

Constraints in Machine Learning

Acknowledging a Fact

ML techniques have reached superhuman performance on many tasks



...All the Facts, Actually

Modern ML methods excel at taking advantage of available data

- They can be robust w.r.t. to noise
- They can approximate highly non-linear relations
- They can handle very large datasets
- ...

However, this is all about **implicit information**

What about **explicit** information? E.g.:

- Locality
- Known physical laws
- Regulations
- Intuitive relations
- ...

Success Stories

Some of the most successful ML methods are based on explicit knowledge

Think of:

- Convolutional networks
- Attention-based architectures (e.g. transformers)
- Graph neural networks
- ...

They all rely on explicit knowledge about the **structure of the problem**

- Locality for CNNs
- Relevance functions for attention
- Known connections for GNNs
- ...

...And Open Problems

Where thing become trickier is with **symbolic** information

...Which is typically encoded in the form of (soft or hard) **constraints**



Let's make a few examples...

Constrained Machine Learning

Example 1: logical rules

E.g. hierarchies in multi-class classification ("A dog is also an animal"):

$$y_{i,dog} \leq y_{i,animal}$$

- This constraint is defined over individual examples

Example 2: shape constraints

E.g. input x_j cannot cause the output to decrease (monotonicity)

$$y_i \leq y_k \quad \forall i, k : x_{i,j} \leq x_{k,j} \wedge x_{i,h} = x_{k,h} \forall h \neq j$$

- This is a relational constraint, i.e. defined over multiple examples

Constrained Machine Learning

Historically, constrained ML has received limited interest

...But things are changing!

- Symbolic knowledge is available for many practical problems
- Fairness in ML can be thought of as a constraint
- Safety in ML can also be stated by means of constraints

Mainstream conferences now often host sessions on related topics:

- Neuro-symbolic AI
- Fairness and trustworthiness in AI
- Hybrid ML-optimization approaches
- ...

About this Lecture

Constraints ML can be taken into account by acting on:

- The architecture
- The training algorithm
- The data

This lecture will contain a few relevant examples of such approaches

The lecture consists of a set of **tutorials**

- We will use (semi) practical example to discuss the techniques
- Everything is a jupyter notebook (and executable)
- We will reproduce the results in real time
- The code will be made available to you can play with that