O2AT-5: Machine Learning

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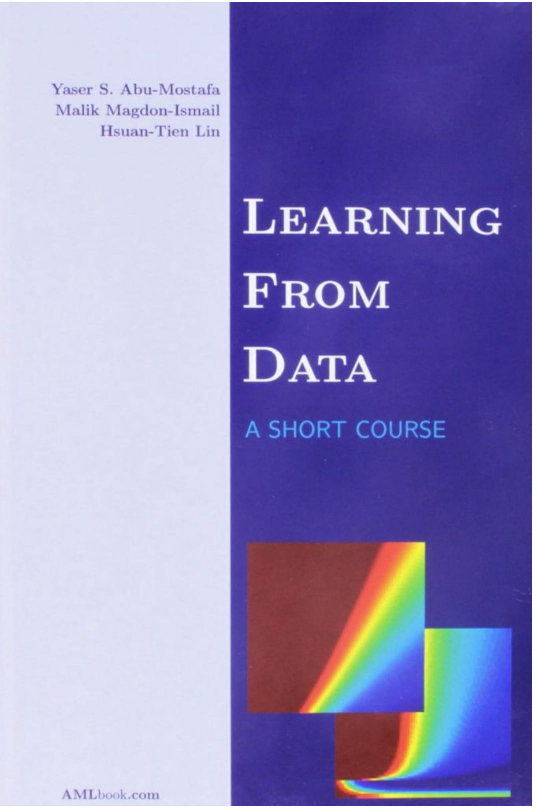
Machine learning: introduction

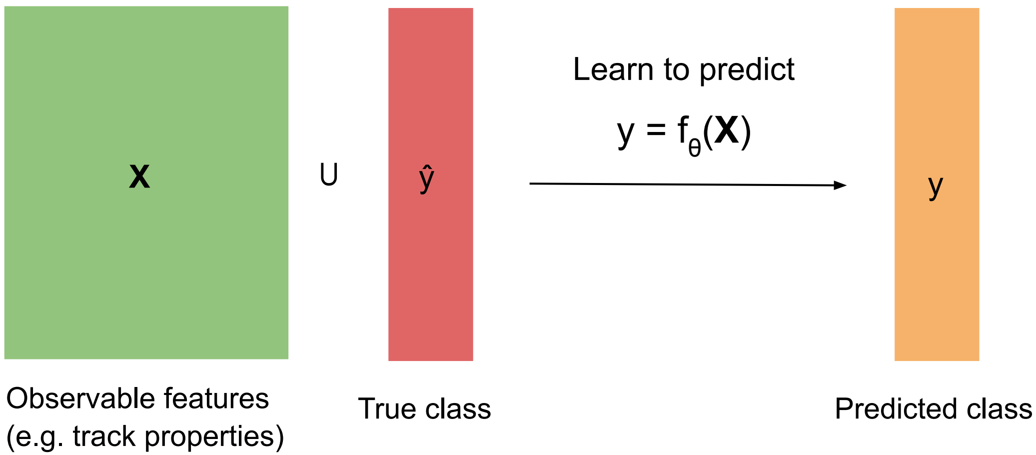
- Machine learning (ML) models are able to perform a task without being explicitly programmed to do so
  - models are built from an input sample data and try to extract patterns from it
  - no need to specify a sequence of instructions to solve the task
- ML is nowadays ubiquitous in real-world applications
  - speech recognition and translation
  - autonomous driving
  - text-to-image generation
  - HEP!
  - ….



https://work.caltech.edu/telecourse

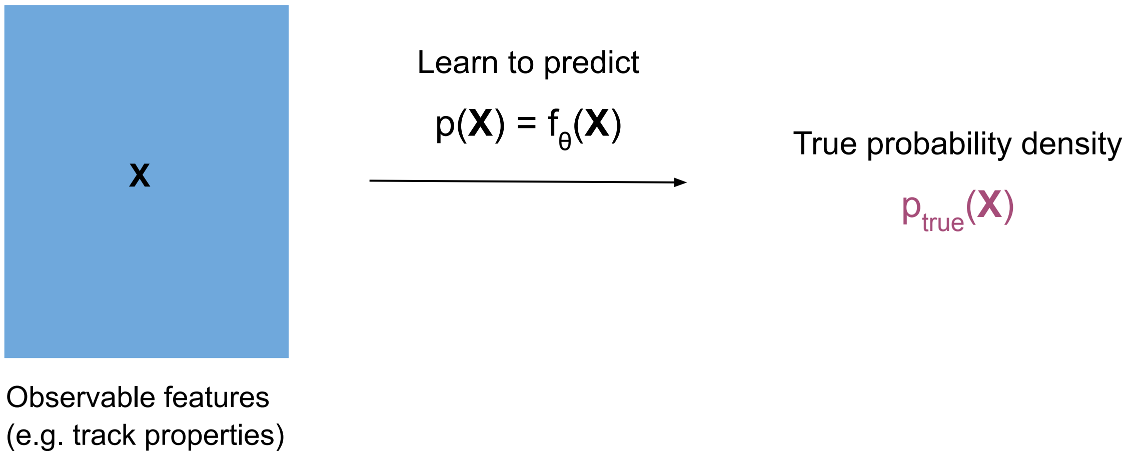
Supervised Learning

- The desired output of the task to be performed is known and a set of examples is available
- Typical tasks
  - classification: distinguish between a pair of or several classes (e.g. signal vs bkg.)
  - regression: predict a continuous value (e.g. particle energy)
- Model "trained" to infer some target starting from the input data
  - ideally the model output matches the target for "unseen" data



Unsupervised Learning

- No examples with known labels are available
  - model “learns” the probability distribution from the input data
- Typical tasks
  - clustering: find structures in the data
  - anomaly detection: identify outliers w.r.t. the input data
  - sampling: generate data from the underlying probability distribution



ML in ALICE: few examples

Signal-vs-background classification

- Boosted Decision Trees (BDTs) and Neural Networks (NN) replacing “traditional” linear selections

Jet p_T reconstruction

- Correction for the background from the underlying event
- Regression task using shallow NN

Heavy flavor jet tagging

- BDTs and Deep Neural Networks (DNN) to tag heavy-flavour jet topologies

HF-hadron trigger

- BDTs to trigger on displaced decay-vertex topologies

Particle identification (PID)

- Exploit complex relationship between track properties and PID (global PID, ITS2 PID..)

Detector calibration

- e.g. : ML to compute corrections of TPC spatial charge distortions
- NN for energy-loss (dE/dx) calibration

Fast simulations

- Use of generative ML to speed-up ALICE detector simulations (e.g. calorimeters..)

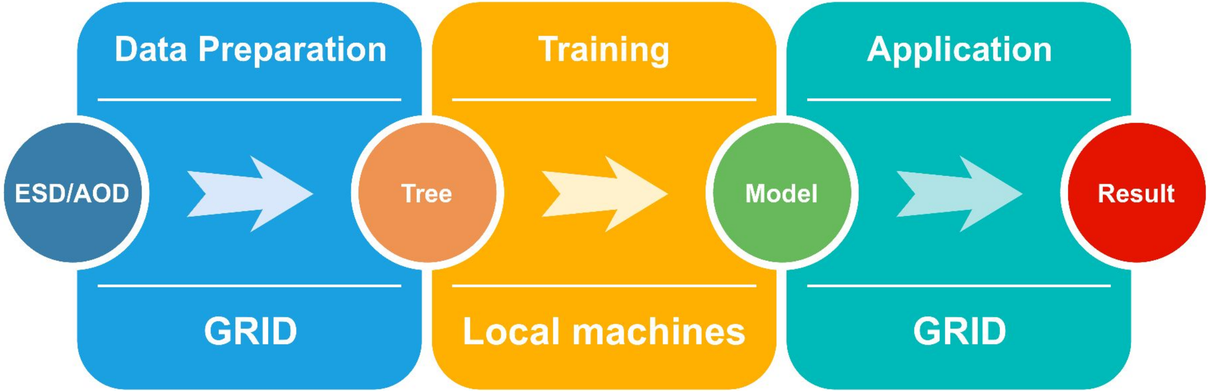
Clustering

- TPC clustering with DNNs

AI-assistants

- Chatbot for ALICE simulations
- Chatbot for ALICE detector operations

ML workflow



Data preparation

- ➢ Information written from AO2D to ROOT TTree
- ➢ Only data needed for training downloaded locally
  - a few GBs independently from the collision system

Training and optimisation

- ➢ Small fraction of real data and all MC simulations used to train/optimise the model
  - a few minutes/hours on laptops or desktops

Inference on full data sample

- ➢ From about 1 to 3 days on the GRID
  - usual time for a train run from the user point of view
  - the ML inference can be added to standard analysis tasks

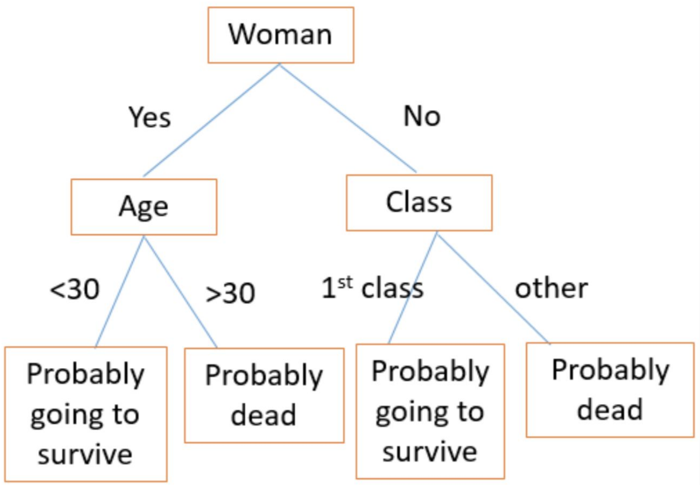
Hands-on session

- Focused on Boosted Decision Trees (BDTs) training and inference for physics analyses
- Divided in two parts

1. Training and testing a BDT model (L. Aglietta)
   - Classification of the $D_s^+ \to K^+K^-\pi^+$ signal
   - Python software strack, hipe4ml package developed in ALICE for ML based physics analyses
2. Apply the BDT to data with a O2Physics task (C. De Martin)
   - Inference using the O2Physics interface for ONNXRuntime

Boosted Decision Trees

- Hands-on session focused on BDTs
- Simple (apparently) supervised learning model well suited for classification and regression problems
- Building block → Decision Tree (DT)
  - A sequence of simple tests on the variables of the candidate
  - Combining all the tests one gets an output as a function of the variables of the single candidate
- Training a DT:
  - each test is built to maximise the separation between the signal and the background classes



DT applied to the Titanic dataset: was the passenger survived?

Boosted Decision Trees

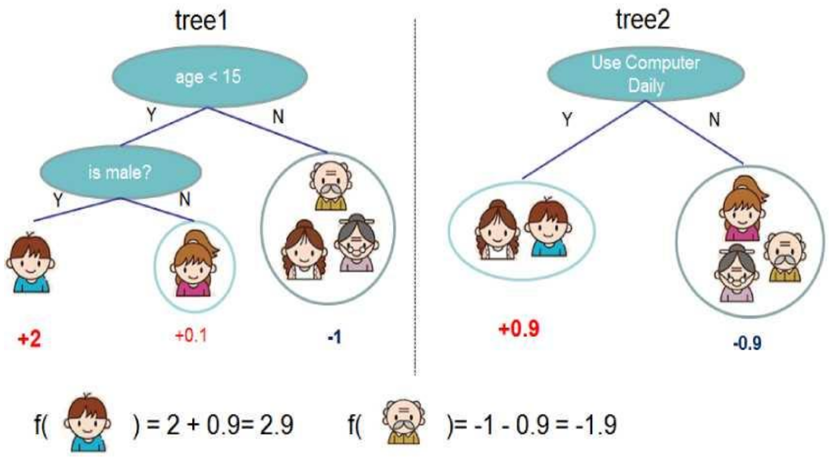
- DT: poor performances on independent samples → overfitting

Boosting

- Many simple (shallow) trees built sequentially
- Each tree is built to compensate the errors of the previous one

Ensemble model

- predictions are made combining the output of all the trees
- Very resilient to overfitting



Do they like computer games?
Score based approach to evaluate it

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ML inference

- ML applications in ALICE usually based on
  - python software stack (scikit-learn, XGBoost, TensorFlow, PyTorch, …)
- Application of models on the GRID (in your analyses!)
  - how to use a model trained in python in the ALICE C++ software?
- Run 3: ONNXRuntime
  - integrated in O2/O2Physics, available on GRID/EPN/FLP
  - supports almost any ML model (BDT, NN, …) and library (XGBoost, PyTorch, TensorFlow, ...)

MLResponse in O2Physics

- MLResponse class implemented in O2Physics
  - link
  - Interface for smooth ML inference

```cpp
// TypeOutputScore is the type of the output score from o2::ml::OnnxModel (float by default)
template <typename TypeOutputScore = float>
class MlResponse
{
 public:
  /// Default constructor
  MlResponse() = default;
  /// Default destructor
  virtual ~MlResponse() = default;
```

```cpp
protected:
 std::vector<o2::ml::OnnxModel> mModels;                  // OnnxModel objects, one for each bin
 uint8_t mNModels = 1;                                    // number of bins
 uint8_t mNClasses = 3;                                   // number of model classes
 std::vector<double> mBinsLimits = {};                    // bin limits of the variable (e.g. pT) used to select which model to use
 std::vector<std::string> mPaths = {""};                  // paths to the models, one for each bin
 std::vector<int> mCutDir = {};                           // direction of the cuts on the model scores (no cut is also supported)
 o2::framework::LabeledArray<double> mCuts = {};          // array of cut values to apply on the model scores
 std::map<std::string, uint8_t> mAvailableInputFeatures; // map of available input features
 std::vector<uint8_t> mCachedIndices;                     // vector of indices correspondance between configurable and available input features
```

MLResponse in O2Physics

- MLResponse class implemented in O2Physics
  - link
  - Interface for smooth ML inference
  - Wrappers based on it for the different PWGs

HfMlResponse.h

HfMlResponseDplusToPiKPi.h

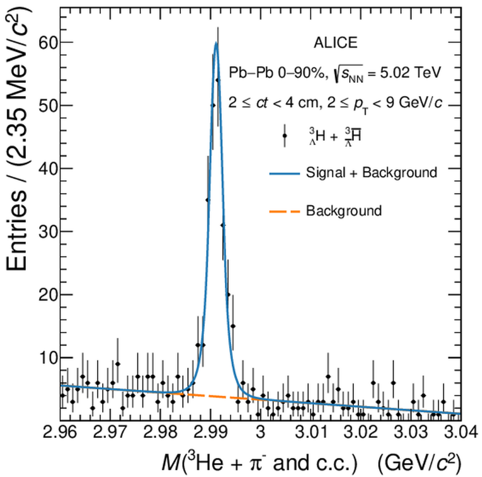
```
/// ML selections
/// \param input is the input features
/// \param pt is the candidate transverse momentum
/// \return boolean telling if model predictions pass the cuts
template <typename T1, typename T2>
bool isSelectedMl(T1& input, const T2& pt)
{
  auto nModel = findBin(&mBinsLimits, pt);
  auto output = getModelOutput(input, nModel);
  uint8_t iClass{0};
  for (const auto& outputValue : output) {
    uint8_t dir = mCutDir.at(iClass);
    if (dir != o2::cuts_ml::CutDirection::CutNot) {
      if (dir == o2::cuts_ml::CutDirection::CutGreater && outputValue > mCuts.get(nModel, iClass)) {
        return false;
      }
      if (dir == o2::cuts_ml::CutDirection::CutSmaller && outputValue < mCuts.get(nModel, iClass)) {
        return false;
      }
    }
    ++iClass;
  }
  return true;
}
```

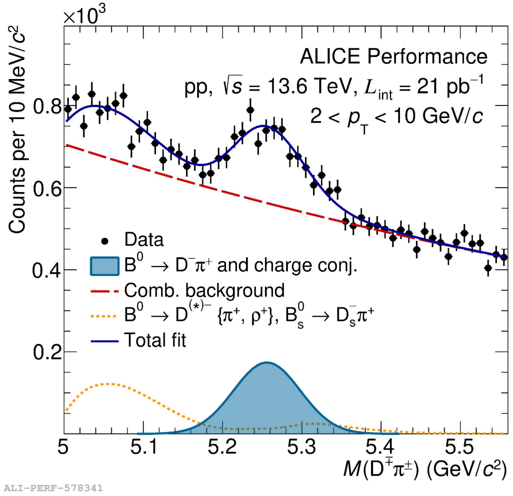
Useful resources - ML

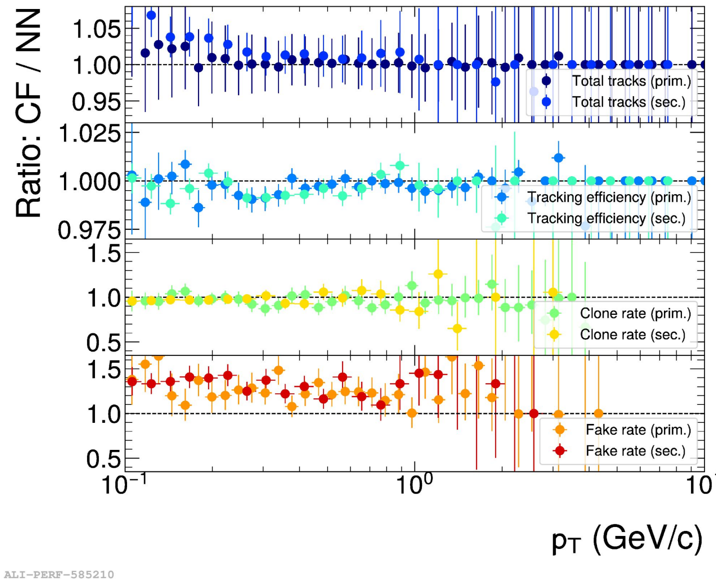
- ML theory from scratch
  - https://work.caltech.edu/telecourse , Learning from Data, Yaser Abu-Mostafa
- Hands-on ML book
  - Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow
- XGBoost BDTs
  - https://xgboost.readthedocs.io/en/stable/tutorials/model.html
- Common ML python libraries
  - https://scikit-learn.org/stable/
  - https://www.tensorflow.org/
  - https://keras.io/
  - https://pytorch.org/
  - https://onnx.ai/

Useful resources - ALICE

- ALICE-ML-Group
  - alice-machine-learning@cern.ch
  - Meetings upon requests/needs
  - https://indico.cern.ch/event/1440815/
  - Contact:
    - Me: francesco.mazzaschi@cern.ch
    - Lee Barnby: lee.barnby@cern.ch







Inter Experimental Machine Learning WG

ALICE

- Lee is the ALICE member of the IML coordination
  - Organisation of ~ monthly meetings and seminars
  - Organisation of the annual IML workshop
    - Last year there were only a few contributions from ALICE — this workshop is a great opportunity to showcase ML related work and increase visibility; we should advertise it better within the collaboration

7th Inter-Experimental LHC Machine Learning Workshop

19–23 May 2025
CERN
Europe/Zurich timezone

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Conclusion

- ML is a powerful tool employed at different levels in ALICE
    - In Run 2 we improved many physics analyses by using ML
    - In Run 3 we are using/developing ML for reconstruction, clustering, PID
- What hands-on session does not /partially cover
    - Neural Networks, ML models optimization, proper choice of the model thresholds, how to deal with systematics
        - For this, please subscribe and follow ALICE ML group meetings!

Reminder

- Tutorial on ML in O2 on Friday, covering BDT training and inference
- Can be run locally or in dedicated SWAN notebooks!
    - link