INTRO TO DECISION TREES

AND BEYOND



[xkcd.com/1838]





[reddit.com]

STATISTICS vs MACHINE LEARNING

What do we want?

- DESCRIBE past trends/effects OR PREDICT "future"?
- Testing HYPOTHESIS OR finding new PATTERNS?

What kind of data is available?

CLASSICAL STATISTICS

- HYPOTHESIS TESTING

OTHER

- ANOMALY DETECTION
- SIMULATIONS
- OPTIMIZATION
- ...and more

SUPERVISED LEARNING

- REGRESSION
- CLASSIFICATION (BINARY vs MANY)

UNSUPERVISED LEARNING

- CLUSTERING
- HIDDEN PATTERNS
- DIMENSIONALITY REDUCTION

DECISION TREE

- classification algorithm
- tree-like structure to model relationships between the data features and possible outcomes
- branching decisions based on conditions
- split based on minimizing entropy in each node
- leaf nodes contain the decision results



Example: Should I take a job offer?

DECISION TREE

PROS

- classification & regression
- intuitive & interpretable
- handling both numerical and categorical data
- access to feature importance
- robust to outliers
- can handle missing data
- relatively fast

CONS

- prone to overfitting
- bias towards features with high cardinality (many unique values)
- data imbalance (accurate predictions for minority class)
- high variance for different subsets of data

FROM SINGLE DT

TO MORE ROBUST MODELS

BAGGING – RANDOM FOREST



[datahacker.rs]

BOOSTED DECISION TREES



ML (TREES & FORESTS) IN HEP

- **Problems of interest:**
 - classification signal vs background, jet finding & identification, regression
 - HL-LHC era high pile-up, demanding on computational resources
 - reduce complexity, find new patterns in data
- Most popular BDT and Neural Networks
- ROOT TMVA package https://root.cern/manual/tmva
 - supervised learning for multivariate classification and regression
 - takes a "signal" and "background" (ROOT) data tree for training (usually from MC)
 - trained model applied to data to distinguish class of interest
- Be cautious!
 - imbalanced problems (e.g. rare signal with large background)
 - train/test data selection (size, representativeness, NO mixing)
 - overfitting

SOME EXAMPLES



Fig. 1. (a) Output of the boosted decision tree used to identify jets originating from b-quarks in ATLAS [7]. (b) Boosted decision tree output used in a fit between data and physics model to extract the $t\bar{t}t\bar{t}$ signal [8].

[arXiv:2206.09645]

BONUS: References, NN (in particle physics)

- A Living Review of ML for Particle Physics: <u>https://github.com/iml-wg/HEPML-LivingReview</u>
- Inter-Experimental LHC Machine Learning Working Group: <u>https://iml.web.cern.ch/homepage</u>
- Nice illustrative intro to neural networks: <u>https://aegeorge42.github.io/</u>
- Scikit-learn: <u>https://scikit-learn.org/stable</u>
- Intro to TensorFlow: <u>https://www.tensorflow.org/tutorials/keras/classification</u>
- Intro to PyTorch: <u>https://pytorch.org/tutorials/beginner/basics/intro.html</u>