

INTRODUCTION



TO STATISTICAL LEARNING

Introduction to Statistical Learning

Boosting - Class 10

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AdaBoost

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Instead of averaging

- Suppose $y \in \{-1, 1\}$
- Recall the final Random Forests model: $\hat{f}(x_0) = \text{sign} \left[\frac{1}{M} \sum_{m=1}^M T_m(x_0) \right]$
- Why not $\hat{f}(x_0) = \text{sign} \left[\sum_{m=1}^M \alpha_m T_m(x_0) \right]$?
 - If M is the number of all possible trees T_m , then finding weights α_m is intractable!
- **Boosting** finds α_m sequentially, *adaptively*:
 - Take a **weak classifier** $G(x)$ with accuracy slightly better than random
 - for any dist. P_T of the training data: $Err_{P_T} = \mathbb{E}_{P_T} (\mathbb{I}[y_i \neq G(x_i)]) \leq \frac{1}{2} - \gamma$
 - Apply it sequentially over modified (weighted) versions of the training data
 - Each time selecting the best α_m to get: $\hat{f}(x_0) = \text{sign} \left[\sum_{m=1}^M \alpha_m G_m(x_0) \right]$

AdaBoost

1. Initialize observations weights $w_i = 1/n$ for $i = 1, \dots, n$
2. For $m = 1$ to M :
 - a. Fit classifier $G_m(x)$ to the training data using **weights** w_i
 - b. Compute weighted classification error:

$$err_m = \frac{\sum_{i=1}^n w_i \mathbb{I}[y_i \neq G_m(x_i)]}{\sum_{i=1}^n w_i}$$

- c. Compute coefficient $\alpha_m = \ln \left[\frac{1 - err_m}{err_m} \right]$
- d. Update weights: $w_i \leftarrow w_i \cdot \exp [\alpha_m \cdot \mathbb{I}[y_i \neq G_m(x_i)]]$
3. Output: $\hat{f}(x) = \text{sign} \left[\sum_{m=1}^M \alpha_m G_m(x) \right]$



What does it mean training a classification tree with weighted data?

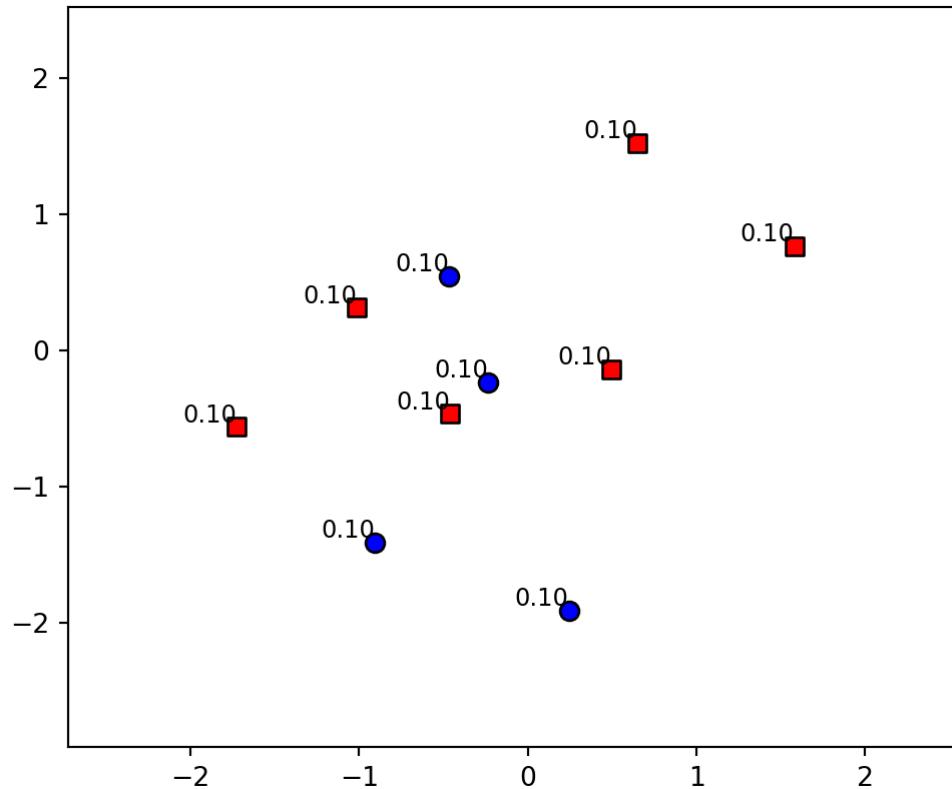
AdaBoost Example

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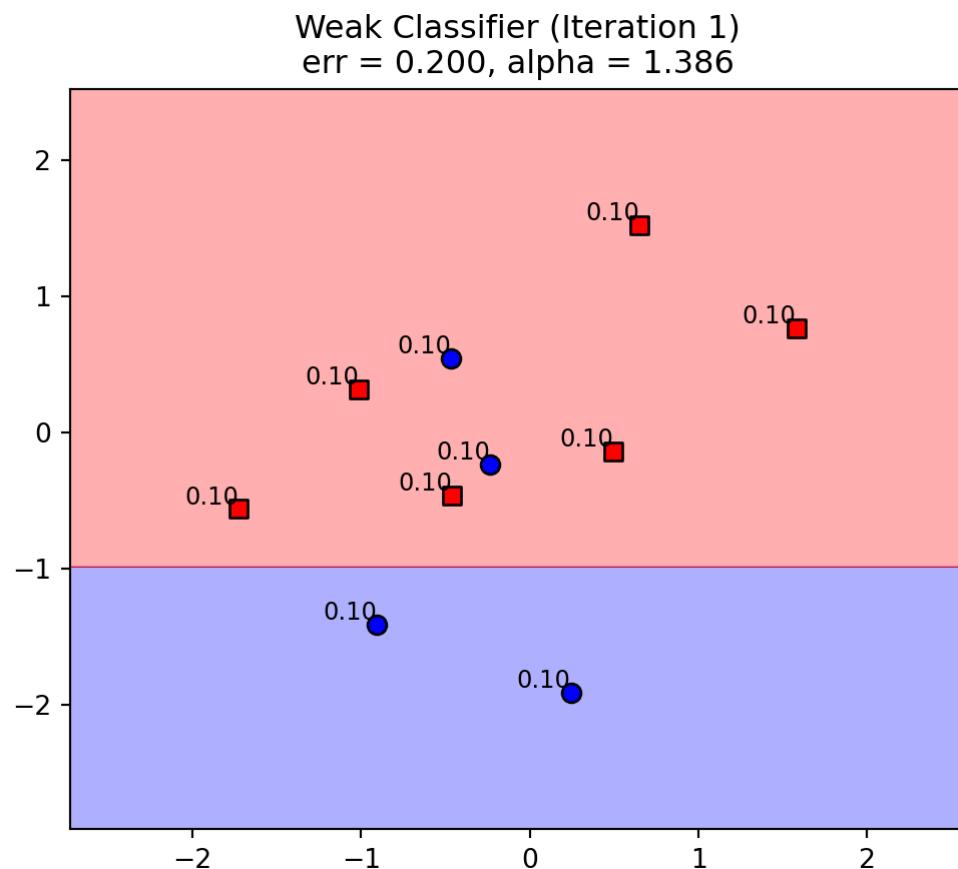
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AdaBoost with Tree Stumps

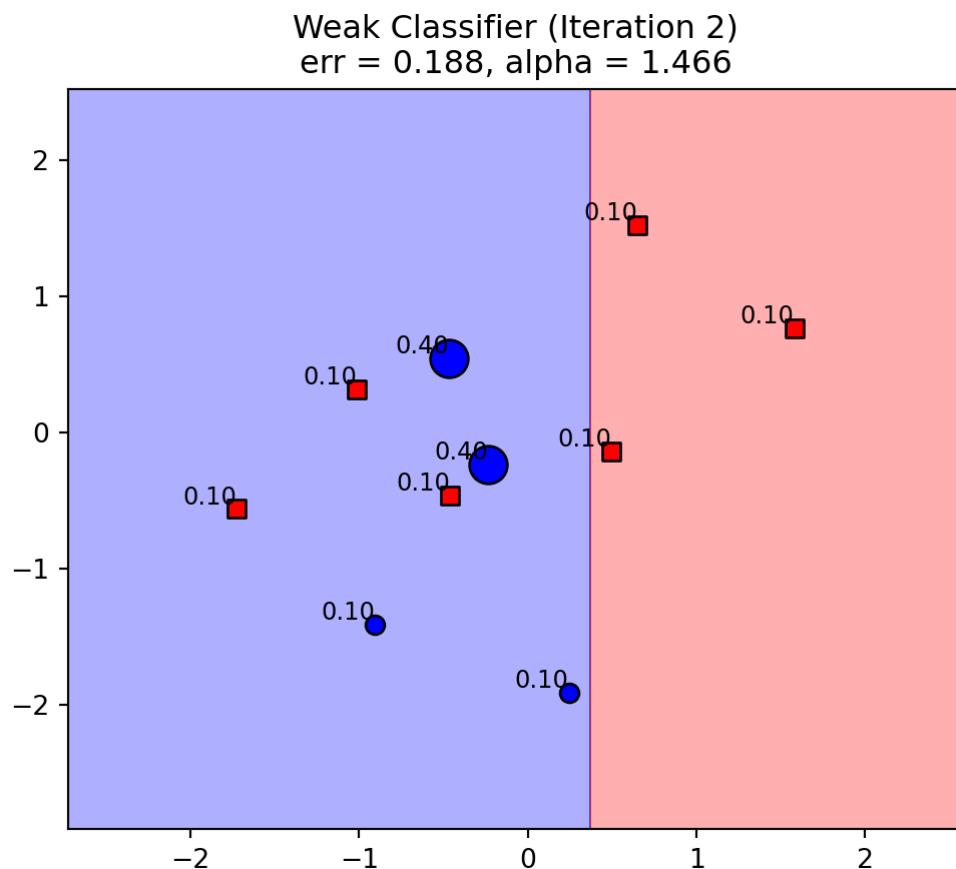


Can a tree stump get to $\overline{err} = 0$? Can a deep decision tree?

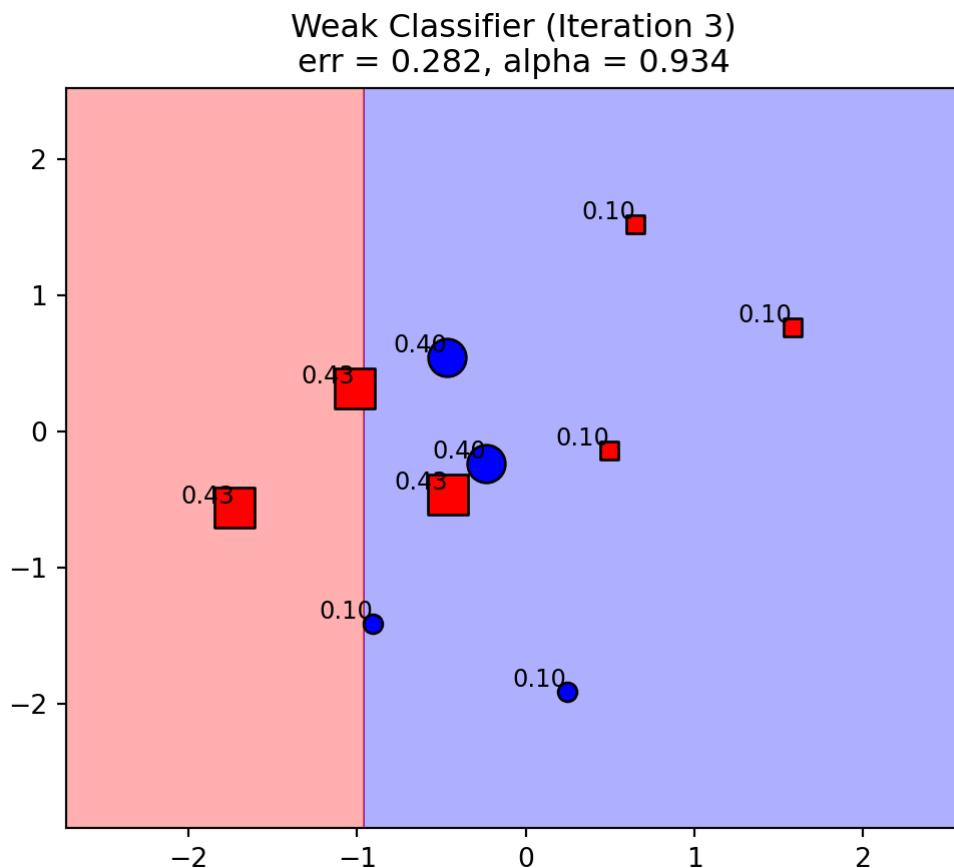
AdaBoost: iteration 1



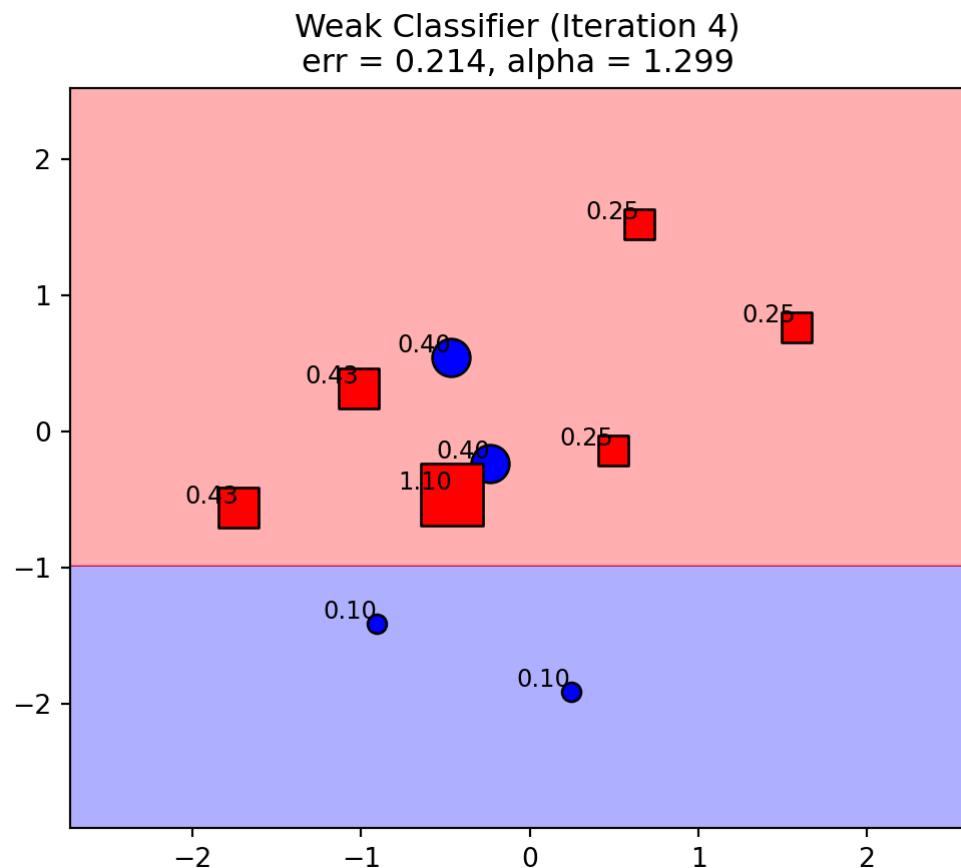
AdaBoost: iteration 2



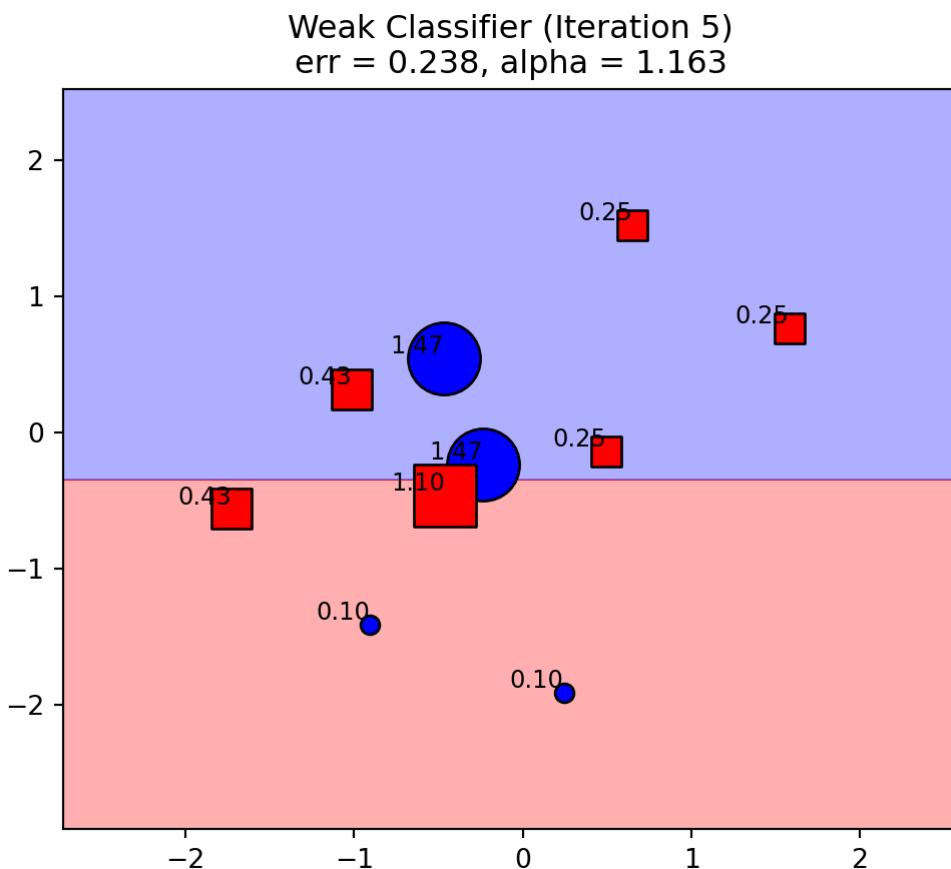
AdaBoost: iteration 3



AdaBoost: iteration 4

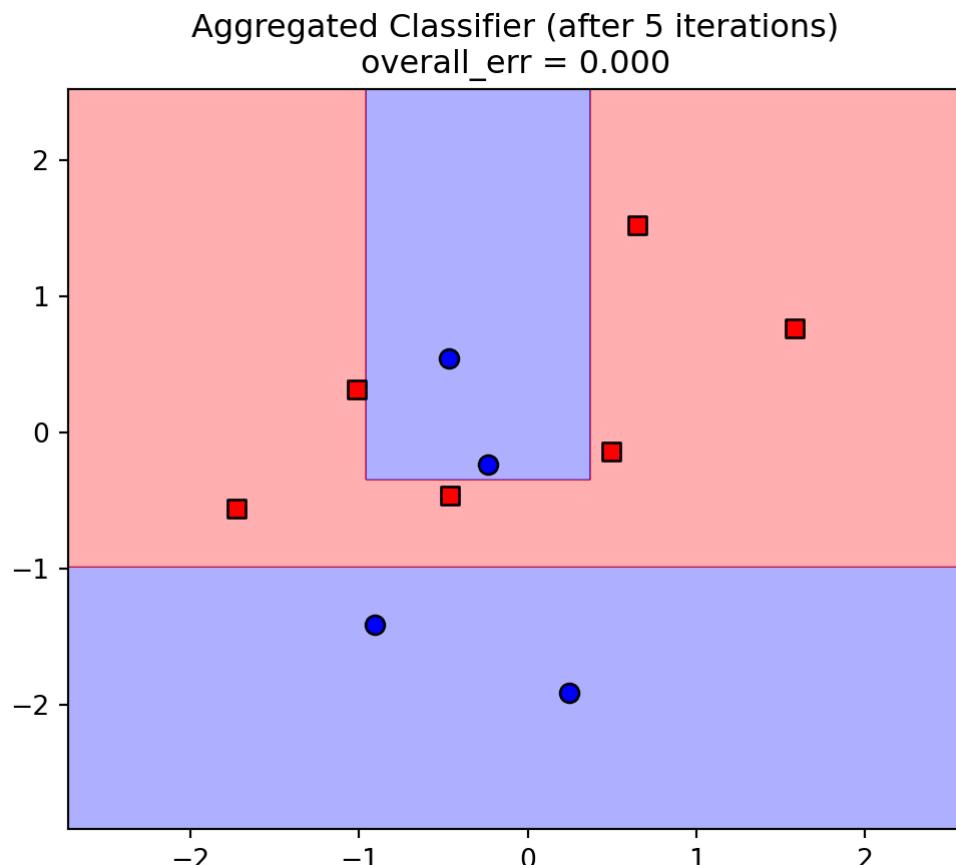


AdaBoost: iteration 5

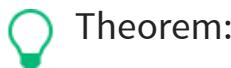


AdaBoost: aggregate

$$\hat{f}(x) = \text{sign} \left[\sum_{m=1}^M \alpha_m G_m(x) \right] =$$
$$= \text{sign} [1.386G_1(x) + 1.466G_2(x) + 0.934G_3(x) + 1.299G_4(x) + 1.126G_5(x)]$$



AdaBoost Guarantee



Theorem:

$$\overline{err} = \sum_{i=1}^n \mathbb{I}[y_i \neq \hat{f}(x_i)] \leq (1 - 4\gamma^2)^{M/2} \leq e^{-2M\gamma^2}$$

- This means for a large enough M we can get \overline{err} as low as we want (on training data)!
- Specifically, to make the upper bound $e^{-2M\gamma^2} < \frac{1}{n}$ (i.e. $\overline{err} = 0$) $\Rightarrow M > \frac{\log(n)}{2\gamma^2}$
- A weak classifier which can only guarantee up to 40% error at each iteration ($\gamma = 0.1$):
 - after $M = 100$ iterations will be boosted to give $\overline{err} \leq (1 - 4 \cdot 0.1^2)^{(100/2)} = 0.96^{50} \approx 0.13$ error
 - if $n = 1000$, need $M > \log(1000)/2 \cdot 0.1^2 \approx 345$ iterations to get $\overline{err} = 0$
- Really nice proof in Freund & Schapire (1997)

AdaBoost as Additive Stagewise Modeling

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Questions from AdaBoost

- Does it optimize a specific loss? Can we plug-in a different loss?
- What about regression?
- What about K -class classification?
- Is there a probabilistic justification? A likelihood-based approach?

AdaBoost sure sounds familiar

Recall: Forward stagewise regression

0. Standardize all features, input some $\tau_{thresh} \in (0, 1)$ and $\varepsilon > 0$ step size
1. Residual $\mathbf{r} = \mathbf{y} - \bar{y}$, $\beta_1, \dots, \beta_p = 0$
2. Find the predictor \mathbf{x}_j most correlated with \mathbf{r} , and let $\tau = \text{Corr}(\mathbf{r}, \mathbf{x}_j)$
3. While $|\tau| > \tau_{thresh}$:
 - i. Update $\beta_j \leftarrow \beta_j + \delta_j$, where $\delta_j = \varepsilon \cdot \text{sign}(\tau)$
 - ii. Update $\mathbf{r} \leftarrow \mathbf{r} - \delta_j \mathbf{x}_j$
 - iii. Find the predictor \mathbf{x}_j most correlated with \mathbf{r} , and let $\tau = \text{Corr}(\mathbf{r}, \mathbf{x}_j)$

A general forward stagewise additive model (FSAM)

1. Initialize $f_0(x) = 0$

2. For $m = 1$ to M :

a. Compute:

$$(\beta_m, \gamma_m) = \arg \min_{\beta, \gamma} \sum_{i=1}^n L(y_i, f_{m-1}(x_i) + \beta b(x_i, \gamma))$$

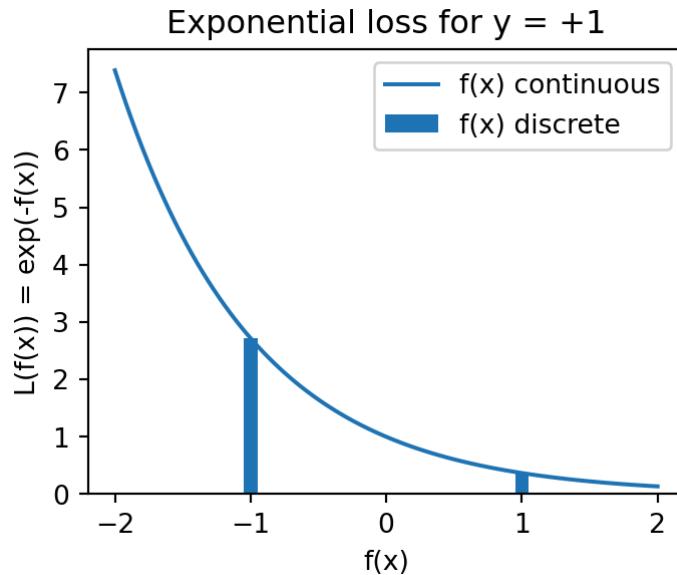
b. Set $f_m(x) = f_{m-1}(x) + \beta_m b(x; \gamma_m)$

3. Output: $\hat{f}(x) = \sum_{m=1}^M \beta_m b(x; \gamma_m)$

 If L is the squared loss, and finding γ_m is finding the j -th predictor \mathbf{x}_j most correlated with the residual
 \Rightarrow this is forward stagewise regression!

Claim: AdaBoost is also a FSAM

- If L is the exponential loss: $L(y, f(x)) = \exp(-yf(x))$
- And, $b(x; \gamma_m) = Gm(x)$
- We get AdaBoost!



Fast forward: plug-in *other* loss functions!

Showing AdaBoost is FSAM

- Recall the goal in FSAM iteration m :

$$(\beta_m, \gamma_m) = \arg \min_{\beta, \gamma} \sum_{i=1}^n L(y_i, f_{m-1}(x_i) + \beta b(x_i, \gamma))$$

- For exponential loss:

$$\begin{aligned} (\beta_m, G_m) &= \arg \min_{\beta, G} \sum_{i=1}^n \exp [-y_i(f_{m-1}(x_i) + \beta G(x_i))] \\ &= \arg \min_{\beta, G} \sum_{i=1}^n \exp [-y_i f_{m-1}(x_i)] \exp [\beta G(x_i)] \\ &= \arg \min_{\beta, G} \sum_{i=1}^n w_i^{(m)} \exp [-\beta y_i G(x_i)] \end{aligned}$$

Getting G_m

- Assuming $\beta > 0$, separate the criterion to “correct” + “incorrect” sums:

$$\begin{aligned} \sum_{i=1}^n w_i^{(m)} \exp [-\beta y_i G(x_i)] &= \\ = e^{-\beta} \sum_{i=1}^n w_i^{(m)} \mathbb{I}[y_i = G(x_i)] + e^{\beta} \sum_{i=1}^n w_i^{(m)} \mathbb{I}[y_i \neq G(x_i)] \end{aligned}$$

- Can also write as:

$$= (e^\beta - e^{-\beta}) \sum_{i=1}^n w_i^{(m)} \mathbb{I}[y_i \neq G(x_i)] + e^{-\beta} \sum_{i=1}^n w_i^{(m)}$$

- AdaBoost stage 2a: G_m minimizing the criterion is minimizing weighted error rate:

$$G_m = \arg \min_G \sum_{i=1}^n w_i^{(m)} \mathbb{I}[y_i \neq G(x_i)]$$

Getting α_m

$$\text{criterion} = (e^\beta - e^{-\beta}) \sum_{i=1}^n w_i^{(m)} \mathbb{I}[y_i \neq G(x_i)] + e^{-\beta} \sum_{i=1}^n w_i^{(m)}$$

$$\frac{\partial \text{criterion}}{\partial \beta} = (e^\beta + e^{-\beta}) \sum_{i=1}^n w_i^{(m)} \mathbb{I}[y_i \neq G(x_i)] - e^{-\beta} \sum_{i=1}^n w_i^{(m)} \rightarrow = 0$$

- Multiply by e^β :

$$(1 + e^{2\beta}) = \frac{\sum_{i=1}^n w_i^{(m)}}{\sum_{i=1}^n w_i^{(m)} \mathbb{I}[y_i \neq G(x_i)]} = \frac{1}{err_m}$$

- Take \ln , we get AdaBoost stages 2b and 2c:

$$\beta_m = \frac{1}{2} \ln \left[\frac{1 - err_m}{err_m} \right] = \frac{1}{2} \alpha_m$$

Getting w_i

- FSAM says:

$$f_m(x) = f_{m-1}(x) + \beta_m b(x; \gamma_m) = f_{m-1}(x) + \frac{1}{2} \alpha_m G_m(x)$$

- Which means next iteration weights are:

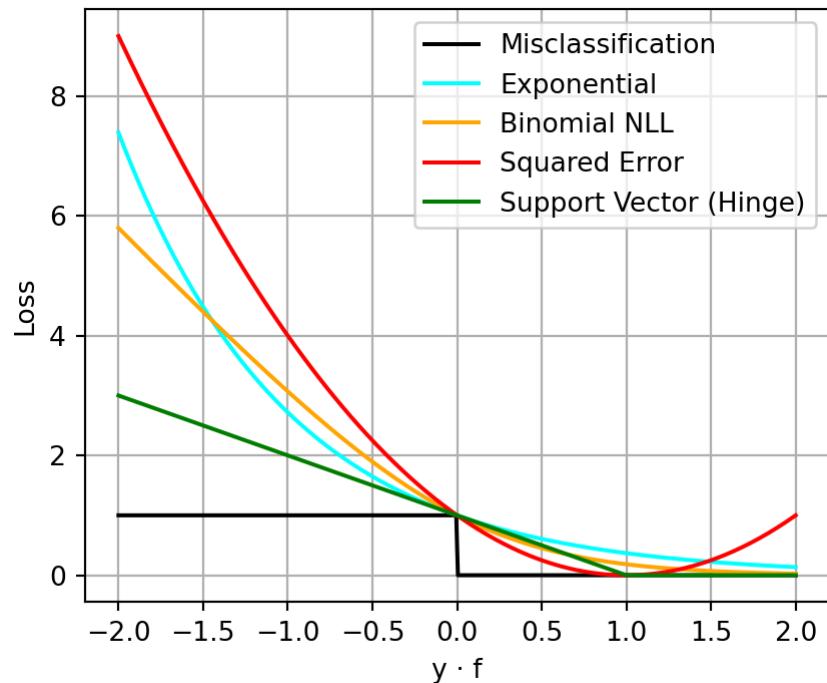
$$\begin{aligned} w_i^{(m+1)} &= \exp[-y_i f_{m+1}(x_i)] = \exp[-y_i(f_m(x) + \frac{1}{2} \alpha_m G_m(x))] = \\ &= w_i^{(m)} \cdot \exp[-\frac{1}{2} \alpha_m y_i G_m(x)] \end{aligned}$$

- Given that $-y_i G_m(x_i) = 2 \cdot \mathbb{I}[y_i \neq G_m(x_i)] - 1$, we can write:

$$w_i^{(m+1)} = w_i^{(m)} \cdot \exp[\alpha_m \cdot \mathbb{I}[y_i \neq G_m(x_i)]] \cdot Const$$

- Equivalent to AdaBoost stage 2d.

Classification losses



(i) The $f(x)$ minimizing exponential loss is also minimizing Binomial negative log-likelihood!

- Misclassification (0/1 loss):

$$L_{\text{misclass}}(y, f) = \begin{cases} 0 & \text{if } y \cdot f(x) > 0 \\ 1 & \text{otherwise} \end{cases}$$

- Exponential loss:

$$L_{\text{exp}}(y, f) = \exp(-y \cdot f(x))$$

- Binomial negative log-likelihood (cross-entropy):

$$L_{\text{bin}}(y, f) = \log(1 + \exp(-2 \cdot y \cdot f(x))) / \log(2)$$

- Squared error loss:

$$L_{\text{sq}}(y, f) = (1 - y \cdot f(x))^2$$

- Support vector (hinge Loss):

$$L_{\text{hinge}}(y, f) = \max(0, 1 - y \cdot f(x))$$

Boosting for Regression

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Recap

What the FSAM framework got us:

$$(\beta_m, \gamma_m) = \arg \min_{\beta, \gamma} \sum_{i=1}^n L(y_i, f_{m-1}(x_i) + \beta b(x_i, \gamma))$$

- Classification:
 - $y \in \{-1, 1\}$, exponential loss, $b(x_i, \gamma)$ are weak learners $G(x) \Rightarrow$ AdaBoost
- Regression:
 - $y \in \mathbb{R}$, squared error loss, $b(x_i, \gamma)$ are single features $\mathbf{x}_j \Rightarrow$ Forward stagewise regression
- What if we want to boost weak learners $G(x)$ for regression?

Boosted trees for regression (I)

- Specifically, let us focus on boosting trees: $f(x) = \sum_{m=1}^M T(x, \Theta_m)$
- Where $T(x, \Theta) = \sum_{j=1}^J \gamma_j \mathbb{I}(X \in R_j)$
- With parameters $\Theta = \{R_j, \gamma_j\}_1^J$
- “Building a regression tree” is equivalent to:

$$\hat{\Theta} = \arg \min_{\Theta} \sum_{i=1}^n (y_i - T(x_i, \Theta))^2$$

Boosted trees for regression (II)

- So FSAM with squared loss, no problem:

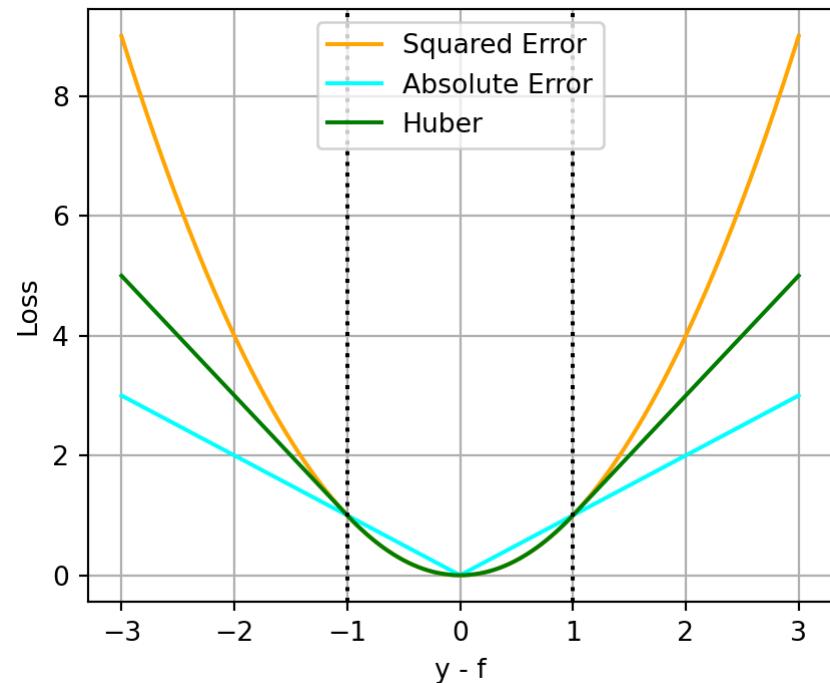
$$\begin{aligned}\Theta_m &= \arg \min_{\Theta} \sum_{i=1}^n L(y_i, f_{m-1}(x_i) + T(x_i, \Theta)) = \\ &= \arg \min_{\Theta} \sum_{i=1}^n (y_i - f_{m-1}(x_i) - T(x_i, \Theta))^2 \\ &= \arg \min_{\Theta} \sum_{i=1}^n (r_{im} - T(x_i, \Theta))^2\end{aligned}$$

- Because we know how to build such trees!
- To sum up: at each iteration m build standard regression tree $T(x, \Theta)$ which best fits the current residuals \mathbf{r}_m



At high-level, similar to AdaBoost!

What about more **robust** losses?



- Squared Error Loss:

$$L_{\text{sq}}(y, f) = (y - f(x))^2$$

- Absolute Error Loss:

$$L_{\text{abs}}(y, f) = |y - f(x)|$$

- Huber Loss:

$$L_{\text{H}}(y, f) = \begin{cases} (y - f(x))^2 & |y - f(x)| \leq \delta \\ 2\delta|y - f(x)| - \delta^2 & \text{otherwise.} \end{cases}$$

Gradient Boosting

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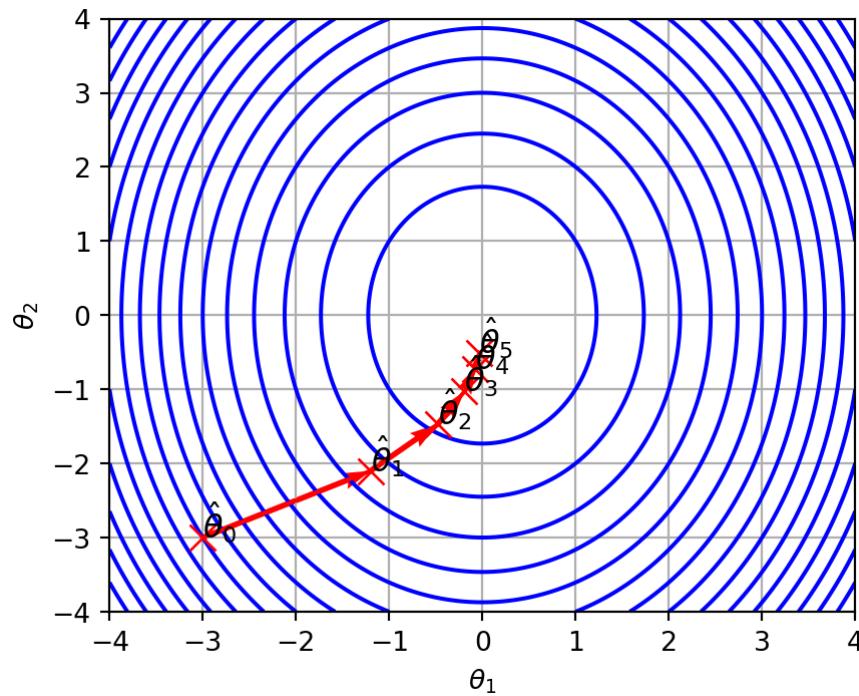


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Gradient descent algorithms

Minimize a function $J(\theta)$ by moving in the opposite direction of the gradient:

$$\hat{\theta}_{i+1} = \hat{\theta}_i - \varepsilon \frac{\partial J(\theta)}{\partial \theta}$$



Gradient boosting machines

- Consider any loss $L(\mathbf{y}, \mathbf{f})$ a function of n data points $\mathbf{f} = (f(x_1), \dots, f(x_n))$
- At each iteration m , calculate the gradient of L by \mathbf{f} , evaluated at \mathbf{f}_{m-1} :

$$\mathbf{g}_m = \frac{\partial L(\mathbf{y}, \mathbf{f})}{\partial \mathbf{f}} \Big|_{\mathbf{f}=\mathbf{f}_{m-1}}$$

- Move a small step ε down this gradient:

$$\mathbf{f}_m = \mathbf{f}_{m-1} - \varepsilon \mathbf{g}_m$$

- Technically, ε can also be optimized at each iteration m to minimize

$$\varepsilon_m = \arg \min_{\varepsilon} L(\mathbf{y}, \mathbf{f}_{m-1} - \varepsilon \mathbf{g}_m)$$

Gradient boosting machines

- Eventually we would get:

$$\mathbf{f}_M = \sum_{i=1}^M \varepsilon_m (-\mathbf{g}_m)$$

- But we are not interested in \mathbf{f}_M for our training data, we wanted a model! What about x_0 ?
 - E.g. $f(x) = \sum_{m=1}^M \varepsilon T(x, \Theta_m)$
- Solution: at each iteration m approximate the negative gradient $-\mathbf{g}_m$ with a weak learner or regression tree!

$$\Theta_m = \arg \min_{\Theta} \sum_{i=1}^n (-g_{im}(L) - T(x_i, \Theta))^2$$

Gradients of common loss functions

setting	loss : $L(y_i, f(x_i))$	gradient: $-g(L(y_i, f(x_i)))$
Regression	$\frac{1}{2}(y_i - f(x_i))^2$	$y_i - f(x_i)$
Regression	$ y_i - f(x_i) $	$\text{sign}(y_i - f(x_i))$
Regression	Huber	$\begin{cases} y_i - f(x_i) & \text{if } y_i - f(x_i) \leq \delta \\ \delta \text{sign}(y_i - f(x_i)) & \text{otherwise} \end{cases}$
Classification*	NLL	$\mathbb{I}[y_i = 1] - \hat{p}_i$

*Here $y \in \{0, 1\}$ and $\hat{p}_i = \frac{\exp(\hat{y}_i)}{1+\exp(\hat{y}_i)} = \frac{\exp(f(x_i))}{1+\exp(f(x_i))}$



Notice for (half) squared loss the gradient is the residuals, as we got earlier.

Gradient boosting trees (simplified)

1. Initialize $f_0(x) = \arg \min_{\gamma} \sum_{i=1}^n L(y_i, \gamma)$ (e.g. $f_0(x) = \bar{y}$)

2. For $m = 1$ to M :

a. Compute pseudo-residuals:

$$\mathbf{r}_m = -\mathbf{g}_m(L) = -\left[\frac{\partial L(\mathbf{y}, \mathbf{f})}{\partial \mathbf{f}} \right]_{\mathbf{f}=\mathbf{f}_{m-1}}$$

b. Fit a **regression tree** to data $(\mathbf{x}, \mathbf{r}_m)$, giving $T(x, \Theta_m)$

c. Update: $f_m(x) = f_{m-1}(x) + \varepsilon T(x, \Theta_m)$ (or ε_m)

3. Output: $\hat{f}(x) = \sum_{m=1}^M \varepsilon T(x, \Theta_m)$



What parameters need tuning?

Example: credit data

