

Boosting

Victor Kitov

Motivation for ensembles

- Consider M classifiers $f_1(x), \dots, f_M(x)$, performing binary classification.
- Let ξ_1, \dots, ξ_M denote indicators of mistakes by f_1, \dots, f_M on particular observation x
- Suppose ξ_1, \dots, ξ_M are independent binomial variables with $P(\xi_i = 1) = p$
- Then $\mathbb{E}\xi_i = p, \text{Var}[\xi_i] = p(1 - p)$
- Consider $F(x)$ be aggregating classifier, assigning x to the class with maximum votes among $f_1(x), \dots, f_M(x)$.

- Consider

$$\eta = \frac{\xi_1 + \dots + \xi_M}{M}$$

- Probability of mistake = probability that majority of ξ_1, \dots, ξ_M are ones = $P(\eta > 0.5)$.
- $P(\eta > 0.5) \rightarrow 0$ as $M \rightarrow \infty$ because $\mathbb{E}\eta = p, \text{Var}[\eta] = \frac{p(1-p)}{M}$.

Linear ensembles

Linear ensemble:

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

Regression: $\hat{y}(x) = F(x)$

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

- Notation: $h_1(x), \dots, h_M(x)$ are called *base learners*, *weak learners*, *base models*.
- Too expensive to optimize $f_0(x), h_1(x), \dots, h_M(x)$ and c_1, \dots, c_M jointly for large M .
- Idea: optimize $f_0(x)$ and then each pair $(h_m(x), c_m)$ greedily.
- After ensemble is built we can fine-tune c_1, \dots, c_M by fitting features $f_0(x), h_1(x), \dots, h_M(x)$ with linear regression/classifier.

Forward stagewise additive modeling (FSAM)

Input: training dataset (x_i, y_i) , $i = 1, 2, \dots, N$; loss function $\mathcal{L}(f, y)$, general form of “base learner” $h(x|\gamma)$ (dependent from parameter γ) and 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 $m = 1, 2, \dots, M$:
 - 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 $h(x) = h(x|\gamma)$ where γ is some fitted parametrization.
- $h(x) \in \{+1, -1\}$
- classification is performed with
$$\hat{y} = \text{sign}\{f_0(x) + c_1 f_1(x) + \dots + c_M f_M(x)\}$$
- optimized loss is $\mathcal{L}(y, f(x)) = e^{-yf(x)}$
- 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 $c_m = \frac{1}{2} \ln((1 - E_m)/E_m)$
- 5 increase all weights, where misclassification with $h^m(x)$ was made:

$$w_i \leftarrow w_i e^{2c_m}, i \in \{i : h^m(x_i) \neq y_i\}$$

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

Adaboost derivation

Set initial approximation, typically $f_0(x) \equiv 0$.

Apply FSAM for $m = 1, 2, \dots, M$:

$$\begin{aligned}
 (c_m, h^m) &= \arg \min_{c_m, h^m} \sum_{i=1}^N \mathcal{L}(f_{m-1}(x_i) + c_m h^m(x), y_i) \\
 &= \arg \min_{c_m, h^m} \sum_{i=1}^N e^{-y_i f_{m-1}(x_i)} e^{-c_m y_i h^m(x)} \\
 &= \arg \min_{c_m, h^m} \sum_{i=1}^N w_i^m e^{-c_m y_i h^m(x_i)}, \quad w_i^m = e^{-y_i f_{m-1}(x_i)}
 \end{aligned}$$

Adaboost derivation

$$\begin{aligned}
\sum_{i=1}^N w_i^m e^{-c_m y_i h^m(x_i)} &= \sum_{i: h^m(x_i)=y_i} w_i^m e^{-c_m} + \sum_{i: h^m(x_i) \neq y_i} w_i^m e^{c_m} \\
&= e^{-c_m} \sum_{i: h^m(x_i)=y_i} w_i^m + e^{c_m} \sum_{i: h^m(x_i) \neq y_i} w_i^m \\
&= e^{c_m} \sum_{i: h^m(x_i) \neq y_i} w_i^m + e^{-c_m} \sum_{i=1}^N w_i^m - e^{-c_m} \sum_{i: h^m(x_i) \neq y_i} w_i^m \\
&= e^{-c_m} \sum_i w_i^m + (e^{c_m} - e^{-c_m}) \sum_{i: h^m(x_i) \neq y_i} w_i^m
\end{aligned}$$

Since $c_m \geq 0$ $h_m(x)$ should be found from

$$h_m(x_i) = \arg \min_h \sum_{i=1}^N w_i^m \mathbb{I}[h(x_i) \neq y_i]$$

Adaboost derivation

Denote $F(c_m) = \sum_{i=1}^n w_i^m \exp(-c_m y_i h^m(x_i))$. Then

$$\frac{\partial F(c_m)}{\partial c_m} = - \sum_{i=1}^N w_i^m e^{-c_m y_i h^m(x_i)} y_i h^m(x_i) = 0$$

$$- \sum_{i: h^m(x_i)=y_i} w_i^m e^{-c_m} + \sum_{i: h^m(x_i) \neq y_i} w_i^m e^{c_m} = 0$$

$$e^{2c_m} = \frac{\sum_{i: h^m(x_i)=y_i} w_i^m}{\sum_{i: h^m(x_i) \neq y_i} w_i^m}$$

$$c_m = \frac{1}{2} \ln \frac{\left(\sum_{i: h^m(x_i)=y_i} w_i^m \right) / \left(\sum_{i=1}^N w_i^m \right)}{\left(\sum_{i: h^m(x_i) \neq y_i} w_i^m \right) / \left(\sum_{i=1}^N w_i^m \right)} = \frac{1}{2} \ln \frac{1 - E_m}{E_m},$$

$$\text{where } E_m := \frac{\sum_{i=1}^N w_i^m \mathbb{I}[h^m(x_i) \neq y_i]}{\sum_{i=1}^N w_i^m}$$

Adaboost derivation

Weights recalculation:

$$w_i^{m+1} \stackrel{df}{=} e^{-y_i f_m(x_i)} = e^{-y_i f_{m-1}(x_i)} e^{-y_i c_m h^m(x_i)}$$

Noting that $-y_i h^m(x_i) = 2\mathbb{I}[h^m(x_i) \neq y_i] - 1$, we can rewrite:

$$\begin{aligned} w_i^{m+1} &= e^{-y_i f_{m-1}(x_i)} e^{c_m(2\mathbb{I}[h^m(x_i) \neq y_i] - 1)} = \\ &= w_i^m e^{2c_m \mathbb{I}[h^m(x_i) \neq y_i]} e^{-c_m} \propto w_i^m e^{2c_m \mathbb{I}[h^m(x_i) \neq y_i]} \end{aligned}$$

Comments:

- We can remove common constants from weights.
- $w_i^{m+1} = w_i^m$ for correctly classified objects by $h_m(x)$.
- $w_i^{m+1} = w_i^m e^{2c_m}$ for incorrectly classified objects by $h_m(x)$.
 - so later classifiers will pay more attention to them

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1 Gradient boosting

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

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

Gradient descend algorithm:

INPUT:

η -parameter, controlling the speed of convergence

M -number of iterations

ALGORITHM:

initialize w

for $m = 1, 2, \dots, M$:

$$\Delta w = \frac{\partial F(w)}{\partial w}$$

$$w = w - \eta \Delta w$$

Modified gradient descent algorithm

INPUT:

M -number of iterations

ALGORITHM:

initialize w

for $m = 1, 2, \dots, M$:

$$\Delta w = \frac{\partial F(w)}{\partial w}$$

$$c^* = \arg \min_c F(w - c\Delta w)$$

$$w = w - c^* \Delta w$$

Gradient boosting

- Now consider $F(f(x_1), \dots, f(x_N)) = \sum_{n=1}^N \mathcal{L}(f(x_n), y_n)$
- 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 $z_i = -\frac{\partial \mathcal{L}(r, y_i)}{\partial r} \Big|_{r=f^{m-1}(x_i)}$
 - fit base learner $h_m(x)$ to $\{(x_i, z_i)\}_{i=1}^N$

Gradient boosting

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

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

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 - 2 fit h_m to $\{(x_i, z_i)\}_{i=1}^N$, for example by solving

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

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- 3 solve univariate optimization problem:

$$\sum_{i=1}^N \mathcal{L}(f_{m-1}(x_i) + c_m h_m(x_i), y_i) \rightarrow \min_{c_m \in \mathbb{R}_+}$$

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- 4 set $f_m(x) = f_{m-1}(x) + c_m h_m(x)$

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- 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

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

Specific cases:

- $\mathcal{L} = \frac{1}{2} (r - y)^2 \Rightarrow -\frac{\partial \mathcal{L}}{\partial r} = -(r - y) = (y - r)$
 - $h_m(x)$ is fitted to compensate regression errors $(y - f_{m-1}(x))$
- $\mathcal{L} = [-ry]_+ \Rightarrow -\frac{\partial \mathcal{L}}{\partial r} = \begin{cases} 0, & ry > 0 \\ y, & ry < 0 \end{cases}$
 - $h_m(x)$ is fitted to $y \mathbb{I}[f(x)y < 0]$

Gradient boosting of trees

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

- 1 Fit constant initial approximation $f_0(x)$:

$$f_0(x) = \arg \min_{\gamma} \sum_{i=1}^N \mathcal{L}(\gamma, y_i)$$

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- 2 For each step $m = 1, 2, \dots, M$:
 - 1 calculate derivatives $z_i = -\frac{\partial \mathcal{L}(r, y)}{\partial r} \Big|_{r=f^{m-1}(x)}$
 - 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) , $i = 1, 2, \dots, N$; loss function $\mathcal{L}(f, y)$ and the number M of successive additive approximations.

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 - 3 for each terminal region R_{jm} , $j = 1, 2, \dots, J_m$ 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

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- 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) , $i = 1, 2, \dots, N$; 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 $m = 1, 2, \dots, M$:
 - ① calculate derivatives $z_i = -\frac{\partial \mathcal{L}(r, y)}{\partial r} \Big|_{r=f^{m-1}(x)}$
 - 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} , $j = 1, 2, \dots, J_m$ 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 $f_M(x)$

Linear loss function approximation

Consider sample (x, y) .

$$\mathcal{L}(f(x) + h(x), y) \approx \mathcal{L}(f(x), y) + h(x) \left. \frac{\partial \mathcal{L}(r, y)}{\partial r} \right|_{r=f(x)}$$

$\Rightarrow h(x)$ should be fitted to $\left. \frac{\partial \mathcal{L}(r, y)}{\partial r} \right|_{r=f(x)}$.

Newton method of optimization

- Suppose we want $F(w) \rightarrow \min_w$
- Let $w^* = \arg \min_w F(w)$
- Then $F'(w^*) = \mathbf{0}$
- Taylor expansion of $F'(w)$ around w to w^* :

$$F'(w^*) = 0 = F'(w) + F''(w)(w^* - w) + o(\|w - w^*\|)$$

- It follows that

$$w^* - w = - \left[F''(w) \right]^{-1} F'(w) + o(\|w - w^*\|)$$

- Iterative scheme for minimization:

$$w \leftarrow w - \left[F''(w) \right]^{-1} F'(w)$$

- it is scaled gradient descent
- speed of convergence faster (uses quadratic approximation in Taylor expansion)
- converges in one step for quadratic $F(w)$.

Quadratic loss function approximation

$$\begin{aligned} & \mathcal{L}(f(x) + h(x), y) = \\ & \mathcal{L}(f(x), y) + h(x) \left. \frac{\partial \mathcal{L}(r, y)}{\partial r} \right|_{r=f(x)} + \frac{1}{2} (h(x))^2 \left. \frac{\partial^2 \mathcal{L}(r, y)}{\partial r^2} \right|_{r=f(x)} = \\ & \frac{1}{2} \left. \frac{\partial^2 \mathcal{L}(r, y)}{\partial r^2} \right|_{r=f(x)} \left(h(x) + \frac{\left. \frac{\partial \mathcal{L}(r, y)}{\partial r} \right|_{r=f(x)}}{\left. \frac{\partial^2 \mathcal{L}(r, y)}{\partial r^2} \right|_{r=f(x)}} \right)^2 + \text{const}(h(x)) \end{aligned}$$

$\Rightarrow h(x)$ should be fitted to $-\frac{\left. \frac{\partial \mathcal{L}(r, y)}{\partial r} \right|_{r=f(x)}}{\left. \frac{\partial^2 \mathcal{L}(r, y)}{\partial r^2} \right|_{r=f(x)}}$ with

weight $\left. \frac{\partial^2 \mathcal{L}(r, y)}{\partial r^2} \right|_{r=f(x)}$

Example: LogitBoost

Binary classification: $y \in \{+1, -1\}$

Assumption:

$$p(y|x) = \frac{1}{1 + e^{-yf(x)}} \quad (1)$$

Properties:

$$p(y|x) \in [0, 1], \quad p(+1|x) + p(-1|x) = 1$$

Function fitting done with maximum likelihood:

$$p(Y|X) = \prod_{i=1}^N p(y_i|x_i) \rightarrow \max_f$$

$$f = \arg \max_f \sum_{i=1}^N \ln p(y_i|x_i) = \arg \min_f \sum_{i=1}^N \ln(1 + e^{-yf(x)})$$

\Rightarrow loss function is $\mathcal{L}(f(x), y) = \ln(1 + e^{-yf(x)})$.

Example: LogitBoost

$\mathcal{L}(r, y) = \ln(1 + e^{-yr})$, so

$$\frac{\partial \mathcal{L}(r, y)}{\partial r} = \frac{e^{-yr}(-y)}{1 + e^{-yr}} = -\frac{y}{1 + e^{yr}}$$

$$\frac{\partial^2 \mathcal{L}(r, y)}{\partial r^2} = -\frac{-ye^{yr}y}{(1 + e^{yr})^2} = \frac{e^{yr}}{(1 + e^{yr})(1 + e^{-yr})} = \frac{1}{(1 + e^{-yr})(1 + e^{yr})}$$

It follows, that $\left. \frac{\partial \mathcal{L}(r, y)}{\partial r} \right|_{r=f(x)} = -y p_{f(x)}(-y)$ and

$$\frac{\partial^2 \mathcal{L}(r, y)}{\partial r^2} = p_{f(x)}(y) (1 - p_{f(x)}(y))$$

$$\Rightarrow h(x) \text{ should be fitted to } -\left. \frac{\frac{\partial \mathcal{L}(r, y)}{\partial r}}{\frac{\partial^2 \mathcal{L}(r, y)}{\partial r^2}} \right|_{r=f(x)} = y (1 + e^{-yf(x)}) = \frac{y}{p_{f(x)}(y)}$$

with weight $\left. \frac{\partial^2 \mathcal{L}(r, y)}{\partial r^2} \right|_{r=f(x)} = p_{f(x)}(y) (1 - p_{f(x)}(y))$

c_m is not fitted because $h(x)$ is fitted directly to local optimum under quadratic approximation.

Logitboost algorithm

Input: training dataset (x_i, y_i) , $i = 1, 2, \dots, N$; number of steps M .

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

Logitboost algorithm

Input: training dataset (x_i, y_i) , $i = 1, 2, \dots, N$; number of steps M .

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Output:

- approximation function $f_M(x) = f_0(x) + \sum_{m=1}^M h_m(x)$
- classifier $\hat{y} = \text{sign}(f_M(x))$
- class probabilities $p(y|x) = \frac{1}{1 + e^{-y f_M(x)}}$

Quadratic loss function approximation - discrete $h(x)$

$$\begin{aligned}
 & \sum_i \mathcal{L}(f(x_i) + h(x_i), y_i) = \\
 & \sum_i \mathcal{L}(f(x_i), y_i) + \sum_i ch(x_i) \left. \frac{\partial \mathcal{L}(r, y_i)}{\partial r} \right|_{r=f(x_i)} + \sum_i \frac{1}{2} (ch(x_i))^2 \left. \frac{\partial^2 \mathcal{L}(r, y_i)}{\partial r^2} \right|_{r=f(x_i)} = \\
 & \sum_i \mathcal{L}(f(x_i), y_i) + \sum_i h(x_i) c \left. \frac{\partial \mathcal{L}(r, y_i)}{\partial r} \right|_{r=f(x_i)} + \sum_i \frac{1}{2} c^2 \left. \frac{\partial^2 \mathcal{L}(r, y_i)}{\partial r^2} \right|_{r=f(x_i)} = \\
 & \sum_i \mathcal{L}(f(x_i), y_i) - c \sum_i y_i p_{f(x_i)}(-y_i) h(x_i) + \frac{1}{2} c^2 \sum_i p_{f(x_i)}(y_i) (1 - p_{f(x_i)}(y_i))
 \end{aligned} \tag{2}$$

$\Rightarrow h(x)$ should be fitted to y_i with weights equal to probability of error $p_{f(x_i)}(-y_i)$.

c is the minimizer of (2) and equal to

$$c^* = \frac{\sum_i y_i p_{f(x_i)}(-y_i) h(x_i)}{\sum_i p_{f(x_i)}(y_i) (1 - p_{f(x_i)}(y_i))}$$

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 $4 \leq J \leq 8$
- 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

Case of $C \geq 3$ classes

- Can fit C independent boostings (one vs. all scheme)
 - $\hat{y} = \arg \max_y f_{my}(x)$
- Alternatively can optimize multivariate $\mathcal{L}(f(x), y) = -\ln p(y|x)$
 - using linear or quadratic approximation
 - for quadratic approximation need to invert $\left. \frac{\partial^2}{\partial r^2} F(r, y) \right|_{r=f(x)}$.
Can use diagonal approximation.

Types of boosting

- Loss function F :
 - $F(|f(x) - y|)$ - regression
 - $-\ln p(y|x)$ or $F(y \cdot \text{score}(y = +1|x))$ - binary classification
 - $-\ln p(y|x)$ - multiclass classification
- Optimization
 - analytical (AdaBoost)
 - gradient based
 - based on quadratic approximation
- Base learners
 - continious
 - discrete
- Classification
 - binary
 - multiclass
- Extensions: shrinkage, subsampling