O2AT-4: Machine Learning

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Machine learning: introduction

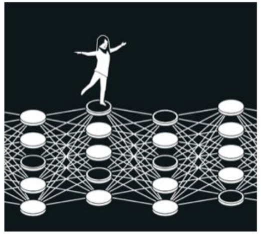
- Machine learning (ML) models are able to perform a task without being explicitly programmed to do so
  - models are built from an input sample data and try to extract patterns from it
  - no need to specify a sequence of instructions to solve the task

- ML is nowadays ubiquitous in real-world applications
  - speech recognition and translation
  - autonomous driving
  - text-to-image generation
  - HEP!
  - ….

The Nobel Prize in Physics 2024

This year's laureates used tools from physics to construct methods that helped lay the foundation for today's powerful machine learning. **John Hopfield** created a structure that can store and reconstruct information. **Geoffrey Hinton** invented a method that can independently discover properties in data and which has become important for the large artificial neural networks now in use.

They used physics to find patterns in information



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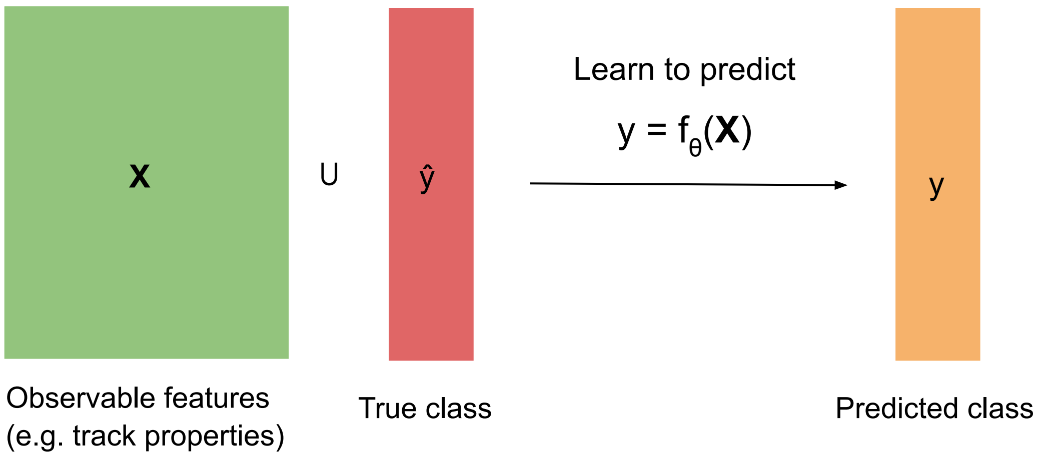
Many people have experienced how computers can translate between languages, interpret images and even conduct reasonable conversations. What is perhaps less well known is that this type of technology has long been important for research, including the sorting and analysis of vast amounts of data. The development of machine learning has exploded over the past fifteen to twenty years and utilises a structure called an artificial neural network. Nowadays, when we talk about *artificial intelligence*, this is often the type of technology we mean.

Although computers cannot think, machines can now mimic functions such as memory and learning. This year's laureates in physics have helped make this possible. Using fundamental concepts and methods from physics, they have developed technologies that use structures in networks to process information.

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

$\mathbf{X}$

Observable features
(e.g. track properties)

Learn to predict

$p(\mathbf{X}) = f_\theta(\mathbf{X})$

True probability density

$p_{true}(\mathbf{X})$

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
  - NNs to combine info from different detectors
  - PID with ITS2 using BDT regression

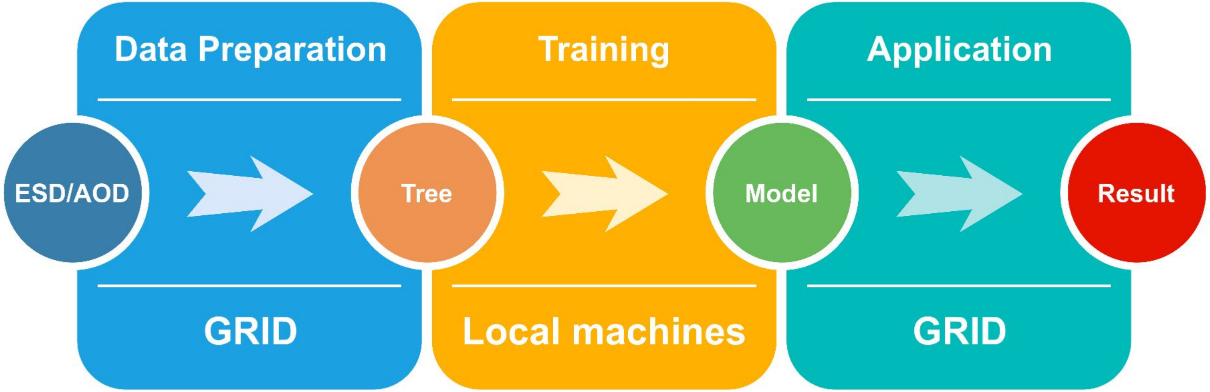
TPC response calibration

- ML to compute corrections of spatial charge distortions
- NN for energy-loss (dE/dx) calibration

Clustering

- TPC clustering with DNNs

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

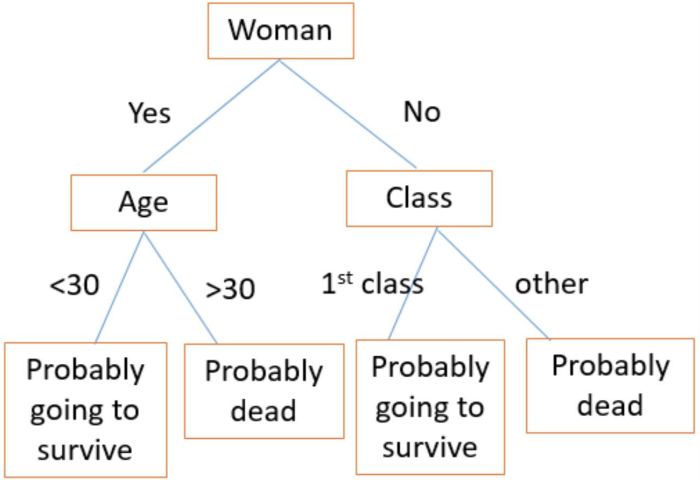
- ➢ From about 1 to 3 days on the GRID
  - ○ usual time for a train run from the user point of view
  - ○ the ML inference can be added to standard analysis tasks

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 (F. Chinu)
     - Classification of the $D_s^+ \rightarrow K^+K^-\pi^+$ signal
     - Python software strack, hipe4ml package developed in ALICE for ML based physics analyses
  2. Apply the BDT to data with a O2Physics task (M. Ciacco)
     - 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

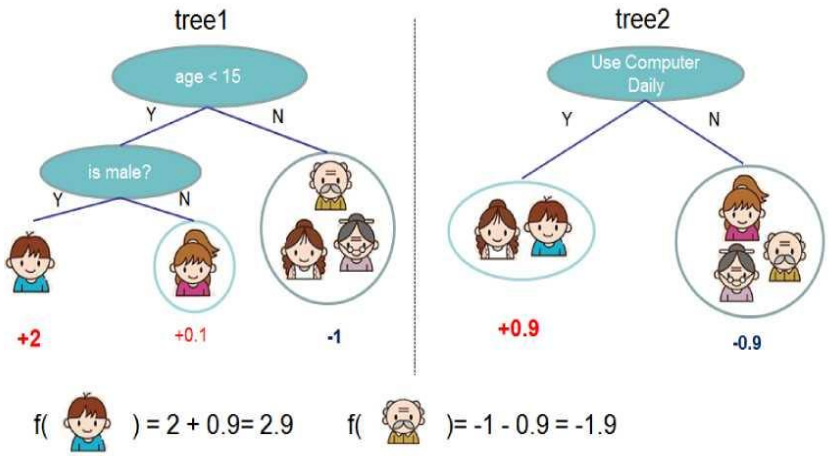
- DT: poor performances on independent samples → overfitting

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

```
// 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;
```

```
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

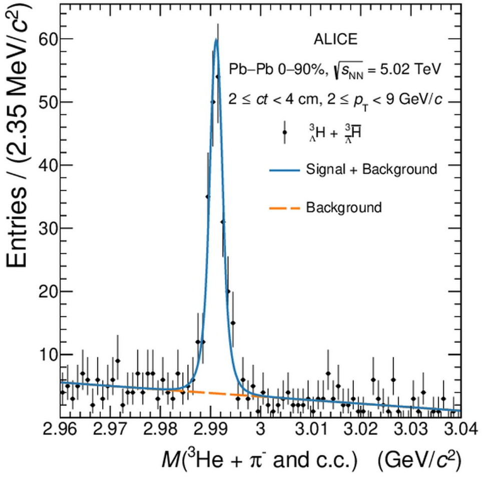
```
/// ML selections
/// \param input is the input features
/// \param pt is the candidate transverse momentum
/// \return boolean telling if model predictions pass the cuts
template <typename T1, typename T2>
bool isSelectedMl(T1& input, const T2& pt)
{
  auto nModel = findBin(&mBinsLimits, pt);
  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;
}
```

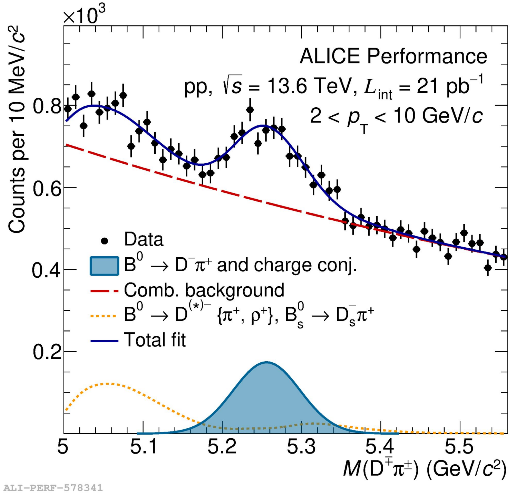
Useful resources - ML

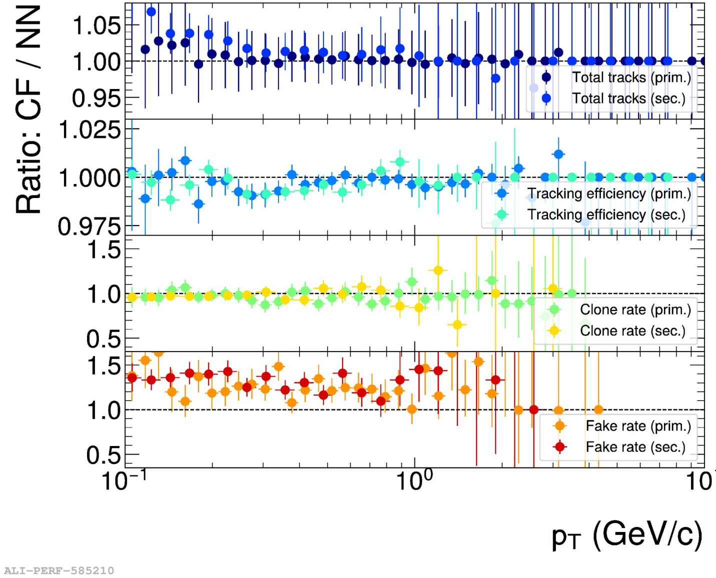
- ML theory from scratch
  - https://work.caltech.edu/telecourse , Learning from Data, Yaser Abu-Mostafa
- Hands-on ML book
  - Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow
- XGBoost BDTs
  - https://xgboost.readthedocs.io/en/stable/tutorials/model.html
- Common ML python libraries
  - 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
    - Fabio Catalano: fabio.catalano@cern.ch







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!
  - https://github.com/AliceO2Group/analysis-tutorials/tree/master/o2at-4