Gradient Boosting

Jan-Philipp Kolb

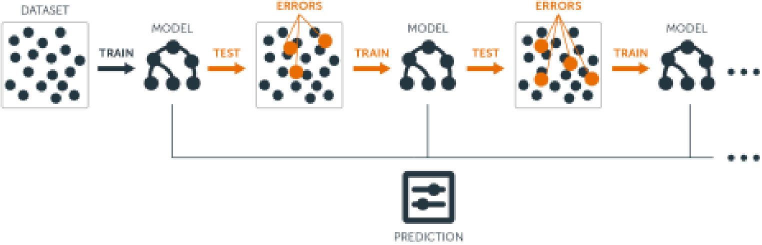
04 Juni, 2019

Gradient Boosting Machines (GBMs)

- GBMs are extremely popular, successful across many domains and one of the leading methods for winning **Kaggle competitions**.
- GBMs build an ensemble of flat and weak successive trees with each tree learning and improving on the previous.
- When combined, these trees produce a powerful "committee" often hard to beat with other algorithms.
- The following slides are based on UC Business Analytics R Programming Guide on **GBM regression**

The idea of GBMs

- Many machine learning models are founded on a single predictive model (i.e. linear regression, penalized models, naive bayes, **svm**).
- Other approaches (bagging, random forests) are built on the idea of building an ensemble of models where each individual model predicts the outcome and the ensemble simply averages the predicted values.
- The idea of boosting is to add models to the ensemble sequentially.
- At each particular iteration, a new weak, base-learner model is trained with respect to the error of the whole ensemble learnt so far.



Advantages of GBMs

Predictive accuracy

- GBMs often provide predictive accuracy that cannot be beat.

Flexibility

- Optimization on various loss functions possible and several hyperparameter tuning options.

No data pre-processing required

- Often works great with categorical and numerical values as is.

Handles missing data

- Imputation not required.

Disadvantages of GBMs

GBMs overemphasize outliers

- This causes overfitting.
- GBMs will continue improving to minimize all errors. Use cross-validation to neutralize.

Computationally expensive

- GBMs often require many trees ($>$1000) which can be time and memory exhaustive.
- The high flexibility results in many parameters that interact and influence heavily the behavior of the approach (number of iterations, tree depth, regularization parameters, etc.).
- This requires a large grid search during tuning.

Interpretability

- GBMs are less interpretable, but this is easily addressed with various tools (variable importance, partial dependence plots, **LIME**, etc.).

Important concepts

Base-learning models

- Boosting is a framework that iteratively improves any weak learning model.
- Many gradient boosting applications allow you to “plug in” various classes of weak learners at your disposal.
- In practice, boosted algorithms often use decision trees as the base-learner.

Training weak models

- A weak model has an error rate only slightly better than random guessing.
- The idea behind boosting is that each sequential model builds a simple weak model to slightly improve the remaining errors.
- Shallow trees represent weak learner - trees with only 1-6 splits.

Benefits of combining many weak models:

- **Speed**: Constructing weak models is computationally cheap.
- **Accuracy improvement**: Weak models allow the algorithm to learn slowly; making minor adjustments in new areas where it does not perform well. In general, statistical approaches that learn slowly tend to perform well.
- **Avoids overfitting**: Making only small incremental improvements with each model in the ensemble allows us to stop the learning process as soon as overfitting has been detected (typically by using cross-validation).

Sequential training with respect to errors

- Boosted trees are grown sequentially;
- Each tree is grown using information from previously grown trees.
- $x \rightarrow$ features and $y \rightarrow$ response:
- The basic algorithm for boosted regression trees can be generalized:

1.) Fit a decission tree: $F_1(x) = y$

2.) the next decission tree is fixed to the residuals of the previous:
$h_1(x) = y - F_1(x)$

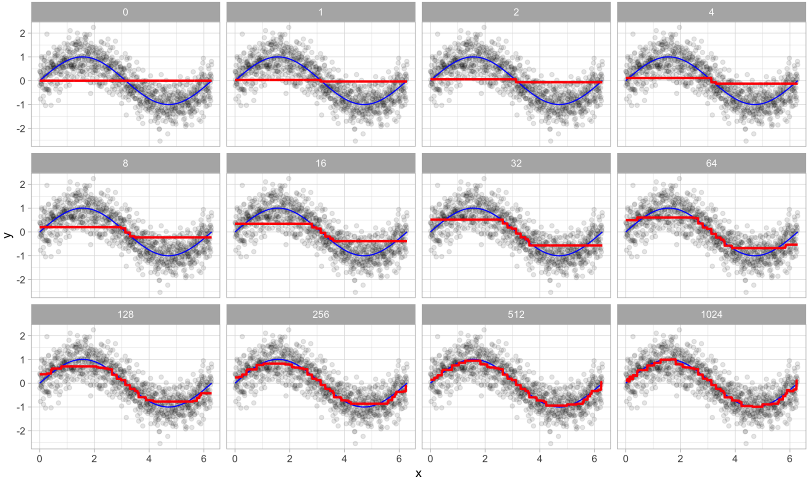
3.) Add this new tree to our algorithm: $F_2(x) = F_1(x) + h_1(x)$

4.) The next decission tree is fixed to the residuals of $h_2(x) = y - F_2(x)$

5.) Add the new tree to the algorithm: $F_3(x) = F_2(x) + h_1(x)$

Continue this process until some mechanism (i.e. cross validation) tells us to stop.

Boosted regression decision stumps as 0-1024 successive trees are added.



Boosted regression figure - explained

- The figure illustrates a single predictor (x) that has a true underlying sine wave relationship (blue line) with y along with some irriducible error.
- The first tree fit in the series is a single decision stump (i.e., a tree with a single split).
- Each following successive decision stump is fit to the previous one's residuals.
- Initially there are large errors, but each additional decision stump in the sequence makes a small improvement in different areas across the feature space where errors still remain.

Loss functions

- Many algorithms, including decision trees, focus on minimizing the residuals and emphasize the MSE loss function.
- In GBM approach, regression trees are fitted sequentially to minimize the errors.
- Often we wish to focus on other loss functions such as **mean absolute error** (MAE)
- Or we want to apply the method to a classification problem with a loss function such as **deviance**.
- With gradient boosting machines we can generalize the procedure to loss functions other than MSE.

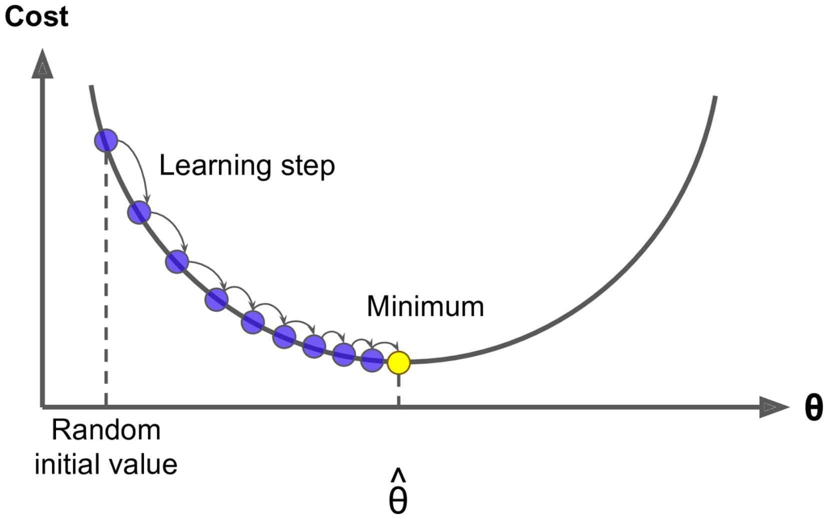
A gradient descent algorithm

- Gradient boosting is considered a **gradient descent** algorithm.
- Which is a very generic optimization algorithm capable of finding optimal solutions to a wide range of problems.
- The general idea of gradient descent is to tweak parameters iteratively in order to minimize a cost function.

Example

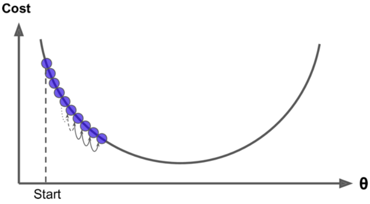
- Suppose you are a downhill skier racing against your friend.
- A good strategy to beat your friend is to take the path with the steepest slope.
- This is exactly what gradient descent does - it measures the local gradient of the loss (cost) function for a given set of parameters (Φ) and takes steps in the direction of the descending gradient.
- Once the gradient is zero, we have reached the minimum.

Gradient descent (Geron, 2017).

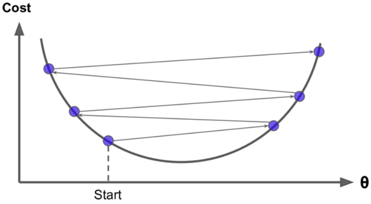


Gradient descent

- Gradient descent can be performed on any loss function that is differentiable.
- This allows GBMs to optimize different loss functions as desired
- An important parameter in gradient descent is the size of the steps which is determined by the learning rate.
- If the learning rate is too small, then the algorithm will take many iterations to find the minimum.
- But if the learning rate is too high, you might jump cross the minimum and end up further away than when you started.



a) too small



a) too big

Tuning GBM

- GBMs are highly flexible - many tuning parameters
- It is time consuming to find the optimal combination of hyperparameters

Number of trees

- GBMs often require many trees;
- GBMs can overfit so the goal is to find the optimal number of trees that minimize the loss function of interest with cross validation.

Tuning parameters

Depth of trees

- The number d of splits in each tree, which controls the complexity of the boosted ensemble.
- Often $d = 1$ works well, in which case each tree is a stump consisting of a single split. More commonly, d is greater than 1 but it is unlikely that $d > 10$ will be required.

Learning rate

- Controls how quickly the algorithm proceeds down the gradient descent.
- Smaller values reduce the chance of overfitting but also increases the time to find the optimal fit.
- This is also called shrinkage.

Tuning parameters (II)

Subsampling

- Controls if a fraction of the available training observations is used.
- Using less than 100% of the training observations means you are implementing **stochastic gradient descent**.
- This can help to minimize overfitting and keep from getting stuck in a local minimum or plateau of the loss function gradient.