Boosting

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Motivation for ensembles

- Consider M classifiers $f_1(x), ...f_M(x)$, performing binary classification.
- Let $\xi_1, ...\xi_M$ denote indicators of mistakes by $f_1, ...f_M$ on particular observation x
- Suppose $\xi_1, ...\xi_M$ are independent binomial variables with $P(\xi_i = 1) = p$
- Then $\mathbb{E}\xi_i = p$, $Var[\xi_i] = p(1-p)$
- Consider $F(x)$ be aggregating classifier, assigning x to the class with maximum votes among $f_1(x), ...f_M(x)$.
- Consider
$$\eta = \frac{\xi_1 + ... + \xi_M}{M}$$
- Probability of mistake = probability that majority of $\xi_1, ...\xi_M$ are ones = $P(\eta > 0.5)$.
- $P(\eta > 0.5) \to 0$ as $M \to \infty$ because $\mathbb{E}\eta = p$, $Var[\eta] = \frac{p(1-p)}{M}$.

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.
- After ensemble is built we can fine-tune $c_1, ...c_M$ by fitting features $f_0(x), h_1(x), ...h_M(x)$ with linear regression/classifier.

Forward stagewise additive modeling (FSAM)

Input: training dataset (x_i, y_i), $i = 1, 2, ...N$; 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 $m = 1, 2, ...M$:
   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.

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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 $\widehat{y} = sign\{f_0(x) + c_1 f_1(x) + ... + c_M f_M(x)\}$
- 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), $i = 1, 2, ...N$; number of additive weak classifiers M, a family of weak classifiers $h(x) \in \{+1, -1\}$, trainable on weighted datasets.

1. Initialize observation weights $w_i = 1/n$, $i = 1, 2, ...n$.
2. for $m = 1, 2, ...M$:
    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 $c_m = \frac{1}{2} \ln\left((1 - E_m)/E_m\right)$
    5. increase all weights, where misclassification with $h^m(x)$ was made:
    $$w_i \leftarrow w_i e^{2c_m},\ i \in \{i :\ h^m(x_i) \neq y_i\}$$

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 $m = 1, 2, ... M$:

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

Adaboost derivation

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

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

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

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

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

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

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

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

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

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:

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

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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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:
η-parameter, controlling the speed of convergence
M-number of iterations

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

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

Gradient boosting

Input: training dataset (x_i, y_i), $i = 1, 2, ...N$; 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

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

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

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

   3. solve univariate optimization problem:

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

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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

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

Specific cases:

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

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

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   1. calculate derivatives $z_i = -\frac{\partial \mathcal{L}(r,y)}{\partial r}|_{r=f^{m-1}(x)}$

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

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   3. for each terminal region R_j^m, $j = 1, 2, ...J_m$ solve univariate optimization problem:

$$\gamma_j^m = \arg\min_\gamma \sum_{x_i \in R_j^m} \mathcal{L}(f_{m-1}(x_i) + \gamma,\ y_i)$$

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   $$\gamma_j^m = \arg\min_\gamma \sum_{x_i \in R_j^m} \mathcal{L}(f_{m-1}(x_i) + \gamma,\ y_i)$$
   4. update $f_m(x) = f_{m-1}(x) + \sum_{j=1}^{J_m} \gamma_j^m \mathbb{I}[x \in R_j^m]$

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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.

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

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_j^m, not globally for the whole classifier $h^m(x)$.
- This is done to increase accuracy: forward stagewise algorithm cannot be applied to find R_j^m, but it can be applied to find γ_j^m, 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

Linear loss function approximation

Consider sample (x, y).

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

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

Newton method of optimization

- Suppose we want $F(w) \to \min_w$
- 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

$$\mathcal{L}(f(x)+h(x),\ y)\approx$$

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

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

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

Case of $C \geq 3$ classes

- Can fit C independent boostings $\{f_y(x)\}_{y=1}^{C}$ (one vs. all scheme)
  - $\widehat{y}(x) = \arg\max_y f_y(x)$
- Alternatively can optimize multivariate $\mathcal{L}(f(x), y) = -\ln p(y|x)$
  - using linear or quadratic approximation
  - for quadratic approximation need to invert $\frac{\partial^2}{\partial r^2} F(r, y)\Big|_{r=f(x)}$.

    Can use diagonal approximation.

Types of boosting

- Loss function F:
  - $F(|f(x)-y|)$ - regression
  - $-\ln p(y|x)$ or $F(y \cdot score(y=+1|x))$ - 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