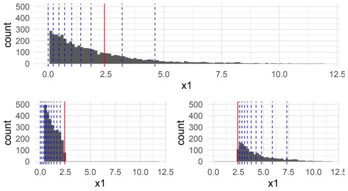
Introduction to Machine Learning

XGBoost



Learning goals

- Overview over XGB
- Regularization in XGB
- Approximate split finding

XBG - EXTREME GRADIENT BOOSTING

- Open-source and scalable tree boosting system
- Efficient implementation in *C++* with interfaces to many other programming languages
- Parallel approximate split finding
- Additional regularization techniques
- Feature and data subsampling
- Cluster and GPU support
- Highly optimized and often achieves top performance in benchmarks – if properly tuned

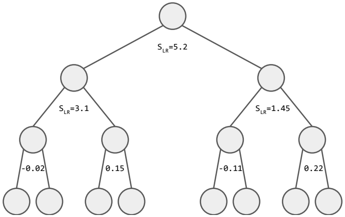
3 EXTRA REGULARIZATION TERMS

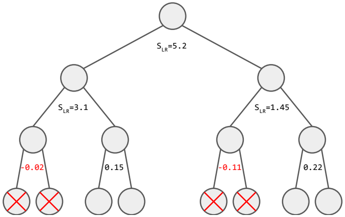
$$\mathcal{R}_{\text{reg}}^{[m]} = \sum_{i=1}^{n} L\left(y^{(i)}, f^{[m-1]}(\mathbf{x}^{(i)}) + b^{[m]}(\mathbf{x}^{(i)})\right) + \lambda_1 J_1(b^{[m]}) + \lambda_2 J_2(b^{[m]}) + \lambda_3 J_3(b^{[m]}),$$

- $J_1(b^{[m]}) = T^{[m]}$: Nr of of leaves to penalize tree depth
- $J_2(b^{[m]}) = \left\|\mathbf{c}^{[m]}\right\|_2^2$: L2 penalty over leaf values
- $J_3(b^{[m]}) = \left\|\mathbf{c}^{[m]}\right\|_1$: L1 penalty over leaf values

TREE GROWING

- Grown to max depth
- Fully expanded and leaves split even if no improvement
- At the end, each split that did not improve risk is pruned





SUBSAMPLING

Data Subsampling: XGB uses stochastic gradient GB.

Feature Subsampling: Similar to `mtry` in a random forest only a random subset of features is used for split finding.

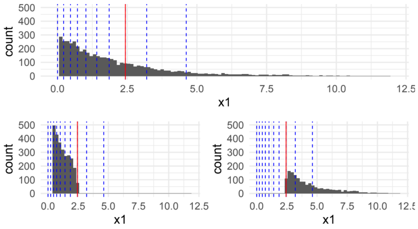
The fraction of features for a split can be randomly sampled for each

1. tree
2. level of a tree
3. split

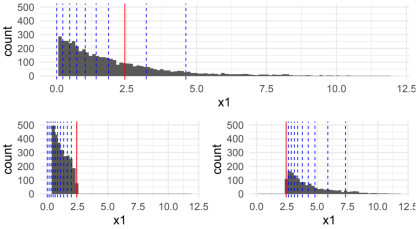
Feature subsampling speeds up training even further and can create a more diverse ensembles that will often perform better.

APPROXIMATE SPLIT-FINDING ALGORITHMS

- Speeds up tree building for large data
- Considers not all, but only *l* splits per feature
- Usually percentiles of the empirical distribution of each feature
- Computed once (global) or recomputed after each split (local)
- Called **Histogram-based Gradient Boosting**



Global



Local

Blue lines are percentiles and red = selected split

DROPOUT ADDITIVE-REGRESSION TREES

DART introduces idea of *dropout* regularization used in DL to boosting

- In iteration m we construct $\hat{b}^{[m]}$
- To compute PRs we need $\hat{f}^{[m-1]}$
- We compute this differently, by using random subset $D \subset \hat{b}^{[1]}, \dots \hat{b}^{[m-1]}$ of size $(m-1) \cdot p_{\text{drop}}$ is ignored
- To avoid *overshot predictions* in ensemble, we scale the BLs at the end of the iteration, by $\frac{1}{|D|+1}\hat{b}^{[m]}$ and $\frac{|D|}{|D|+1}\hat{b} \quad \forall \hat{b} \in D$.

- $p_{\text{drop}} = 0$: Ordinary GB
- $p_{\text{drop}} = 1$: All BLs are trained independently, and equally weighted. Model is very similar to random forest.

$\Rightarrow$ p_{drop} is smooth transition from GB to RF

PARALLELISM AND GPU COMPUTATION

- GB is inherently sequential, not easy to parallelize
- **But:** Building of BLs can be parallelized
- Data sort and split eval in different branches of tree BLs can be computed in parallel by using efficient block data structures
- Can also gain huge speed-up by moving from CPU to GPU

OVERVIEW OF IMPORTANT HYPERPARAMETERS

HP (as named in software)	Type	Typical Range	Trafo	Default	Description
`eta`	R	$[-4, 0]$	10^x	0.3	learning rate (also called ν) shrinks contribution of each boosting update
`nrounds`	I	$\{1, \dots, 5000\}$	–	–	number of boosting iterations. Can also be optimized with early stopping.
`gamma`	R	$[-7, 6]$	2^x	0	minimum loss reduction required to make a further partition on a leaf node of the tree
`max_depth`	I	$\{1, \dots, 20\}$	–	6	maximum depth of a tree
`colsample_bytree`	R	$[0.1, 1]$	–	1	subsample ratio of columns for each tree
`colsample_bylevel`	R	$[0.1, 1]$	–	1	subsample ratio of columns for each depth level
`lambda`	R	$[-10, 10]$	2^x	1	L_2 regularization term on weights
`alpha`	R	$[-10, 10]$	2^x	0	L_1 regularization term on weights
`subsample`	R	$[0.1, 1]$	–	1	subsample ratio of the training instances