Introduction to Regressor BDT

Offshell Workshop Tutorial

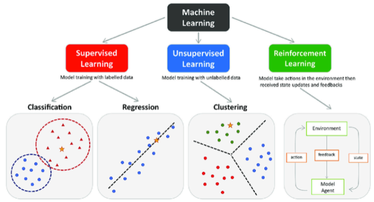
John Rotter (Rice)
Graduate Student

RICE

Previous Tutorials

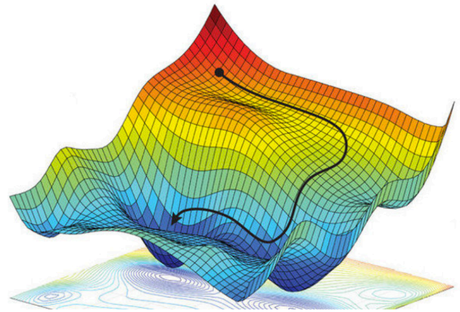
What is Machine Learning?

- Data driven general solution to a complex problem - Universal Function Approximators!
- The name “Learning” comes from personification of the algorithm but it is really just an optimization problem and **not a sentient being**
- Supervised Learning is when the algorithm is given a deterministic task
  - **Training involves a correction based on the prediction.**



How to Reward the Machine

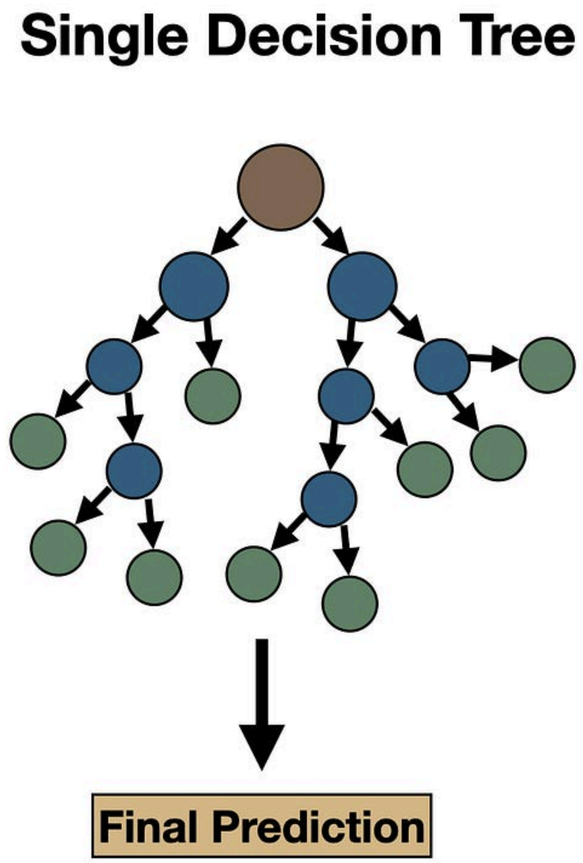
- To motivate an algorithm to perform as intended, its performance will need to be quantified
- Often this is done using a Loss Function which gives a penalty to wrong answer
- The Loss Function will return a larger value for wrong answers and zero for correct answers
- **Minimizing the Loss Function will lead to more and more correct answers**



https://indico.cern.ch/event/1375252/timetable/#16-machine-learning

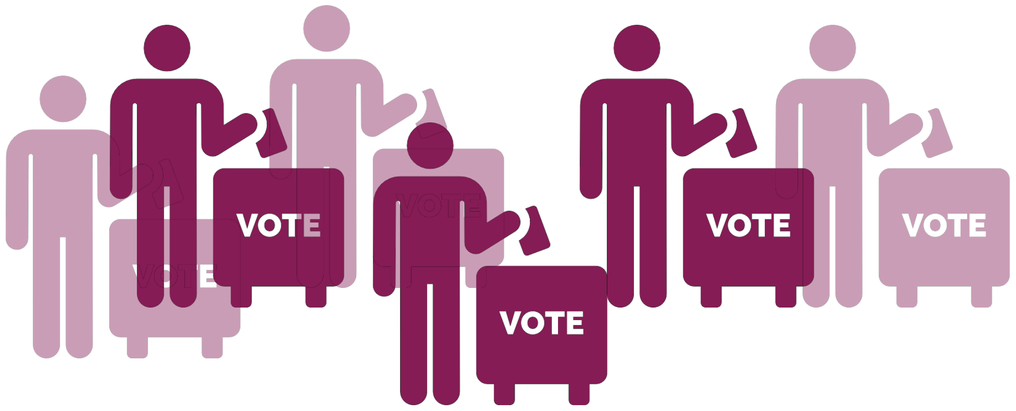
Weak Learners

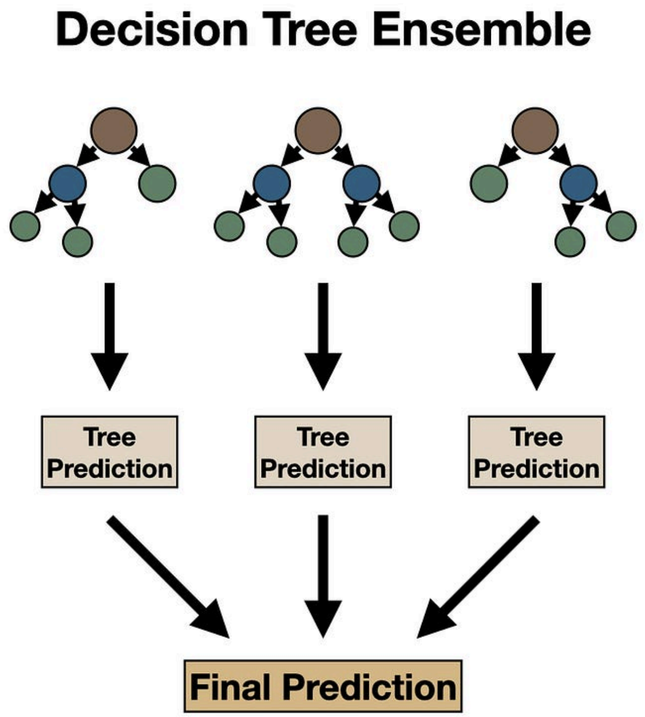
- Weak learners are small networks or trees that perform just barely better than guessing
- The idea is that it is still learning but is not learning the full model
- Cannot be trained to arbitrary level of accuracy



Ensemble of Weak Learners

- Many weak learners together can form a **Strong Learner** when chained together
- The idea is that each weak learner can learn about a subset of the structure of the algorithm
- The strong learner can recursively train more weak learners based on the error of the current ensemble!



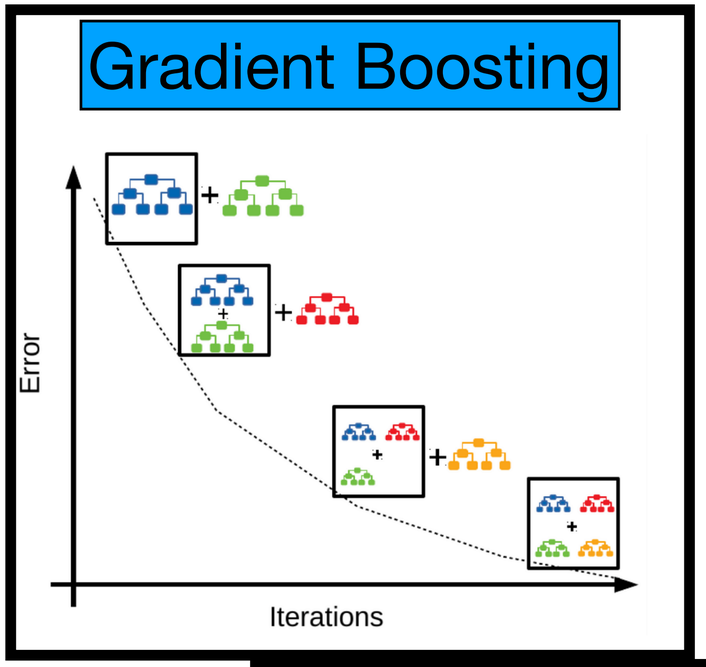


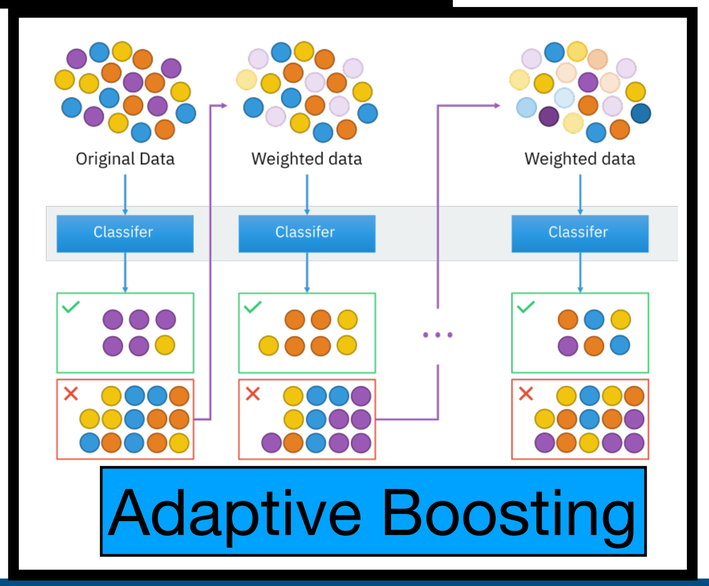
Boosted Decision Trees (BDTs)

- BDTs are a supervised learning technique which **utilizes weak learners in an ensemble to make some prediction**

- They can be used for regression or categorization

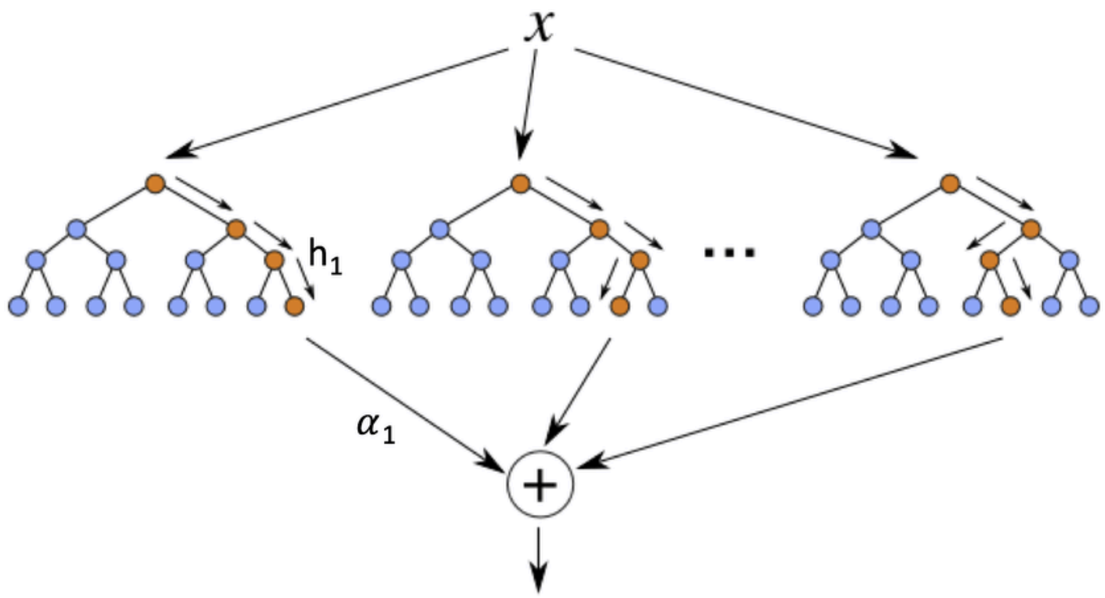
- Boosting refers to how the trees “grow” in the forest
  - Gradient Boosting (GBoost)
  - Adaptive Boosting (AdaBoost)
  - Extreme Gradient Boosting (XGBoost) - Parallelized Gradient Boosting





BDT Leaves and Predictions

- Based on the BDT structure chosen, the prediction method may vary
- For BDTs in XGBoost, trees can be traversed and will terminate at a “leaf”
- These “leaves” will all contribute some small weight, α_i
- Summing these weights yields the prediction
- Sometimes this summation can also have a function when used in classification such as a sigmoid or softmax



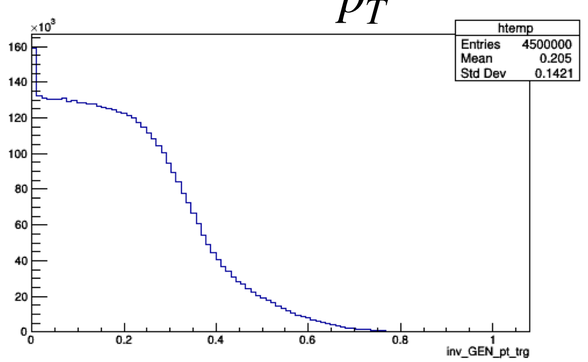
Training a Regressor BDT using XGBoost

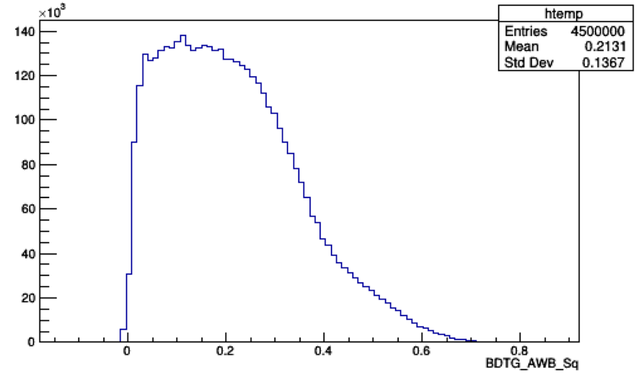
- When training any algorithm, a testing, training, and validation are randomly split to identify performance of the training
- Training data includes events whose output is already known
- The input data is fed into the BDT for each event and trained on a small batch of events
- Each time the BDT is evaluated, the residual is calculated and a new tree is appended to minimize the residual
- This is done until the forest size reaches the limit we set in the hyperparameters

Target Variables

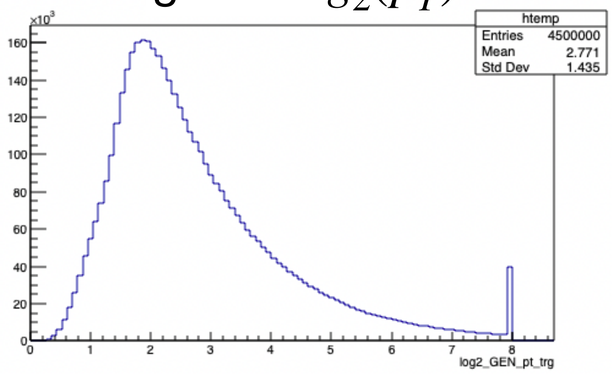
- With machine learning algorithms, the regression generally performs better with smooth output spaces
- The algorithm will tend to smooth over sharp peaks
- Playing with the target variable to choose the smoothest output space will improve performance!

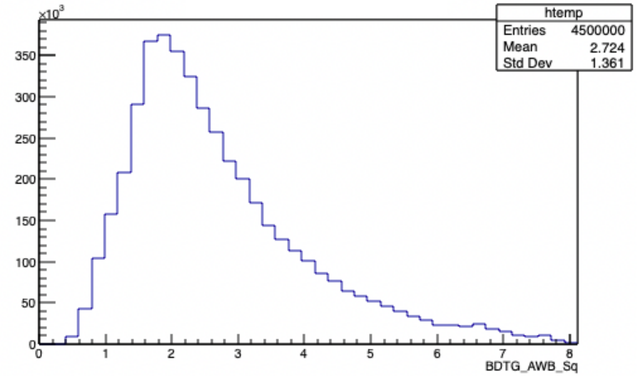
Target of $\frac{1}{p_T}$ → BDT Prediction





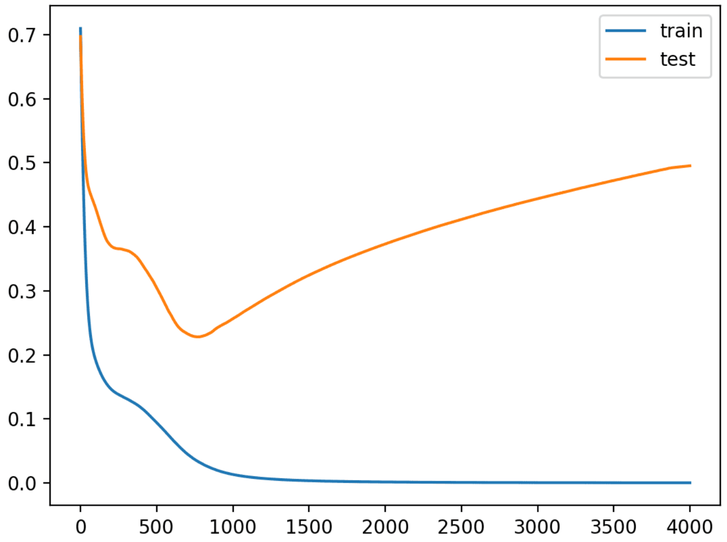
Target of $log_2(p_T)$ → BDT Prediction

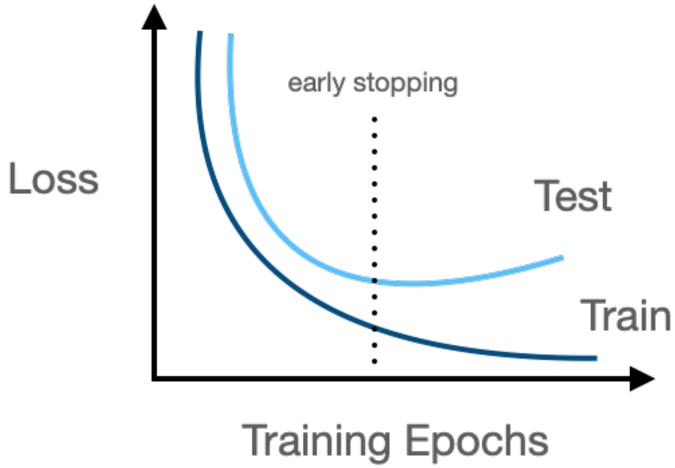




Overtraining or Overfitting

- **Overtraining** is still an issue with BDTs
- This mainly results from using incorrect tree structure or too large of forests for the input datasets





Input Variables

- One of the largest setbacks of BDTs compared to NN is that the input variables must be well defined

- Unlike NN, BDTs will produce binary cuts based on the input variables and will optimize the cuts and leaf weights **based on a given input variable** as opposed to connections **between input variables.**

- As a result, it is important to construct input variables that will be useful to the BDT rather than give default values

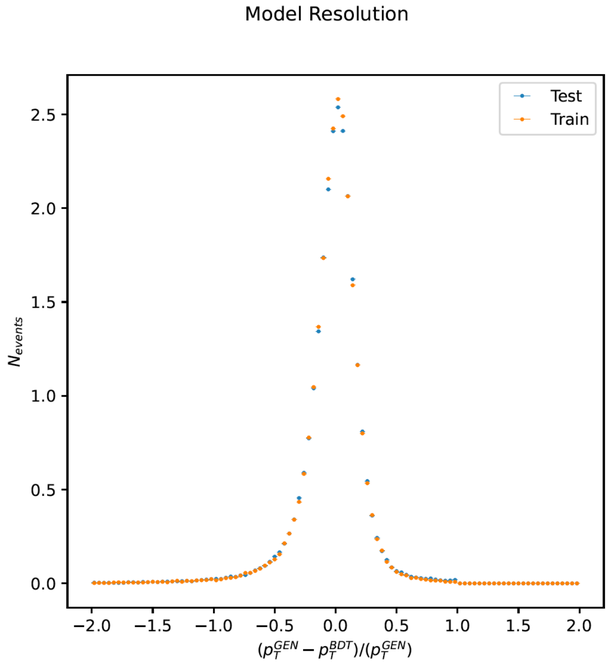
- For Example: ϕ_A and ϕ_B are not useful on their own, but $\Delta\phi_{AB}$ is useful for the BDT! A NN may be able to create a similar variable over many layers but a BDT will try to create logic from ϕ_A and ϕ_B in separate weak learners.

Hyperparameters

- Regressor BDTs have tons of hyperparameters to mess with
- To name a few:
  - Batch Size
  - Number of Trees
  - Tree Depth
  - Learning Rate
  - Event weights
  - Target Variable
  - Loss function
  - Boosting Algorithm (And optimizer)

The Tutorial

- We will be training a regressor BDT to learn to regress a muons momentum in CMS based on hits in the muon chambers!
- We will be looking at simulated events that contain many variables given from the CSCs in the endcap
- The main metric we will be plotting will be the resolution of our regressor!



https://github.com/Offshell-Workshop-LPC/Offshell-Workshop-ML-Tutorials/tree/main/Tutorial_3