Boosting

Victor Kitov

v.v.kitov@yandex.ru

Yandex School of Data Analysis

General idea

- Bagging, Random forest, extra random trees fit independent models.
  - can be done in parallel
  - sampling: objects - with replacement, features - without replacement.
  - base learners-complex
- Boosting fits models sequentially and they depend on each other.
  - each model is fitted to correct errors of the ensemble of previous models.
  - base learners-simple

Linear ensembles

Linear ensemble:

$$F(x) = f_0(x) + c_1 h_1(x) + ... + c_M h_M(x)$$

Regression: $\widehat{y}(x) = F(x)$
Binary classification: $score(y|x) = F(x)$, $\widehat{y}(x) = \text{sign } F(x)$

- Notation: $h_1(x), ...h_M(x)$ are called *base learners, weak learners, base models.*
- Too expensive to optimize $f_0(x), h_1(x), ...h_M(x)$ and $c_1, ...c_M$ jointly for large M.
- Idea: optimize $f_0(x)$ and then each pair $(h_m(x), c_m)$ greedily.

Forward stagewise additive modeling (FSAM)

Input: training dataset (x_i, y_i), $i = 1, 2, ...N$; loss function $\mathcal{L}(f, y)$, parametrized base learner $h(x|\theta)$ and initial approximation $f(x|\theta')$, the number M of successive additive approximations.

Forward stagewise additive modeling (FSAM)

Input: training dataset (x_i, y_i), $i = 1, 2, ...N$; loss function $\mathcal{L}(f, y)$, parametrized base learner $h(x|\theta)$ and initial approximation $f(x|\theta')$, the number M of successive additive approximations.

1. Fit initial approximation $f_0(x) = \arg\min_f \sum_{i=1}^N \mathcal{L}(f(x_i), y_i)$

Forward stagewise additive modeling (FSAM)

Input: training dataset (x_i, y_i), $i = 1, 2, ...N$; loss function $\mathcal{L}(f, y)$, parametrized base learner $h(x|\theta)$ and initial approximation $f(x|\theta')$, the number M of successive additive approximations.

1. Fit initial approximation $f_0(x) = \arg\min_f \sum_{i=1}^N \mathcal{L}(f(x_i), y_i)$
2. For $m = 1, 2, ...M$:
    1. find next best classifier

$$(c_m, h_m) = \arg\min_{h,c} \sum_{i=1}^{N} \mathcal{L}(f_{m-1}(x_i) + ch(x_i),\ y_i)$$

Forward stagewise additive modeling (FSAM)

Input: training dataset (x_i, y_i), $i = 1, 2, ...N$; loss function $\mathcal{L}(f, y)$, parametrized base learner $h(x|\theta)$ and initial approximation $f(x|\theta')$, the number M of successive additive approximations.

1. Fit initial approximation $f_0(x) = \arg\min_f \sum_{i=1}^N \mathcal{L}(f(x_i), y_i)$
2. For $m = 1, 2, ...M$:
    1. find next best classifier
$$(c_m, h_m) = \arg\min_{h,c} \sum_{i=1}^{N} \mathcal{L}(f_{m-1}(x_i) + ch(x_i),\ y_i)$$
    2. set
$$f_m(x) = f_{m-1}(x) + c_m h_m(x)$$

Output: approximation function
$f_M(x) = f_0(x) + \sum_{m=1}^{M} c_m h_m(x)$

Comments on FSAM

- Number of steps M should be determined by performance on validation set.
- Step 1 need not be solved accurately, since its mistakes are expected to be corrected by future base learners.
  - we can take $f_0(x) = \arg\min_{\beta\in\mathbb{R}} \sum_{i=1}^{N} \mathcal{L}(\beta, y_i)$ or simply $f_0(x) \equiv 0$.
- By similar reasoning there is no need to solve 2.1 accurately
  - typically very simple base learners are used such as trees of depth=1,2,3.
- For some loss functions, such as $\mathcal{L}(y, f(x)) = e^{-yf(x)}$ we can solve FSAM explicitly.
- For general loss functions gradient boosting scheme should be used.

Adaboost (discrete version): assumptions

- binary classification task $y \in \{+1, -1\}$
- family of base classifiers $h(x) = h(x|\theta)$ where θ is some fitted parametrization.
- $h(x) \in \{+1, -1\}$
- classification is performed with $\widehat{y} = sign\{f_0(x) + c_1 f_1(x) + ... + c_M f_M(x)\}$
- optimized loss is $L(y, f(x)) = e^{-yf(x)}$
- FSAM is applied

Adaboost (discrete version): algorithm

Input: training dataset (x_i, y_i), $i = 1, 2, \dots N$; number of additive weak classifiers M, a family of weak classifiers $h(x) \in \{+1, -1\}$, trainable on weighted datasets.

1. Initialize observation weights $w_i = 1/n$, $i = 1, 2, \dots n$.
2. for $m = 1, 2, \dots M$:
    1. fit $h^m(x)$ to training data using weights w_i
    2. compute weighted misclassification rate:
       $$E_m = \frac{\sum_{i=1}^{N} w_i \mathbb{I}[h^m(x) \neq y_i]}{\sum_{i=1}^{N} w_i}$$
    3. if $E_M > 0.5$ or $E_M = 0$: terminate procedure.
    4. compute $\alpha_m = \ln\left((1 - E_m)/E_m\right)$
    5. increase all weights, where misclassification with $h^m(x)$ was made:
       $$w_i \leftarrow w_i e^{\alpha_m},\ i \in \{i : h^m(x_i) \neq y_i\}$$

Output: composite classifier $f(x) = \text{sign}\left(\sum_{m=1}^{M} \alpha_m h^m(x)\right)$

Table of Contents

Motivation

- Problem: For general loss function L FSAM cannot be solved explicitly
- Analogy with function minimization: when we can't find optimum explicitly we use numerical methods
- Gradient boosting: numerical method for iterative loss minimization

Gradient descent algorithm

$$F(w) \to \min_w, \quad w \in \mathbb{R}^N$$

Gradient descend algorithm:

```
INPUT:
$\eta$-parameter, controlling the speed of convergence
$M$-number of iterations

ALGORITHM:
initialize $w$
for $m = 1, 2, ...M$:
    $\Delta w = \frac{\partial F(w)}{\partial w}$
    $w = w - \eta \Delta w$
```

Modified gradient descent algorithm

```
INPUT:
$M$-number of iterations

ALGORITHM:
initialize $w$
for $m = 1, 2, ...M$:
    $\Delta w = \frac{\partial F(w)}{\partial w}$
    $c^* = \arg\min_c F(w - c\Delta w)$
    $w = w - c^* \Delta w$
```

Gradient boosting

- Now consider $F\left(f(x_1),...f(x_N)\right)=\sum_{n=1}^{N}\mathcal{L}\left(f(x_n),y_n\right)$
- Gradient descent performs pointwise optimization, but we need generalization, so we optimize in space of functions.
- Gradient boosting implements modified gradient descent in function space:
  - find $z_i=-\frac{\partial\mathcal{L}(r,y)}{\partial r}|_{r=f^{m-1}(x)}$
  - fit base learner $h_m(x)$ to $\{(x_i,z_i)\}_{i=1}^{N}$

Gradient boosting

Input: training dataset (x_i, y_i), $i = 1, 2, ...N$; loss function $\mathcal{L}(f, y)$ and the number M of successive additive approximations.

1. Fit initial approximation $f_0(x)$ (might be taken $f_0(x) \equiv 0$)

Gradient boosting

Input: training dataset (x_i, y_i), $i = 1, 2, ...N$; loss function $\mathcal{L}(f, y)$ and the number M of successive additive approximations.

1. Fit initial approximation $f_0(x)$ (might be taken $f_0(x) \equiv 0$)
2. For each step $m = 1, 2, ...M$:

Gradient boosting

Input: training dataset (x_i, y_i), $i = 1, 2, ...N$; loss function $\mathcal{L}(f, y)$ and the number M of successive additive approximations.

1. Fit initial approximation $f_0(x)$ (might be taken $f_0(x) \equiv 0$)
2. For each step $m = 1, 2, ...M$:
    1. calculate derivatives $z_i = -\frac{\partial \mathcal{L}(r, y_i)}{\partial r}|_{r=f^{m-1}(x_i)}$

Gradient boosting

Input: training dataset (x_i, y_i), $i = 1, 2, ...N$; loss function $\mathcal{L}(f, y)$ and the number M of successive additive approximations.

1. Fit initial approximation $f_0(x)$ (might be taken $f_0(x) \equiv 0$)
2. For each step $m = 1, 2, ...M$:
    1. calculate derivatives $z_i = -\frac{\partial \mathcal{L}(r, y_i)}{\partial r}|_{r=f^{m-1}(x_i)}$
    2. fit h_m to $\{(x_i, z_i)\}_{i=1}^N$, for example by solving

$$\sum_{n=1}^N (h_m(x_n) - z_n)^2 \to \min_{h_m}$$

Gradient boosting

Input: training dataset (x_i, y_i), $i = 1, 2, ...N$; loss function $\mathcal{L}(f, y)$ and the number M of successive additive approximations.

1. Fit initial approximation $f_0(x)$ (might be taken $f_0(x) \equiv 0$)
2. For each step $m = 1, 2, ...M$:
    1. calculate derivatives $z_i = -\frac{\partial \mathcal{L}(r, y_i)}{\partial r}|_{r=f^{m-1}(x_i)}$
    2. fit h_m to $\{(x_i, z_i)\}_{i=1}^{N}$, for example by solving
    $$\sum_{n=1}^{N} (h_m(x_n) - z_n)^2 \to \min_{h_m}$$
    3. solve univariate optimization problem:
    $$\sum_{i=1}^{N} \mathcal{L}\left(f_{m-1}(x_i) + c_m h_m(x_i), y_i\right) \to \min_{c_m \in \mathbb{R}_+}$$

Gradient boosting

Input: training dataset (x_i, y_i), $i = 1, 2, ...N$; loss function $\mathcal{L}(f, y)$ and the number M of successive additive approximations.

1. Fit initial approximation $f_0(x)$ (might be taken $f_0(x) \equiv 0$)
2. For each step $m = 1, 2, ...M$:
    1. calculate derivatives $z_i = -\frac{\partial \mathcal{L}(r, y_i)}{\partial r}|_{r=f^{m-1}(x_i)}$
    2. fit h_m to $\{(x_i, z_i)\}_{i=1}^N$, for example by solving
       $$\sum_{n=1}^{N} (h_m(x_n) - z_n)^2 \to \min_{h_m}$$
    3. solve univariate optimization problem:
       $$\sum_{i=1}^{N} \mathcal{L}\left(f_{m-1}(x_i) + c_m h_m(x_i), y_i\right) \to \min_{c_m \in \mathbb{R}_+}$$
    4. set $f_m(x) = f_{m-1}(x) + c_m h_m(x)$

Gradient boosting

Input: training dataset (x_i, y_i), $i = 1, 2, ...N$; loss function $\mathcal{L}(f, y)$ and the number M of successive additive approximations.

1. Fit initial approximation $f_0(x)$ (might be taken $f_0(x) \equiv 0$)
2. For each step $m = 1, 2, ...M$:
   1. calculate derivatives $z_i = -\frac{\partial \mathcal{L}(r, y_i)}{\partial r}\big|_{r=f^{m-1}(x_i)}$
   2. fit h_m to $\{(x_i, z_i)\}_{i=1}^{N}$, for example by solving
   $$\sum_{n=1}^{N}(h_m(x_n) - z_n)^2 \to \min_{h_m}$$
   3. solve univariate optimization problem:
   $$\sum_{i=1}^{N}\mathcal{L}\left(f_{m-1}(x_i) + c_m h_m(x_i), y_i\right) \to \min_{c_m \in \mathbb{R}_+}$$
   4. set $f_m(x) = f_{m-1}(x) + c_m h_m(x)$

Output: approximation function $f_M(x) = f_0(x) + \sum_{m=1}^{M} c_m h_m(x)$

Gradient boosting: examples

In gradient boosting

$$\sum_{n=1}^{N}\left(h_m(x_n)-\left(-\frac{\partial\mathcal{L}(r,y_n)}{\partial r}|_{r=f^{m-1}(x_n)}\right)\right)^2\to\min_{h_m}$$

Commonly used loss-functions[1]:

- $\mathcal{L}=\frac{1}{2}(r-y)^2$
- $\mathcal{L}=e^{-ry}$
- $\mathcal{L}=[-ry]_+$
- $\mathcal{L}=\ln\left(1+e^{-ry}\right)$

[1]Estimate targets for them.

Gradient boosting of trees

Input: training dataset (x_i, y_i), $i = 1, 2, ...N$; loss function $\mathcal{L}(f, y)$ and the number M of successive additive approximations.

1. Fit constant initial approximation $f_0(x)$:
   $f_0(x) = \arg\min_\gamma \sum_{i=1}^N \mathcal{L}(\gamma, y_i)$

Gradient boosting of trees

Input: training dataset (x_i, y_i), $i = 1, 2, ...N$; loss function $\mathcal{L}(f, y)$ and the number M of successive additive approximations.

1. Fit constant initial approximation $f_0(x)$: $f_0(x) = \arg\min_\gamma \sum_{i=1}^N \mathcal{L}(\gamma, y_i)$
2. For each step $m = 1, 2, ...M$:

Gradient boosting of trees

Input: training dataset (x_i, y_i), $i = 1, 2, ...N$; loss function $\mathcal{L}(f, y)$ and the number M of successive additive approximations.

1. Fit constant initial approximation $f_0(x)$: $f_0(x) = \arg\min_\gamma \sum_{i=1}^N \mathcal{L}(\gamma, y_i)$
2. For each step $m = 1, 2, ...M$:
    1. calculate derivatives $z_i = -\frac{\partial \mathcal{L}(r, y_i)}{\partial r}|_{r=f^{m-1}(x_i)}$

Gradient boosting of trees

Input: training dataset (x_i, y_i), $i = 1, 2, ...N$; loss function $\mathcal{L}(f, y)$ and the number M of successive additive approximations.

1. Fit constant initial approximation $f_0(x)$:
   $f_0(x) = \arg\min_\gamma \sum_{i=1}^N \mathcal{L}(\gamma, y_i)$
2. For each step $m = 1, 2, ...M$:
   1. calculate derivatives $z_i = -\frac{\partial \mathcal{L}(r, y_i)}{\partial r}|_{r=f^{m-1}(x_i)}$
   2. fit regression tree h^m on $\{(x_i, z_i)\}_{i=1}^N$ with some loss function, get leaf regions $\{R_{jm}\}_{j=1}^{J_m}$.

Gradient boosting of trees

Input: training dataset (x_i, y_i), $i = 1, 2, ...N$; loss function $\mathcal{L}(f, y)$ and the number M of successive additive approximations.

1. Fit constant initial approximation $f_0(x)$:
   $f_0(x) = \arg\min_\gamma \sum_{i=1}^N \mathcal{L}(\gamma,\, y_i)$
2. For each step $m = 1, 2, ...M$:
   1. calculate derivatives $z_i = -\frac{\partial \mathcal{L}(r, y_i)}{\partial r}\big|_{r=f^{m-1}(x_i)}$
   2. fit regression tree h^m on $\{(x_i, z_i)\}_{i=1}^N$ with some loss function, get leaf regions $\{R_{jm}\}_{j=1}^{J_m}$.
   3. for each terminal region R_{jm}, $j = 1, 2, ...J_m$ solve univariate optimization problem:

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

Gradient boosting of trees

Input: training dataset (x_i, y_i), $i = 1, 2, ...N$; loss function $\mathcal{L}(f, y)$ and the number M of successive additive approximations.

1. Fit constant initial approximation $f_0(x)$:
   $f_0(x) = \arg\min_\gamma \sum_{i=1}^N \mathcal{L}(\gamma, y_i)$
2. For each step $m = 1, 2, ...M$:
   1. calculate derivatives $z_i = -\frac{\partial \mathcal{L}(r, y_i)}{\partial r}|_{r=f^{m-1}(x_i)}$
   2. fit regression tree h^m on $\{(x_i, z_i)\}_{i=1}^N$ with some loss function, get leaf regions $\{R_{jm}\}_{j=1}^{J_m}$.
   3. for each terminal region R_{jm}, $j = 1, 2, ...J_m$ solve univariate optimization problem:
   $$\gamma_{jm} = \arg\min_\gamma \sum_{x_i \in R_{jm}} \mathcal{L}(f_{m-1}(x_i) + \gamma, y_i)$$
   4. update $f_m(x) = f_{m-1}(x) + \sum_{j=1}^{J_m} \gamma_{jm} \mathbb{I}[x \in R_{jm}]$

Gradient boosting of trees

Input: training dataset (x_i, y_i), $i = 1, 2, ...N$; loss function $\mathcal{L}(f, y)$ and the number M of successive additive approximations.

1. Fit constant initial approximation $f_0(x)$:
   $f_0(x) = \arg\min_\gamma \sum_{i=1}^N \mathcal{L}(\gamma, y_i)$
2. For each step $m = 1, 2, ...M$:
   1. calculate derivatives $z_i = -\frac{\partial \mathcal{L}(r, y_i)}{\partial r}\big|_{r=f^{m-1}(x_i)}$
   2. fit regression tree h^m on $\{(x_i, z_i)\}_{i=1}^N$ with some loss function, get leaf regions $\{R_{jm}\}_{j=1}^{J_m}$.
   3. for each terminal region R_{jm}, $j = 1, 2, ...J_m$ solve univariate optimization problem:

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

   4. update $f_m(x) = f_{m-1}(x) + \sum_{j=1}^{J_m} \gamma_{jm} \mathbb{I}[x \in R_{jm}]$

Output: approximation function $f_M(x)$

Modification of boosting for trees

- Compared to first method of gradient boosting, boosting of regression trees finds additive coefficients individually for each terminal region R_{jm}, not globally for the whole classifier $h^m(x)$.
- This is done to increase accuracy: forward stagewise algorithm cannot be applied to find R_{jm}, but it can be applied to find γ_{jm}, because second task is solvable for arbitrary L.
- Max leaves J
    - interaction between no more than $J-1$ terms
    - usually $J \leq 8$
    - M controls underfitting-overfitting tradeoff and selected using validation set

Shrinkage & subsampling

- Shrinkage of general GB, step (d):

$$f_m(x) = f_{m-1}(x) + \nu c_m h_m(x)$$

- Shrinkage of trees GB, step (d):

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

- Comments:
  - $\nu \in (0, 1]$
  - $\nu \downarrow \implies M \uparrow$
- Subsampling
  - increases speed of fitting
  - may increase accuracy

Types of boosting

- Loss function F:
  - $\mathcal{L}(|f(x) - y|)$ - regression
  - $\mathcal{L}(y \cdot score(y = +1|x))$ - binary classification
  - multiclass classification - may extend with one vs. all scheme
- Optimization
  - analytical (AdaBoost)
  - gradient based
- Base learners: continious, discrete
- Extensions: shrinkage, subsampling