Universal Boost Decision Trees: A Unified Framework to Translate Optimization Methods to Boosting Algorithms

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Abstract

A general paradigm is developed to translate optimization methods to 'boosting' algorithms. The gradient boost decision trees inspire higher order boost decision trees. And we translate the augmented Lagrangian methods to boosting algorithms with regularized cost fucntion. The interaction of optimization methods and boosting algorithms is discussed in surrogate boosting decision trees. It is first time to connent almost all optimization methods and boosting algorithms. It is why we call it as 'universal boost'. Although it is limited on boosted decision trees, the idea is easy to generalize to any boosting machine.

1 Introduction

Jerome Friedman et al assert that the Discrete AdaBoost algorithm (population version) builds an additive logistic regression model via Newton-like updates for minimizing $E(e^{-yf(x)})$. Jyrki Kivinen, Manfred K. Warmuth, Chunhua Shen, Hanxi Li study some boosting algorithms from a entropy minimization perspective. The gradient boost machine algorithms seems far from continuous optimization methods. Gradient boost machine is usually considered as functional gradient descent. There are many *gradient-like boosting machines* to fit the profitable directions different from negative gradients such as AnyBoost, Functional Frank-Wolfe Boosting, XGBoost, Historical Gradient Boost Machine, Accelerated Gradient Boosting, Accelerating Gradient Boosting Machine, NGBoost.

It seems that optimization methods can be mapped to boosting algorithms. However, it is not clear how to translate continuous optimization methods to their functional version such as ADMM. We will show that there is a unified framework to translate each optimization method to boosting algorithm.

2 Gradient Boost Decision Trees

Boosted decision tree or multiple additive regression tree is the sum of successive decision tree

$$F(x) = \sum_{n=1}^{T} f_t(x)$$

where f_n relies on the outputs of its 'parent tree' f_{n-1} for $n = 2, 3, \cdots, N$.

The following algorithm describe the gradient boost decision as boosted decision trees

Algorithm 1 Gradient Boost Decision Trees

```
 1: Input training data set $\{(x_n, y_n) \mid x_n \in \mathrm{X} \subset \mathbb{R}^p, y_n \in \mathbb{R}, n = 1, 2, \cdots, N\}$
 2: Initialize $f_0 = \arg\min_\gamma \sum_{i=1}^{N} L(x_i, \gamma)$
 3: for $t = 1, 2, \ldots, T$ do
 4:     for $i = 1, 2, \ldots, N$ do
 5:         Compute $r_{i,t} = -[\frac{\partial L(\mathrm{y}_i, f(x_i))}{\partial f(x_i)} \mid_{f=F^{(t-1)}}]$.
 6:     end for
 7:     Fit a regression tree to the targets $r_{i,t}$ giving terminal regions
                $R_{j,m}, j = 1, 2, \ldots, J_m$.
 8:     for $j = 1, 2, \ldots, J_m$ do
 9:         Compute $\gamma_{j,t} = \arg\min_\gamma \sum_{x_i \in R_{j,m}} L(\mathrm{y}_i, F^{(t-1)}(x_i) + \gamma)$.
10:     end for
11:     $f_t = \sum_{j=1}^{J_m} \gamma_{j,t} \mathbb{I}(x \in R_{j,m})$
12:     Update $F^{(t)} = F^{(t-1)} + \nu f_t, \nu \in (0, 1)$
13: end for
14: Output $F^{(T)}$.
```

In gradient boost decision tree, it takes additive training:

$$\gamma_{j,t} = \arg\min_\gamma \sum_{x_i \in R_{j,m}} L(\mathrm{y}_i, \underbrace{F^{(t-1)}(x_i) + \gamma}_{\text{additive training}})$$

which results as weighted sum of decision trees. Here $\gamma_{j,t}$ is expected to be parallel of $-[\frac{\partial L(\mathrm{y}_i, f(x_i))}{\partial f(x_i)} \mid_{f=F^{(t-1)}}] = -g_{t-1,i}$ thus $F^{(t)}(x_i) \approx F^{t-1}(x_i) - \alpha g_{t-1,i}$.

If let $F^{(t-1)}(x_i) = \tilde{y}_i$, the following inequality holds for some $\alpha \in (0, 1)$ if the loss function L is smooth

$$\sum_{i=1}^{N} L(\mathrm{y}_i, \tilde{y}_i) \geq \sum_{i=1}^{N} L(\mathrm{y}_i, \tilde{y}_i - \alpha[\frac{\partial L(\mathrm{y}_i, \tilde{y}_i)}{\partial \tilde{y}_i}]).$$

This is basic idea of gradient descent. And the gradient descent is updated by

$$\theta^{(t+1)} = \theta^{(t)} - \alpha_t \nabla_\theta L(\theta^{(t)})$$

for $t = 0, 1, 2, \cdots, T-1$. The final result of gradient descent is

$$\theta^{(T)} = \theta^{(0)} - \sum_{t=1}^{T-1} \alpha_t \nabla_\theta L(\theta^{(t)}).$$

If we replace the $\theta^{(T)}(\theta^{(0)})$ with the gradient boost decision trees $F^{(T)}(f_0)$ and $-\nabla_\theta L(\theta^{(t)})$ with the decision tree f_t for $t = 1, 2, \cdots, T-1$, we will obtain

$$F^{(T)} = f_0 + \sum_{t=1}^{T-1} \alpha_t f_t.$$

In gradient boost decision trees, a tree f_t is used to fit the negative gradient $-\frac{\partial L(\mathrm{y}_i, \tilde{y}_i)}{\partial \tilde{y}_i}$ for $i = 1, 2, \cdots, N$ so that it brings some noise or error in this step. So we say that it is analogous to gradient descent.

In optimization, we call the point γ at point $\tilde{y}_i$ as profitable direction if

$$\sum_{i=1}^{N} L(\mathrm{y}_i, \tilde{y}_i) \geq \sum_{i=1}^{N} L(\mathrm{y}_i, \tilde{y}_i + \gamma).$$

There are many *gradient-like boosting machines* to fit the descent directions different from negative gradients such as Functional Frank-Wolfe Boosting, XGBoost, Historical Gradient Boost Machine, Accelerated Gradient Boosting, Accelerating Gradient Boosting Machine, NGBoost. It is also the basic idea behind AnyBoost.

What is more, Historical Gradient Boost Machine, Accelerated Gradient Boosting, Accelerating Gradient Boosting Machine extend the gradient boost methods to momentum boost methods. XGBoost extend the gradient boost methods to second order boost methods. Any techniques in gradient-based optimization methods can be applied to gradient boost decision trees such as the distributed optimization techniques, acceleration techniques, variance reduction techniques.

Note that the following relation always holds for most loss function:

$$\ell(\mathrm{y}_i, f(x_i)) = 0 \iff \mathrm{y}_i = f(x_i) \iff \frac{\partial \ell(\mathrm{y}_i, f(x_i))}{\partial f(x_i)} \mid_{f=F^{(t-1)}} = 0$$

which means if $f(x_i) = \mathrm{y}_i$ the value 0 will be learnt in next decision tree. In another words, the gradient is always to be 0 when the loss is 0. And the outputs is a constant in vanilla decision tree for different input in the same leaf so that the new targets $r_{i,t}$ and $r_{j,t}$ are equal if x_i, x_j are output in the same leaf and $y_i = y_j$. As a result, such pair x_i, x_j tends to be in the same terminal region in the next tree. The samples in the same terminal region with different targets tend to be seperated in the next tree. The gradients is used to build the next decision tree.

"If I have seen further, it is by standing on the shoulders of giants." The new targets $\{f_{t-1}(x_i) - \alpha_{i,t} g_{i,t}\}$ are the shoulders of giants in decision tree for $i = 1, 2, \cdots, N, t = 1, 2, \cdots, T$. In next section, we will translate higher order optimization methods to boosting algorithms.

3 Higher Order Boost Decision Trees

XGBoost extends the gradient boost to the second order boost method. We can generalize much higher order boost decision tree. Even gradient is computed in xGBoost, it is univariate rather than multivariate so that quasi-Newton methods cannot play a role in our framework.

Halley's method is a third order method to find the roots of nonlinear equations. At point X_n, the next point X_{n+1} in Halley's method is found by :

$$X_{n+1} = X_n - \frac{2f(X_n)f'(X_n)}{2[f'(X_n)]^2 - f(X_n)f''(X_n)}. \tag{1}$$

It is proved to be cubical convergence insofar as the number of significant digits eventually triples with each iteration. See some examples of Halley's method visualized by Herb Susmann.

Now we apply Halley's method to the equation $g(x) = 0$:

$$x_{n+1} = x_n - \frac{2g(x_n)g'(x_n)}{2[g'(x_n)]^2 - g(x_n)g''(x_n)} \tag{2}$$

where $g(x) = \frac{\partial L(\mathrm{y}, f(x))}{\partial f(x)}$, i.e., $g(x)$ is the derivative function of the ouput of x. It is a fixed point iteration to find the minimal values of $L(\mathrm{y}, f(x))$.

Then we translate the Halley's method to a third order boosting algorithm.

Algorithm 2 Third Order Boost Decision Trees

```
1:  Input training data set ${(x_n, y_n) \mid x_n \in \mathrm{X} \subset \mathbb{R}^p, y_n \in \mathbb{R}, n = 1, 2, \cdots, N}$
2:  Initialize $f_0 = \arg\min_{\gamma} \sum_{i=1}^{N} L(x_i, \gamma)$
3:  for $t = 1, 2, \dots, T$ do
4:      for $i = 1, 2, \dots, N$ do
5:          Compute $r_{i,t} = T_t(x_i)$
6:      end for
7:      Fit a regression tree to the targets $r_{i,t}$ giving terminal regions
            $R_{j,m}, j = 1, 2, \dots, J_m.$
8:      for $j = 1, 2, \dots, J_m$ do
9:          Compute $\gamma_{j,t} = \arg\min_{\gamma} \sum_{x_i \in R_{j,m}} L(\mathrm{y}_i, F^{(t-1)}(x_i) + \gamma)$.
10:     end for
11:     $f_t = \sum_{j=1}^{J_m} \gamma_{j,t} \mathbb{I}(x \in R_{j,m})$.
12:     Update $F^{(t)} = F^{(t-1)} + f_t$.
13: end for
14: Output $F^{(T)}$.
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Here $T_t(x_i) = -\frac{2g_t(x_i)g'_t(x_i)}{2[g'_t(x_i)]^2 - g_t(x_i)g''_t(x_i)}$ and $g_t(x_i) = \frac{\partial L(\mathrm{y}_i, f(x_i))}{\partial f(x_i)} \mid_{f=F^{(t-1)}}$, $g'_t(x_i) = \frac{\mathrm{d} g_t(x_i)}{\mathrm{d} f(x_i)} \mid_{f=F^{(t-1)}}$, $g''_t(x_i) = \frac{\mathrm{d} g'_t(x_i)}{\mathrm{d} f(x_i)} \mid_{f=F^{(t-1)}}$. Note that it works only when $2[g_t'(x_i)]^2 - g_t(x_i)g_t''(x_i) \neq 0$. And when $g(x) = 0 \quad \forall x \in \mathbb{R}$, it finds a fixed point. When $g_t''(x_i) = 0$, it is exactly the Newton's method. All the technoques used in xGBoost can apply to this third order boost decision trees. So that it is a direct extension of xGBoost.

4 Surrogate Boost Decision Trees

The surrogate principle is to optimze a simple surrogate objective function at each iteration instead of the original complex objective function. For example, our aim is to solve an optimization problem of the following form

$$\arg\min_{\boldsymbol{x}\in\mathcal{X}} f(\boldsymbol{x}). \tag{3}$$

Given initial estimates $\boldsymbol{x}_0$ and surrogate objective function $Q(x_t, x)$, it is updated via

$$\boldsymbol{x}_{t+1} = \arg\min_{x} Q(x_t, x),$$

and it is usually $f(\boldsymbol{x}_{t+1}) \leq f(\boldsymbol{x}_t)$. Generally, it is required that $\lim_{t\to\infty} x_t = x^* \in \arg\min_{\boldsymbol{x}\in\mathcal{X}} f(\boldsymbol{x})$. The surrogate objective function $Q(x_t, x)$ is usually simpler to optimze than original function $f(\boldsymbol{x})$.

Algorithm 3 Surrogate Boost Decision Trees

```
1: Input training data set $\{(x_n, y_n) \mid x_n \in \mathrm{X} \subset \mathbb{R}^p, y_n \in \mathbb{R}, n = 1, 2, \cdots, N\}$
2: Initialize $f_0 = \arg\min_\gamma \sum_{i=1}^N L(x_i, \gamma)$
3: for $t = 1, 2, \dots, T$ do
4:     for $i = 1, 2, \dots, N$ do
5:         Compute $r_{i,t} = \arg\min_x Q(f_t(x_i), F^{(t-1)}(x_i) + x)$.
6:     end for
7:     Fit a regression tree to the targets $r_{i,t}$ giving terminal regions
               $R_{j,m}, j = 1, 2, \dots, J_m.$
8:     for $j = 1, 2, \dots, J_m$ do
9:         Compute $\gamma_{j,t} = \arg\min_\gamma \sum_{x_i \in R_{j,m}} L(\mathrm{y}_i, F^{(t-1)}(x_i) + \gamma)$.
10:    end for
11:    $f_t = \sum_{j=1}^{J_m} \gamma_{j,t} \mathbb{I}(x \in R_{j,m})$.
12:    Update $F^{(t)} = F^{(t-1)} + f_t$.
13: end for
14: Output $F^{(T)}$.
```

In this framework, we can extend the NGBoost to 'expectation maximization' type boosting algorithms.

A unifying principle: surrogate minimization

5 ADMM Boost Decision Trees

Now we take alternating direction method of multipliers (ADMM) into consideration.

ADMM is aimed to solve the following convex optimization problem:

$$\min F(x, y)\{= f(x) + g(y)\} \text{ subject to } \quad Ax + By = b \tag{4}$$

where $f(x)$ and $g(y)$ is convex; A and B are matrices. Its augmented Lagrangian is defined as $L_\beta(x, y) = f(x) + g(y) - \lambda^T(Ax + By - b) + \frac{\beta}{2}\|Ax + By - b\|_2^2$. ADMM at step t is described as following:

1. $x^{k+1} = \arg\min_{x\in\mathbf{X}} L_\beta(x, y^k, \lambda^k)$;
2. $y^{k+1} = \arg\min_{y\in\mathbf{Y}} L_\beta(x^{k+1}, y, \lambda^k)$;
3. $\lambda^{k+1} = \lambda^k - \beta(Ax^{k+1} + By^{k+1} - b)$.

The aim boosting algorithms is to find a decision tree f^* to minimize the following function

$$\arg\min_f \sum_{i=1}^N \ell(y_i, f(x_i)) + r\sum_{i=1}^N |f(x_i)| \text{ subject to } z_i = f(x_i)$$

where $\ell(y_i, f(x_i))$ is the loss of sample (x_i, y_i) and $r\sum_{i=1}^N |f(x_i)|$ is the regularization term. Note that the loss function $\ell(\cdot,\cdot)$ is usually convex and f is a decision tree (region-wise linear function), so the above cost function is convex.

Here the augmented Lagragian is given by

$$\begin{aligned} L_\beta^{(t)}(\gamma_i, z_i, \lambda_i) = &\ \ell(y_i, f_{t-1}(x_i) + \gamma_i) \\ &+ r|z_i|_1 - \langle z_i - (f_{t-1}(x_i) + \gamma_i), \lambda_i\rangle \\ &+ \frac{\beta}{2}|z_i - (f_{t-1}(x_i) + \gamma_i)|. \end{aligned}$$

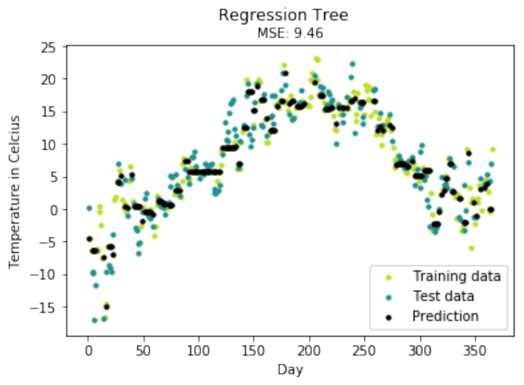
And $f(\cdot)$ is a decision tree; $\ell(\cdot,\cdot)$ is the loss function.

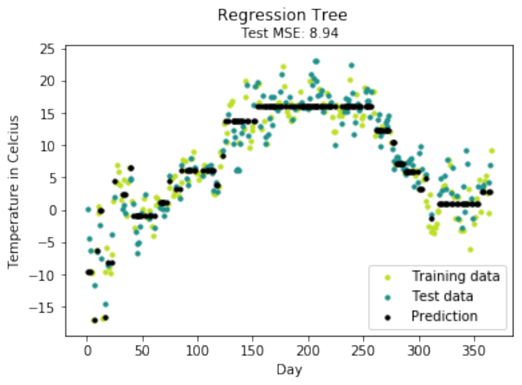
This scheme is more suitable for the regularized cost function. In general, all the optimization methods for the optimizaion problem 4 can be tranlated to boosting algorithms. It is the first time to translate the augmented Lagragian method to boosting algorithms. And this framework can be generalized to any operator splitting optimization methods.

Algorithm 4 ADMM Boost Decision Trees

```
1: Input training data set $\{(x_n, y_n) \mid x_n \in \mathrm{X} \subset \mathbb{R}^p, y_n \in \mathbb{R}, n = 1, 2, \cdots, N\}$
2: Initialize $f_0 = \arg\min_\gamma \sum_{i=1}^N L(x_i, \gamma)$
3: for $t = 1, 2, \ldots, T$ do
4:     for $i = 1, 2, \ldots, N$ do
5:         Compute $r_{i,t} = \arg\min_{\gamma_i} L_\beta^{(t)}(\gamma_i, z_i, \lambda_i)$.
6:     end for
7:     Fit a regression tree to the targets $r_{i,t}$ giving terminal regions
           $$R_{j,m}, j = 1, 2, \ldots, J_m.$$
8:     for $j = 1, 2, \ldots, J_m$ do
9:         Compute $\gamma_{j,t} = \arg\min_\gamma \sum_{x_i \in R_{j,m}} L(\mathrm{y}_i, \gamma)$.
10:    end for
11:    $f_t = \sum_{j=1}^{J_m} \gamma_{j,t} \mathbb{I}(x \in R_{j,m})$.
12:    Update $F^{(t)} = F^{(t-1)} + f_t$.
13: end for
14: Compute $z^{t+1} = \arg\min_z \sum_{i=1}^N L_\beta^{(t)}(r_{i,t}, z_i, \lambda_i^t)$.
15: Compute $\lambda^{t+1} = \arg\min_\lambda \sum_{i=1}^N L_\beta^{(t)}(r_{i,t}, z_i^{t+1}, \lambda_i)$
16: Output $F^{(T)}$.
```

6 Experiments





7 Conclusion