Introduction to Machine Learning

XBoosting Trees and Random Forests

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Outline

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Partition

Tree partition of the space

- They partition the space of all joint predictor variable values into disjoint regions:

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Thus, a constant γ_j is assigned to each such region

$$\boldsymbol{x} \in R_j \Rightarrow f(\boldsymbol{x}) = \gamma_j$$

Outline

Finally, we can see a tree as

Formal, Equation

$$T(\boldsymbol{x}|\Theta) = \sum_{j=1}^{J} \gamma_j I(\boldsymbol{x} \in R_j)$$

- $\Theta = \{R_j, \gamma_j\}_{j=1}^{J}$

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Then, we have the following Loss function for Θ

$$L(\boldsymbol{x}_i, \gamma_j|\Theta) = I[y_i \neq \gamma_j]$$

This is a problem

We have an Empirical Risk used to obtain the parameters

$$\widehat{\Theta} = \arg\min_{\Theta} \sum_{j=1}^{J} \sum_{\boldsymbol{x}_i \in R_j} L\left(\boldsymbol{x}_i, \gamma_j | \Theta\right)$$

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This is a combinatorial problem

- This can be quite difficult to solve

We can solve it, if ...

Finding R_j

- Note also that finding the R_j entails estimating also γ_j.

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Normally, for this type of problems we use given that they are NP-Complete

- Recursive Branch and Bound algorithms

Pseudo-code for Branch-and-Bound

We have

BRANCH-AND-BOUND(P_0)

1. *Start with some problem* P_0
2. *Let* $\mathcal{S} = \{P_0\}$, *the set if active subproblems*
3. *bestsofar*$=\infty$

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12. *return bestsofar*

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Therefore

We use a smoother criterion that the one by $I[y_i \neq \gamma_j]$

$$\widetilde{\Theta} = \arg\min_{\Theta} \sum_{i=1}^{N} \widetilde{L}\left(T\left(\boldsymbol{x}_i|\Theta\right), y_i|\Theta\right)$$

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Here, we do the following

- $\widehat{\gamma}_j = \overline{y}_j$, the mean of the y_i falling in the region R_j.

Therefore

For misclassification loss

- $\widehat{\gamma}_j$ is the modal class of the observations falling in R_j.

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How do we estimate R_j

- We can use Gini or Shannon Entropy...

Outline

We are ready to define

The Boosted tree model is a sum of such trees

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This comes from the Boosting classic cost function

$$C(\boldsymbol{x}_i) = \alpha_1 y_1(\boldsymbol{x}_i) + \alpha_2 y_2(\boldsymbol{x}_i) + ... + \alpha_M y_M(\boldsymbol{x}_i) \quad (1)$$

Thus, at each stage

We need to solve the following cost function

$$\widehat{\Theta} = \arg\min_{\Theta_m} \sum_{i=1}^{N} L\left(y_i, f_{m-1}\left(\boldsymbol{x}_i\right) + T\left(\boldsymbol{x}_i|\Theta_m\right)\right)$$

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For the region set and constants $\Theta_m = \{R_{jm}, \gamma_{jm}\}_{j=1}^{J_m}$

- Of the next tree give the previous model $f_{m-1}\left(\boldsymbol{x}_i\right)$

This can be solved by

Forward Stage-wise Additive Modeling.

1. Init $f_0 = 0$
2. For $m = 1$ to M:
3. Compute

$$(\beta_m, \gamma_m) = \arg\min_{\beta,\gamma} \sum_{i=1}^{N} L\left(y_i, f_{m-1}\left(\boldsymbol{x}_i\right) + \beta b\left(\boldsymbol{x}_i|\gamma\right)\right)$$

4. Set $f_m\left(\boldsymbol{x}\right) = f_m\left(\boldsymbol{x}\right)$

- Here $b\left(\boldsymbol{x}_i|\gamma\right)$ simple functions of the multivariate argument $\boldsymbol{x}$.

Now

Given the regions R_{jm}

$$\widehat{\gamma}_{jm} = \arg\min_{\gamma_{jm}} \sum_{\boldsymbol{x}_i \in R_{jm}} L\left(y_i, f_{m-1}\left(\boldsymbol{x}_i\right) + \gamma_{jm}\right)$$

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Nevertheless, finding the regions can be difficult

- For a few special cases, the problem simplifies.

Outline

We can use AdaBoost

We can use the exponential Loss

$$\widehat{\Theta}_m = \arg\min_{\Theta_m} \sum_{i=1}^{N} w_i^{(m)} \exp\left\{-y_i T\left(|\Theta_m\right)\right\}$$

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Now, we have a conundrum

- We can decide to use a Robust Loss function
  - Absolute Error, the Huber loss

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This will be make our life quite difficult

- Therefore, we opt for loss functions that can simplify our algorithms

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We have the following loss function

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Where

$$\boldsymbol{f} = \{f(\boldsymbol{x}_1), f(\boldsymbol{x}_2), ..., f(\boldsymbol{x}_N)\}$$

Thus, we have

As a Solution, we have a sum of component vectors

$$\boldsymbol{f}_M = \sum_{m=0}^{M} \boldsymbol{h}_m, \ \boldsymbol{h}_m \in \mathbb{R}^N$$

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Thus, we select

- $\boldsymbol{h}_m = -\rho_m \boldsymbol{g}_m$ where ρ_m is a scalar and $\boldsymbol{g}_m \in \mathbb{R}^N$ is the gradient of

$$L(\boldsymbol{f}) = \sum_{i=1}^{N} L(y_i, \boldsymbol{f}(\boldsymbol{x}_i))$$

  - Evaluated at $\boldsymbol{f} = \boldsymbol{f}_{m-1}$

Then

The components

$$\boldsymbol{g}_{im} = \frac{\partial L\left(y_i, \boldsymbol{f}\left(\boldsymbol{x}_i\right)\right)}{\partial \boldsymbol{f}\left(\boldsymbol{x}_i\right)}\Big|_{\boldsymbol{f}(\boldsymbol{x}_i)=\boldsymbol{f}_{m-1}(\boldsymbol{x}_i)}$$

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Where

$$\rho_m = \arg\min_{\rho} L\left(\boldsymbol{f}_{m-1} - \rho \boldsymbol{g}_m\right)$$

Then, we have the classic Gradient Descent

$$\boldsymbol{f}_m = \boldsymbol{f}_{m-1} - \rho_m \boldsymbol{g}_m$$

Therefore

We have the following Gradients for some common Loss functions

Setting	Loss Function	Gradient $-\partial L(y_i, \boldsymbol{f}(\boldsymbol{x}_i))/\partial \boldsymbol{f}(\boldsymbol{x}_i)$
Regression	$\frac{1}{2}\left[y_i - f\left(\boldsymbol{x}_i\right)\right]^2$	$y_i - f\left(\boldsymbol{x}_i\right)$
Regression	$\left\|y_i - f\left(\boldsymbol{x}_i\right)\right\|$	$sign\left[y_i - f\left(\boldsymbol{x}_i\right)\right]$
Classification	$-\sum_{k=1}^{K} \log p_k\left(\boldsymbol{x}_i\right)$	k^{th} component $I\left(y = G_k\right) - p_k\left(\boldsymbol{x}_i\right)$

Final Algorithm

Gradient Tree Boosting Algorithm

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3. Output $\widehat{f}(\boldsymbol{x}) = f_M(\boldsymbol{x})$

How do we get the Right size for the Trees

We could see this as a separated procedure

- A very large (oversized) tree is first induced,
  - A bottom-up procedure is employed to prune it to the estimated optimal number of terminal nodes.

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Problem

- The first trees are too Large, reducing performance...

We can do better

We can restrict the trees to have the same size on the number of Terminal Regions

$$J_m = J \ \forall m$$

- At each iteration a J-terminal node regression tree is induced.

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Therefore

- Thus J becomes a meta-parameter of the entire boosting procedure.

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Another parameter to estimate

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A Large M can lead to Overfitting

- A convenient way to estimate M^* is to monitor prediction risk as a function of M on a validation sample.
  - Other Techniques are Shrinkage and Subsampling

For More on this

Take a Look at

- The Elements of Statistical Learning by Hastie et al. Chapter 10.11 and 10.12

In the Case of Shrinkage

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The parameter ν is controlling the learning rate of the boosting procedure.

- Smaller values of ν (more shrinkage) result in larger training risk for the same number of iterations M.

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A Popular Algorithm

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- 17 solutions used XGBoost.

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As solely algorithm

- Or with a combination of neural network algorithms as ensembles method.

Ensemble Learning

Definition

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Basically

1. Bootstrap aggregating (bagging)
2. Boosting
3. Bayesian parameter averaging
4. Bayesian model combination
5. etc

Outline

Cost Function Ensemble

For a given data set

$$\mathcal{D} = \{(\boldsymbol{x}_i, y_i) \,|\, |\mathcal{D}| = N, \boldsymbol{x}_i \in \mathbb{R}^m, y_i \in \mathbb{R}\}$$

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A Tree Ensemble model

$$\widehat{y}_i = \phi\left(\boldsymbol{x}_i\right) = \sum_{k=1}^{K} f_k\left(\boldsymbol{x}_i\right)$$

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Where, the space of regression trees (CART)

$$\mathcal{F} = \left\{f_k\left(\boldsymbol{x}\right) = w_{q(\boldsymbol{x})}\right\}\left(q : \mathbb{R}^m \rightarrow T, w \in \mathbb{R}^T\right)$$

Remarks

$q : \mathbb{R}^m \rightarrow T, w \in \mathbb{R}^T$

- q represents the structure of a tree that maps an example to the corresponding leaf index.
- T is the number of leaves in the tree.
- Each f_k corresponds to an independent tree structure q and leaf weights w.

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Something Notable

- Unlike decision trees, each regression tree contains a continuous score on each of the leaf.
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For this

- we use w_i to represent score on i^{th} leaf.

Final Cost Function

XGBoost minimize the following function

$$\mathcal{L}(\phi) = \sum_i l(\hat{y}_i, y_i) + \sum_k \Omega(f_k)$$

$$\text{whre } \Omega(f) = \gamma T + \frac{1}{2}\lambda \|w\|^2$$

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Remarks

- l is a differentiable convex loss function.
- Ω penalize the complexity of the regression tree.
- $\frac{1}{2}\lambda \|w\|^2$ helps to smooth the final learned weights to avoid over-fitting.

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Optimizing in an Additive Manner

For this, the model is trained in an additive manner

- Given $\widehat{y}_i^{(t)}$ be the prediction of the i^{th} instance at the t^{th} iteration,

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We rewrite the cost function as

$$\mathcal{L}^{(t)}(\phi) = \sum_i l\left(\widehat{y}_i^{(t-1)} + f_t(\boldsymbol{x}_i), y_i\right) + \Omega(f_t)$$

- This means we greedily add the f_t that most improves our model.

Then, we can use the Taylor Second Optimization

Second-order approximation

$$\mathcal{L}^{(t)} \simeq \sum_{i=1}^{N} \left[l\left(\widehat{y}_i^{(t-1)}, y_i\right) + g_i f_t\left(\boldsymbol{x}_i\right) + \frac{1}{2} h_i f_t^2\left(\boldsymbol{x}_i\right) \right] + \Omega\left(f_t\right)$$

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Where

- $g_i = \partial_{\widehat{y}^{(t-1)}} l\left(\widehat{y}_i^{(t-1)}, y_i\right)$ and $h_i = \partial^2_{\widehat{y}^{(t-1)}} l\left(\widehat{y}_i^{(t-1)}, y_i\right)$

Outline

Furthermore

We have the following cost function after removing constant terms

$$\mathcal{L}^{(t)} \simeq \sum_{i=1}^{N} \left[g_i f_t\left(\boldsymbol{x}_i\right) + \frac{1}{2} h_i f_t^2\left(\boldsymbol{x}_i\right) \right] + \Omega\left(f_t\right)$$

Furthermore

We have the following cost function after removing constant terms

$$\mathcal{L}^{(t)} \simeq \sum_{i=1}^{N} \left[g_i f_t\left(\boldsymbol{x}_i\right) + \frac{1}{2} h_i f_t^2\left(\boldsymbol{x}_i\right) \right] + \Omega\left(f_t\right)$$

Which can be expanded by defining $I_j = \{i | q\left(\boldsymbol{x}_i\right) = j\}$

$$\begin{aligned}
\mathcal{L}^{(t)} &= \sum_{i=1}^{N} \left[g_i f_t\left(\boldsymbol{x}_i\right) + \frac{1}{2} h_i f_t^2\left(\boldsymbol{x}_i\right) \right] + \gamma T + \frac{1}{2} \lambda \sum_{j=1}^{T} w_j^2 \\
&= \sum_{j=1}^{T} \left[\left(\sum_{i \in I_j} g_i \right) w_j + \frac{1}{2} \left(\sum_{i \in I_j} h_i + \lambda \right) w_j^2 \right] + \lambda T
\end{aligned}$$

Then, for a fixed structure $q(\boldsymbol{x})$

we can compute the optimal weight for a leaf

$$w_j^* = -\frac{\sum_{i \in I_j} g_i}{\sum_{i \in I_j} h_i + \lambda}$$

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Additionally, we can use the following function to score the structure of q

$$\mathcal{L}^{(t)}(q) = -\frac{1}{2} \sum_{j=1}^{T} \frac{\left(\sum_{i \in I_j} g_i\right)^2}{\sum_{i \in I_j} h_i + \lambda} + \gamma T$$

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The previous equations can be used

- As a scoring function to measure the quality of a tree structure q

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Something Notable

- This score is like the impurity score for evaluating decision trees

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Letting $I = I_L \cup I_R$, then the reduction is given by

$$\mathcal{L}_{split} = \frac{1}{2}\left[\frac{\left(\sum_{i\in I_L} g_i\right)^2}{\sum_{i\in I_L} h_i + \lambda} + \frac{\left(\sum_{i\in I_R} g_i\right)^2}{\sum_{i\in I_R} h_i + \lambda} - \frac{\left(\sum_{i\in I} g_i\right)^2}{\sum_{i\in I} h_i + \lambda}\right] - \gamma$$

Outline

Basic Exact Greedy Algorithm

A Big Problem

- One of the key problems in tree learning is to find the best split by

$$\mathcal{L}_{split}$$

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In order to do generate these splits

- A split finding algorithm enumerates over all the possible splits on all the features

Example, Exact Greedy Algorithm

Something Notable

1. **Input:** I, instance set of current node
2. **Input:** m, feature dimension

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6. $\quad G_L = 0$ and $H_L = 0$
7. $\quad$ for j in $sorted\left(I, \text{by } x_{jk}\right)$ do
8. $\quad\quad G_L = G_L + g_j,\ H_L = H_L + h_j.$
9. $\quad\quad G_R = G - G_L,\ H_R = H - H_L.$
10. $\quad\quad score = \max\left\{score, \frac{G_L^2}{H_L+\lambda} + \frac{G_R^2}{H_R+\lambda} - \frac{G^2}{H+\lambda}\right\}$

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11. **Output**: Split with Max Score

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Quite computationally demanding

- This can be improved!!!

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Quite computationally demanding

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For this

- The algorithm must first sort the data according to feature values.
- Then, it visits the data in sorted order to accumulate the gradient statistics.

Therefore

Better to have an approximation

- Thus, people proposed the use the percentiles of feature distributions
  - To find the splitting points or candidate points

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Then, it maps the continuous features into buckets split by these candidate points

- Basically you could use homogeneity via the Shannon Entropy
  - Or any other possible one

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Aggregates the statistics on the buckets

- Then, It finds the best solution based on this statistics

The Two Variants for Splitting

The global variant

- It proposes all the candidate splits during the initial phase of tree construction

The Two Variants for Splitting

The global variant

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The local variant

- The local variant re-proposes after each split!!!

Outline

Approximate Algorithm for Split Finding

Algorithm

1. for $k = 1$ to m:
2. Propose $S_k =$ by using weighted percentiles at the feature k
3. Proposal can be done per tree (global) or per split
4. for $k = 1$ to m:
5. $G_{kv} = \sum_{j \in \{j | s_{k,v} \geq x_{jk} > s_{k,v-1}\}} g_j$
6. $H_{kv} = \sum_{j \in \{j | s_{k,v} \geq x_{jk} > s_{k,v-1}\}} h_j$

However

An important subject

- How the Weighted Quantile Sketch works?

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Weighted Quantile Sketch

- To understand the method in XGBoost

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Weighted Quantile Sketch

- To understand the method in XGBoost

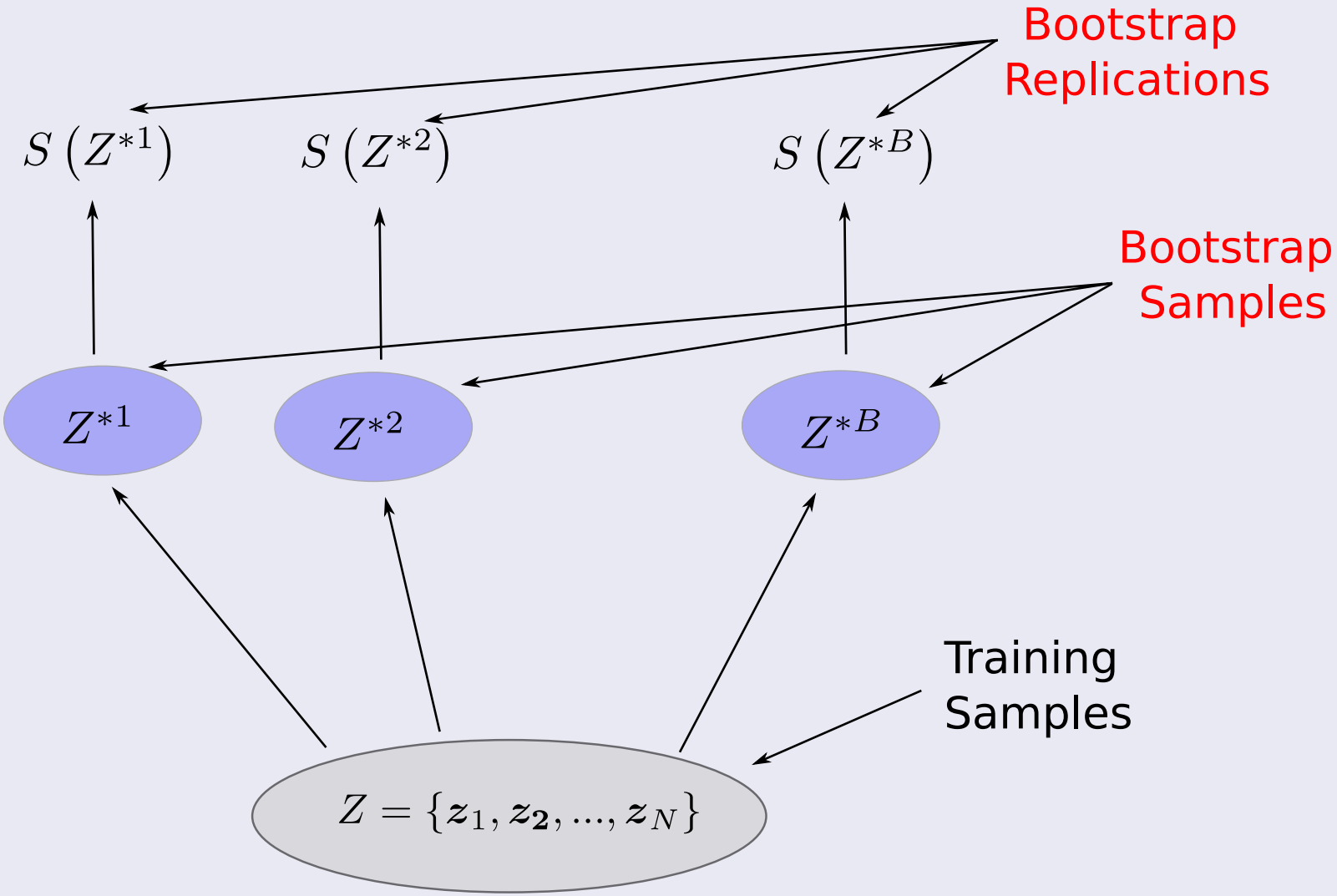
It is part of the original implementation

- Chen, Tianqi, and Carlos Guestrin. "Xgboost: A scalable tree boosting system." In Proceedings of the 22nd ACM SIGKDD international conference on knowledge discovery and data mining, pp. 785-794. 2016.

Outline

Reminder

Bootstrap aggregating/ bagging



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This is perfect given

- If we can decrease the variance of the decision trees
  - We obtain a more precise classifier.

Outline

The Model

In a series of papers and technical reports

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By using ensembles of trees

- In Breiman's approach, each tree in the collection is formed by first selecting at random
  - At each node, a small of input coordinates/features

Then, we use such features to obtain the best split

- For the subsets at the nodes...

For example, using the idea of Bootstrap

Draw a bootstrap sample Z of size N from the training data

- Grow a random-forest tree T_b

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Finally

Output the ensemble of trees $\{T_b\}_{b=1}^{B}$

In another example

The following procedure is then repeated $\lceil \log_2 k_n \rceil$

1. At each node, a feature of $\boldsymbol{x} = (x_1, x_2, ..., x_d)^T$ is selected, with the jth feature having a probability $p_{nj} \in (0, 1)$ of being selected.
2. At each node, after feature selection, the split is at the midpoint of the chosen side.

Therefore

A Random Forest

- It is a predictor consisting of a collection of randomized base trees

$$\{T_b(\boldsymbol{x}, \Theta_m, \mathcal{D}_n) | m > 1\}$$

where $\mathcal{D}_n = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$

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where $\mathcal{D}_n = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$

Here, $\Theta_1, \Theta_2, \ldots$ are i.i.d. outputs of a randomizing variable Θ

$$\widehat{y}(X, \mathcal{D}_n) = E_\Theta [T_b(X, \Theta, \mathcal{D}_n) |]$$

We tend to use the sample mean

Regression

$$\widehat{y} = \frac{1}{B}\sum_{b=1}^{B} T_b\left(x\right)$$

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Classification, given $C_b(x)$ the classification prediction of the T_b tree

$$\widehat{C}_b(x) = \text{majority vote}\left\{C_b(x)\right\}_{b=1}^{B}$$

The nice part is that

Given that trees are notoriously noisy

- When we average over them, we obtained better accurate predictions

For More

Take a Look at

- The Elements of Statistical Learning by Hastie et al. Chapter 15