Introduction to Machine Learning

XBoosting Trees and Random Forests

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Outline

1. Boosting Trees
   - Introduction
   - Cost Functions for Trees
   - Using a Smoother Version
   - Boosted Tree Model
   - AdaBoost for Classification Trees
   - Numerical Optimization via Gradient Boosting
2. XGBoost
   - Introduction
   - Cost Function
   - Solving some Issues
   - Taylor Expansion
   - Split Finding Algorithms
     - Generic Approximated Version
3. Random Forest
   - Introduction
   - From Bootstrap to Random Forest

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Partition

Tree partition of the space

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

$$R_j,\ j = 1, 2, ..., J$$

Thus, a constant γ_j is assigned to each such region

$$x \in R_j \Rightarrow f(x) = \gamma_j$$

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Finally, we can see a tree as

Formal, Equation

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

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

Then, we have the following Loss function for Θ

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

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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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We can solve it, if ...

Finding R_j

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

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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*$=\infty$
4. *While* $\mathcal{S} \neq \emptyset$
5. *choose a subproblem (Partial Solution)* $P \in \mathcal{S}$ *and remove it from* $\mathcal{S}$
6. *expand it into smaller subproblems* $P_1, P_2, ..., P_k$
7. *For each* P_i
8. *if* P_i *is a complete solution:*
9. *update bestsofar*
10. *else*
11. *if lowerbound*$(P_i) <$*bestsofar: add* P_i *to* $\mathcal{S}$
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Therefore

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

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

Here, we encounter a problem

- Given R_j, How do we estimate γ_j?

Here, we do the following

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

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We are ready to define

The Boosted tree model is a sum of such trees

$$f_M(\boldsymbol{x}) = \sum_{i=1}^{N} T(\boldsymbol{x}|\Theta_m)$$

This comes from the Boosting classic cost function

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

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Thus, at each stage

We need to solve the following cost function

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

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

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

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- 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}

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

Nevertheless, finding the regions can be difficult

- For a few special cases, the problem simplifies.

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We can use AdaBoost

We can use the exponential Loss

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

Now, we have a conundrum

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

This will be make our life quite difficult

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

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Therefore

We have the following loss function

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

Minimizing can be viewed as a numerical optimization

$$\hat{f} = \arg\min_{f} L(f)$$

Where

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

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Thus, we have

As a Solution, we have a sum of component vectors

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

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

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Then

The components

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

Where

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

Then, we have the classic Gradient Descent

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

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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

1. $f_0(\boldsymbol{x}) = \arg\min_\gamma \sum_{i=1}^{N} L(y_i, \gamma)$
2. For $m = 1$ to M:
   - For $i = 1, 2, ..., N$ compute:
   $$r_{im} = \left[\frac{\partial L(y_i, f(\boldsymbol{x}_i))}{\partial f(\boldsymbol{x}_i)}\right]_{f(\boldsymbol{x}_i)=f_{m-1}(\boldsymbol{x}_i)}$$
   - Fit a regression tree to the targets r_{im} giving terminal regions R_{mj}, $j = 1, 2, ..., J_m$
   - For $j = 1, 2, ..., J_m$ compute
   $$\gamma_{jm} = \arg\min_\gamma \sum_{\boldsymbol{x}_i \in R_{jm}} L(y_i, f_{m-1}(\boldsymbol{x}_i) + \gamma)$$
   - Update $f_m(\boldsymbol{x}) = f_{m-1}(\boldsymbol{x}) + \sum_{j=1}^{J_m} \gamma_{jm} I(\boldsymbol{x} \in R_{jm})$
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2. For $m = 1$ to M:
   - For $i = 1, 2, ..., N$ compute:

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

   - Fit a regression tree to the targets r_{im} giving terminal regions R_{mj} $j = 1, 2, ..., J_m$
   - For $j = 1, 2, ..., J_m$ compute

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

   - Update $f_m(\boldsymbol{x}) = f_{m-1}(\boldsymbol{x}) + \sum_{j=1}^{J_m} \gamma_{jm} I(\boldsymbol{x} \in R_{jm})$
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.

Problem

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

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

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What about M the number of trees

Another parameter to estimate

- The other meta-parameter of gradient boosting is the number of boosting iterations M.

Here, a problem is that a Large M

- It is clear that the Empirical Risk is reduced at each iteration.

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

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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

Instead of using

$$f_m(\boldsymbol{x}) = f_{m-1}(\boldsymbol{x}) + \sum_{j=1}^{J_m} \gamma_{jm} I(\boldsymbol{x} \in R_{jm})$$

We modify by a parameter ν

$$f_m(\boldsymbol{x}) = f_{m-1}(\boldsymbol{x}) + \nu \sum_{j=1}^{J_m} \gamma_{jm} I(\boldsymbol{x} \in R_{jm})$$

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

It has been a winner 29 Kaggle challenges (2015)

- 17 solutions used XGBoost.

As solely algorithm

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

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Definition

- In statistics and machine learning, ensemble methods use multiple learning algorithms to obtain

Basically

1. Bootstrap aggregating (bagging)
2. Boosting
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Cost Function Ensemble

For a given data set

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

A Tree Ensemble model

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

Where, the space of regression trees (CART)

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

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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.
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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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- 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,

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.

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Then, we can use the Taylor Second Optimization

Second-order approximation

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

Where

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

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Furthermore

We have the following cost function after removing constant terms

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

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$$= \sum_{j=1}^{T} \left[\left(\sum_{i \in I_j} g_i \right) w_j + \frac{1}{2} \left(\sum_{i \in I_j} h_i + \lambda \right) w_j^2 \right] + \lambda T$$

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\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

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

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

Something Notable

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- Normally, it is impossible to enumerate all the possible tree structures q.

Therefore

- A greedy algorithm that starts from a single leaf and iteratively adds branches to the tree is used instead.

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

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

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Basic Exact Greedy Algorithm

A Big Problem

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

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

In order to do generate these splits

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

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Example, Exact Greedy Algorithm

Something Notable

1. **Input:** I, instance set of current node
2. **Input:** m, feature dimension
3. $gain = 0$
4. $G = \sum_{i \in I} g_i$ and $H = \sum_{i \in I} h_i$
5. for $k = 1$ to m do:
6. $G_L = 0$ and $H_L = 0$
7. for j in $sorted\left(I, \text{by } x_{jk}\right)$ do
8. $G_L = G_L + g_j$, $H_L = H_L + h_j$
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11. **Output:** Split with Max Score

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

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

- Basically you could use homogeneity via the Shannon Entropy
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Aggregates the statistics on the buckets

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The Two Variants for Splitting

The global variant

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

The local variant

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

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Outline

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   - Introduction
   - Cost Functions for Trees
   - Using a Smoother Version
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   - AdaBoost for Classification Trees
   - Numerical Optimization via Gradient Boosting
2. XGBoost
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   - Split Finding Algorithms
     - Generic Approximated Version
3. Random Forest
   - Introduction
   - From Bootstrap to Random Forest

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?

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.

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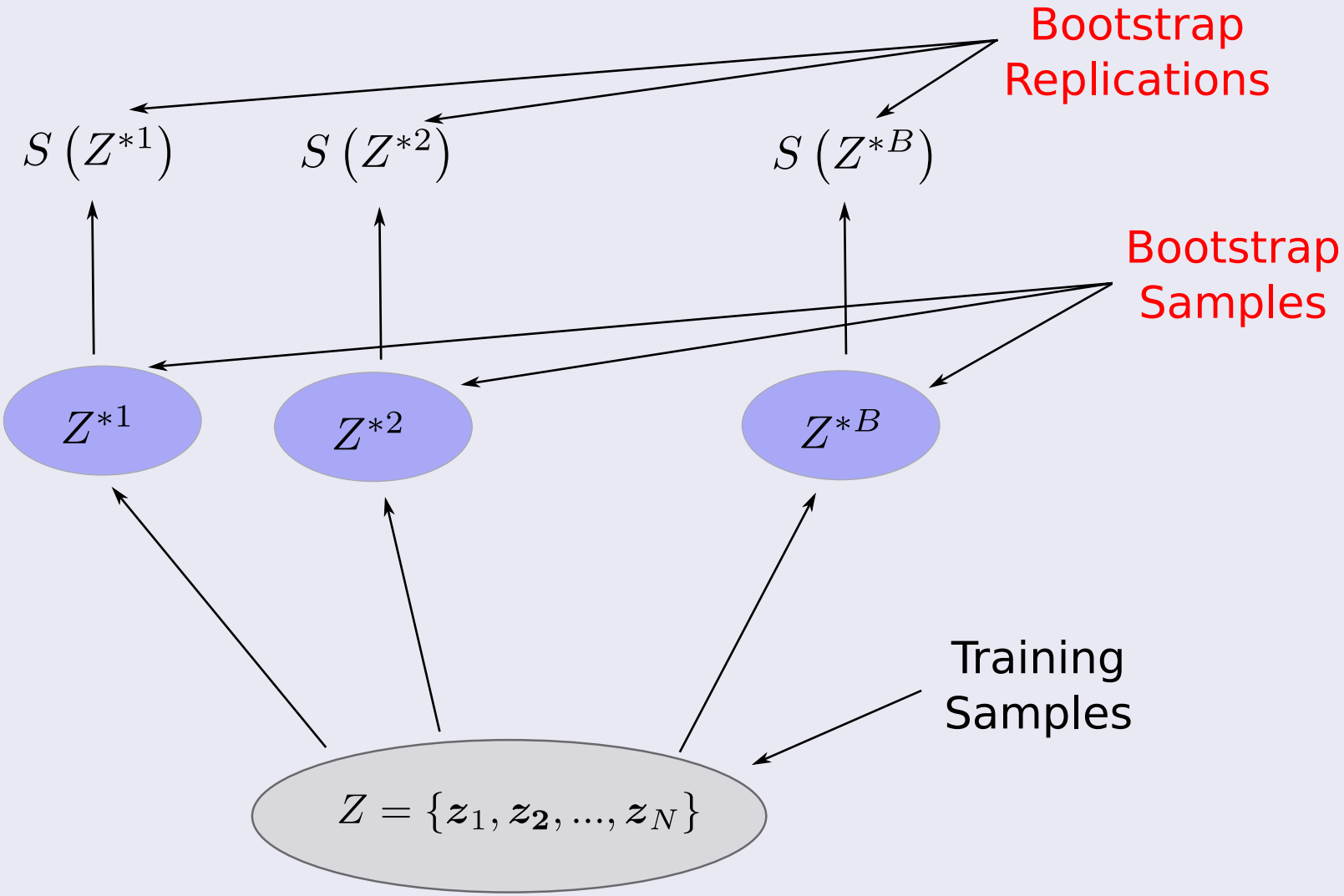
Reminder

Bootstrap aggregating/ bagging



Main Idea

We have then

- The essential idea in bagging is to average many noisy but approximately unbiased models.

Thus, you reduce the variance

- And given that trees capture complex interactions

This is perfect given

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

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The Model

In a series of papers and technical reports

- In a series of papers and technical reports - Leo Breiman demonstrated the substantial gains in classification and regression

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...

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

- Grow a random-forest tree T_b

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

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

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Regression

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

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

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

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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