lambda \sum_{i,j} |W_{ij}|$
- **Dropout**:
  - New hyperparameter p_k for layer k: the **dropout rate**
  - Each learning step, with independently randomly set all outputs from a neuron to 0
- **Early stopping**:
  - retain a test dataset (from the training dataset)
  - evaluate performance on the held-out set
  - stop when this no longer increases

Reflection

- Understand the tools available for neural networks
- Be able to use high-level implementations efficiently

Further reading

- Keras and PyTorch
- Tensorflow or keras?
- A performance focussed comparison: TensorFlow, PyTorch or MXNet?
- Tensorboard
- Brilliant.org on Backpropagation
- Practical Advice for Building Deep Neural Networks