CSCE 421: Machine Learning

Lecture 12: Boosting

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CSCE 421

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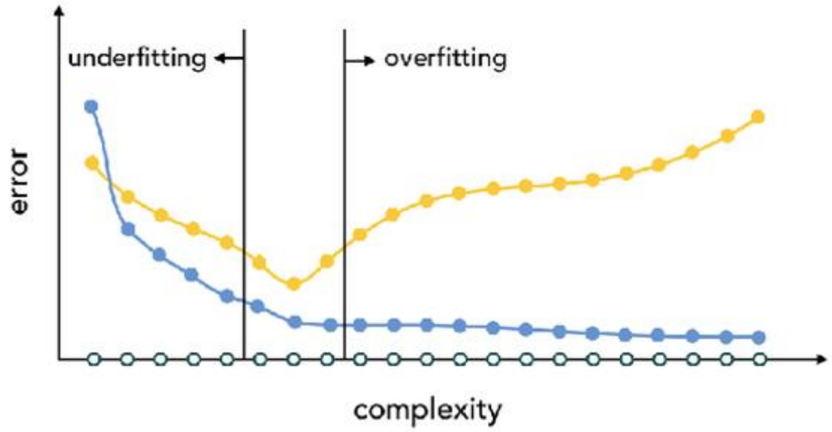
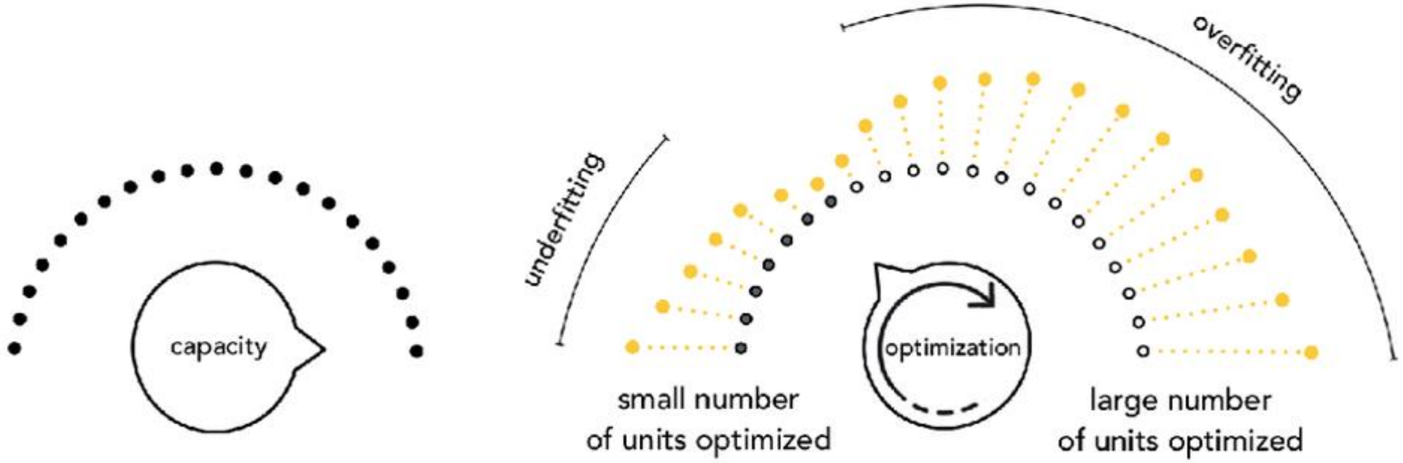
Goals

- Review Gradient Boosting
- Introduce Gradient Boosting for Classification
- Python Code!

Boosting Capacity





Initial Round (Round 0)

- Start with model:

$$model_0(x, \theta) = w_0$$

- Whose weight set $\theta_0 = \{w_0\}$, which contains a single bias weight which minimizes least squares (notation from Watt, Borhani, and Kastaggelos – P is people):

$$\frac{1}{p}\sum_{p=1}^{P}\left(model_0\left(x_p, \theta_0\right) - y_p\right)^2 = \frac{1}{p}\sum_{p=1}^{P}\left(w_0 - y_p\right)^2$$

- This optimal w_0 remains fixed forever forward

Round 1 of Boosting

- Having tuned the only parameter, we now boost its complexity by adding weighted unit $f_{s_1}(x)\, w_1$:

$$model_1(x, \theta_1) = model_0(x, \theta_0) + f_{s_1}(x)\, w_1$$

- To determine which unit in our set F best lowers the training error, we pick the $f_s \in F$ that minimizes the cost:

$$\frac{1}{p} \sum_{p=1}^{P} \left(model_0\left(x_p, \theta_0\right) + f_{s_1}\left(x_p\right) w_1 - y_p\right)^2 =$$

$$\frac{1}{p} \sum_{p=1}^{P} \left(w_0 + f_{s_1}\left(x_p\right) w_1 - y_p\right)^2$$

Round m > 1 of Boosting

$$model_{m-1}(x, \theta_{m-1}) = \; w_0 + \; f_{s_1}(x) * \; w_1 + f_{s_2}(x) * \; w_2 + \ldots + f_{s_{m-1}}(x) * \; w_{m-1}$$

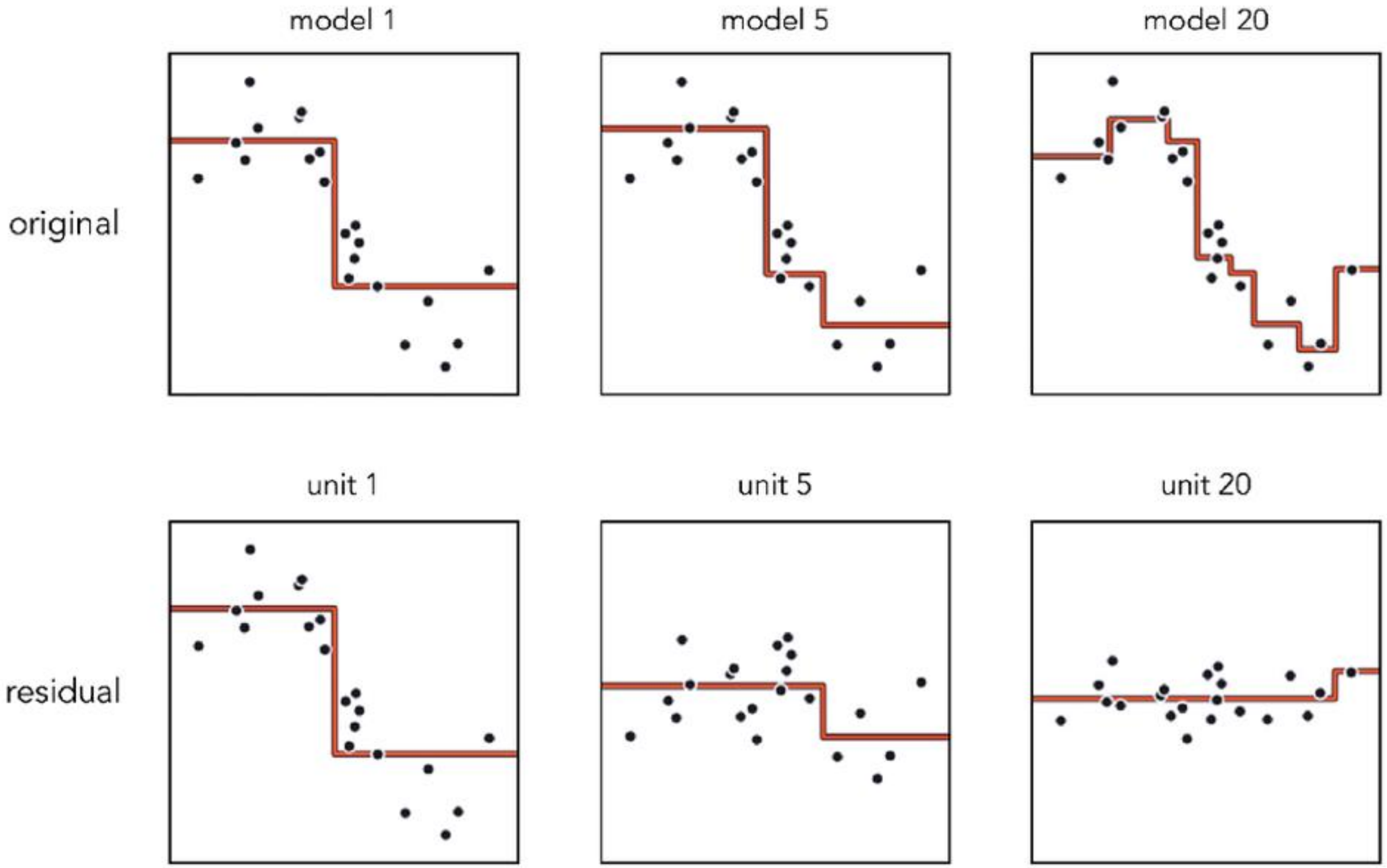
- We then seek out the best next unit to add

$$model_m(x, \theta_m) = model_{m-1}(x, \theta_{m-1}) + f_{s_m}(x)\, w_m$$

- By minimizing

$$\frac{1}{p}\sum_{p=1}^{P}\left(model_{m-1}(x_p, \theta_{m-1}) + f_{s_m}(x_p)\, w_m - \; y_p\right)^2 \; =$$
$$\frac{1}{p}\sum_{p=1}^{P}\left(w_0 + f_{s_1}(x_p)\, w_1 + \; \ldots + f_{s_m}(x_p)\, w_m - y_p\right)^2$$

Visualization using trees



Boosting for Regression Trees: Algorithm

1. Set $\hat{f}(x) = 0$ and error $r_i = y_i$
2. For b = 1, 2, … , B repeat:
   a. Fit a tree $\widehat{f^b}$ with d splits (d + 1 terminal nodes) to the training data (X, r)
   b. Update $\hat{f}$ by adding in a shrunken version of the new tree

   $$\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \hat{f}^b(x)$$

   c. Update the residuals

   $$r_i \leftarrow r_i - \lambda \hat{f}^b(x_i)$$

3. Output the boosted model

$$\hat{f}(x) = \sum_{b=1}^{B} \lambda \hat{f}^b(x)$$

Boosted Decision Trees

- Learn slowly from shallow trees
- Given a current model – calculate residuals
- Build next tree to improve on the remaining residuals
- Slowly improve where the model does not currently perform well
- Boosted classification becomes a bit trickier in how it updates
- Some key notation reminders from last time:
  - Boosting learns slowly from a bunch of weak classifiers
  - Boosting learns a strong classifier, this model can often be denoted as G, f, or H in common texts. Similarly, weights may vary in notation (w or α for example)

Boosting for Classification

- Consider a dataset $D = \{(x_p, y_p)\}_{p=1}^{P}$, where $y \in \{-1, +1\}$
- Would like to learn:

$$F(x) = w_o + \sum_{m=1}^{M} w_m f_m(x)$$

- So that we may classify based upon

$$F(x) = sign(w_o + \sum_{m=1}^{M} w_m f_m(x))$$

Boosting for Classification: Learning the Boundary

- Consider a dataset $D = \{(x_p, y_p)\}_{p=1}^{P}$, where $y \in \{-1, +1\}$
- Let's revisit Misclassification, just like with Logistic Regression:

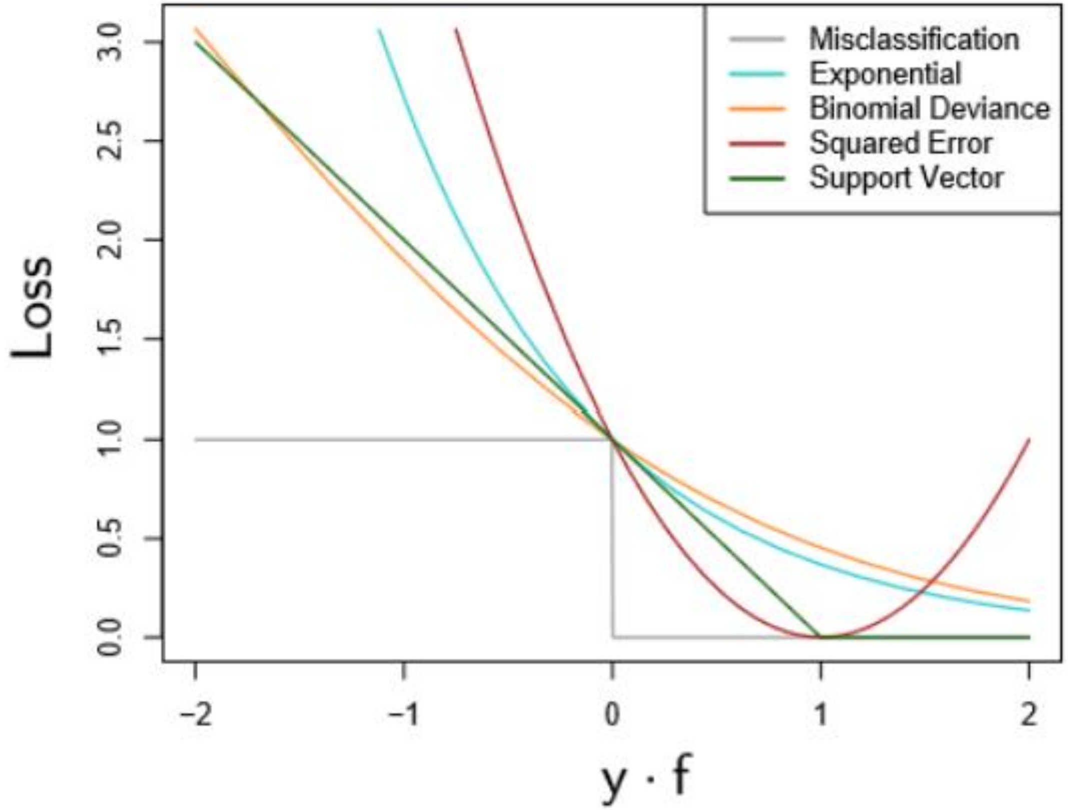
$$L(y, f(x)) = \overline{Err} = \frac{1}{P}\sum_{p=1}^{P} I\,(y_p \neq \hat{y}_p)$$

- Where we seek to minimize:

$$\min_f \sum_{p=1}^{P} L(y_p, f(x_p))$$

- Where $L(y, f(x))$ is a loss function set up above as the 0-1 binary loss

Types of Loss: A Review



Convex Optimizations of Binary Loss

- Reminder – the Binary 0-1 loss is not differentiable
- Might consider the squared error loss

$$f^*(x) = \underset{f}{\operatorname{argmin}} E_{y\,|\,x}\left[(Y - f(x))^2\right] = E[Y \mid X]$$

Convex Optimizations of Binary Loss

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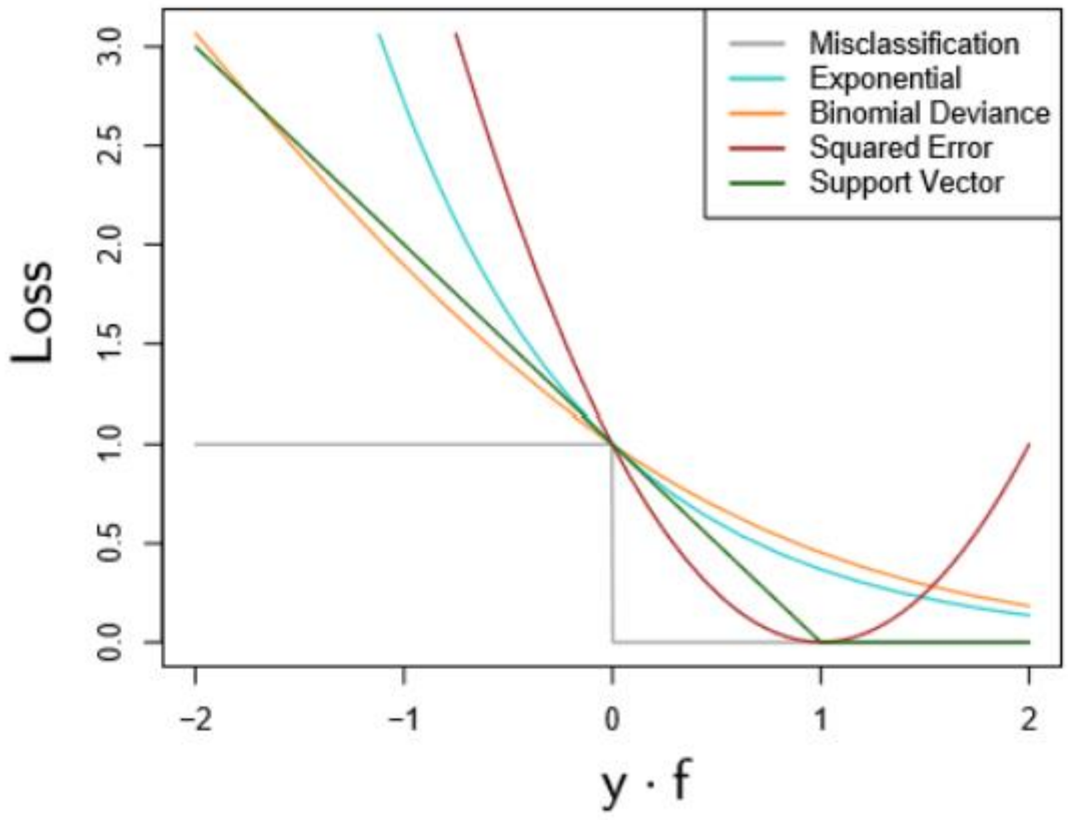
$$f^*(x) = \underset{f}{\operatorname{argmin}} E_{y\,|\,x}\,[(Y\ - f(x))^2] = E[Y\ |\ X]$$

- But this cannot be computed because it requires p(y|x) to be known
- this is known as the population minimizer and we seek to approximate this probability in boosting.

Types of Loss: A Review



Convex Optimizations of Binary Loss

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$$f^*(x) = \underset{f}{\operatorname{argmin}} E_{y \mid x} [(Y - f(x))^2] = E[Y \mid X]$$

- Log Loss:

$$f^*(x) = \frac{1}{2} \log \frac{p(y = 1 \mid x)}{p(y = -1 \mid x)}$$

Convex Optimizations of Binary Loss

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$$f^*(x) = \underset{f}{\operatorname{argmin}} E_{y\,|\,x}\left[(Y - f(x))^2\right] = E[Y \mid X]$$

- Log Loss:

$$L(y, f(x)) = \frac{1}{2}\log\frac{p(y = 1\,|x)}{p\,(y = -1\,|x)}$$

- Exponential Loss:

$$L(y, f(x)) = \exp(-y * f(x))$$

Convex Optimizations of Binary Loss

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- Exponential Loss:

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Turns out, these two have same optimal solution

Learning from Exponential Loss

- Exponential Loss:

$$L(y, f(x)) = \exp(-y * f(x))$$

- Means we would like to solve:

$$(\beta_m, F_m) = \underset{\beta,F}{\operatorname{argmin}} \sum_{p=1}^{P} exp\left[-y_p f_m\left(x_p\right) + \beta F(x_p)\right]$$

(this is called forward stagewise additive modeling)

Learning from Exponential Loss

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$$(\beta_m, F_m) = \underset{\beta,F}{\operatorname{argmin}} \sum_{p=1}^{P} exp\left[-y_p f_m\left(x_p\right) + \beta F(x_p)\right]$$

- Which can be re-written as:

$$(\beta_m, F_m) = \underset{\beta,F}{\operatorname{argmin}} \sum_{p=1}^{P} w_p^{(m)} exp\left[-\beta y_p F(x_p)\right]$$

Learning from Exponential Loss

- Exponential Loss Optimization:

$$(\beta_m, F_m) = \underset{\beta,F}{\operatorname{argmin}} \sum_{p=1}^{P} w_p^{(m)} exp\left[-\beta y_p F(x_p)\right]$$

- For $\beta > 0$, to minimize misclassifications:

$$F_m = \underset{F}{\operatorname{argmin}} \sum_{p=1}^{P} w_p^{(m)} I\left(y_p \neq F(x_p)\right)$$

$$= e^{-\beta} \sum_{y_p = F(x_p)} w_p^{(m)} + e^{\beta} \sum_{y_p \neq F(x_p)} w_p^{(m)}$$

$$= \left(e^{\beta} - e^{-\beta}\right) \sum_{p=1}^{P} w_p^{(m)} I\left(y_p \neq F(x_p)\right) + e^{\beta} \sum_{p=1}^{P} w_p^{(m)}$$

Exponential Loss = Log Loss

- Plugging back to solve for β_m yields:

$$\beta_m = \frac{1}{2}\log\frac{1 - err_m}{err_m}$$

- Where

$$err_m = \frac{\sum_{p=1}^{P} w_p^{(m)} I\left(y_p \neq F(x_p)\right)}{\sum_{p=1}^{P} w_p^{(m)}}$$

Creating Update Rules

- Update our approximate f as

$$f_m(x) = f_{m-1}(x) + \beta_m F_m(x)$$

- Which updates weights as

$$w_p^{(m+1)} = w_p^{(m)} e^{\alpha_m I(y_p \neq F_m(x_p))} e^{\beta_m}$$

Why does this work?

$$f^*(x) = \underset{f}{\operatorname{argmin}} E_{y\,|\,x}\left[e^{-Y*f(x)}\right] = \frac{1}{2}\log\frac{p(Y=1\,|x)}{p\,(Y=-1\,|x)}$$

Where

$$p(Y=1\,|x) = \frac{1}{1+\ e^{-2f^*(x)}}$$

Convex Optimizations of Binary Loss

- Reminder – the Binary 0-1 loss is not differentiable
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$$f^*(x) = \underset{f}{\operatorname{argmin}}\, E_{y\,|\,x}\left[(Y - f(x))^2\right] = E[Y \mid X]$$

- Log Loss:

$$L(y, f(x)) = \frac{1}{2}\log\frac{p(y = 1\,|x)}{p\,(y = -1\,|x)}$$

- Exponential Loss:

$$L(y, f(x)) = \exp(-y * f(x))$$

Name	Loss	Derivative	f^*	Algorithm
Squared error	$\frac{1}{2}(y_i - f(\mathbf{x}_i))^2$	$y_i - f(\mathbf{x}_i)$	$\mathbb{E}[y\|\mathbf{x}_i]$	L2Boosting
Absolute error	$\|y_i - f(\mathbf{x}_i)\|$	$\operatorname{sgn}(y_i - f(\mathbf{x}_i))$	$\operatorname{median}(y\|\mathbf{x}_i)$	Gradient boosting
Exponential loss	$\exp(-\tilde{y}_i f(\mathbf{x}_i))$	$-\tilde{y}_i \exp(-\tilde{y}_i f(\mathbf{x}_i))$	$\frac{1}{2}\log\frac{\pi_i}{1-\pi_i}$	AdaBoost
Logloss	$\log(1 + e^{-\tilde{y}_i f_i})$	$y_i - \pi_i$	$\frac{1}{2}\log\frac{\pi_i}{1-\pi_i}$	LogitBoost

How to optimize Boosting for Classification

- Key to the classification algorithm, if log-loss looks like:

$$L\big(y, f(x)\big) = \frac{1}{2}\log\frac{p(y = 1\,|x)}{p\,(y = -1\,|x)}$$

- Then the initial best estimate is $f_0(x) = \bar{y}$, in other words

$$f_0(x) = \frac{1}{2}\log\frac{\bar{y}}{1 - \bar{y}}$$

Notation Change!

- Because the regression concept of residual is going to change to classification concept of weight, we need to re-use the term “w”
- So we change

$$F(x) = sign(w_o + \sum_{m=1}^{M} w_m f_m(x))$$

- To

$$F(x) = sign(\sum_{m=1}^{M} \alpha_m f_m(x))$$

AdaBoost M1

1. Initialize observation weights to $w_i = \frac{1}{P}, i = 1, 2, \ldots, P$

AdaBoost M1

1. Initialize observation weights to $w_p = \frac{1}{P}, p = 1, 2, \dots, P$
2. For m = 1 to M:
   a. Fit a classifier $f_m(x)$ to the training data using weights w_p
   b. Compute error as:
   $$err_m = \frac{\sum_{p=1}^{P} w_p \; I\left(y_p \neq f_m(x_p)\right)}{\sum_{p=1}^{P} w_p}$$
   c. Compute classifier weight as:
   $$\alpha_m = \log \frac{1 - err_m}{err_m}$$
   d. Re-weigh observations as:
   $$w_p \leftarrow w_p * \exp\left[\alpha_m * I\left(y_p \neq f_m(x_p)\right)\right] \; \forall\, p$$

AdaBoost M1

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   c. Compute classifier weight as:
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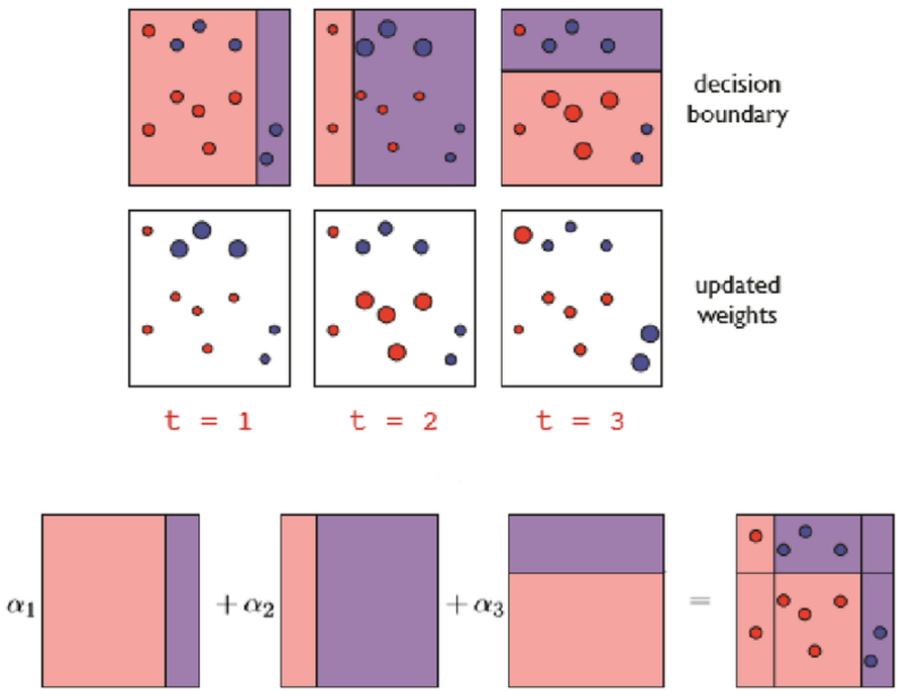
   d. Re-weigh observations as:
   $$w_p \leftarrow w_p * \exp\left[\alpha_m * I\left(y_p \neq f_m(x_p)\right)\right] \; \forall\, p$$
3. Output:
   $$F(x) = sign\left(\sum_{m=1}^{M} \alpha_m f_m(x)\right)$$

Visualization of AdaBoost



Other Boosting: Logit Boost

- AdaBoost with exponential loss puts a lot of weight on misclassified examples
- Hard to interpret probabilities from f(x)
- If we use log-loss instead of exponential – mistakes are only punished linearly
- And this generalizes to multiple classes

$$p(y = 1\,|x) = \frac{e^{f(x)}}{e^{-f(x)} + \ e^{f(x)}} = \frac{1}{1 + \ e^{-2f(x)}}$$

With loss

$$L_m(\phi) = \sum_{p=1}^{P} \log(1 + \exp(-2y_p\left(f_{m-1}(x_p) + \ \phi(x_p)\right)))$$

Logit Boost

1. Initialize observation weights to $w_p = \frac{1}{P}, p = 1, 2, \dots, P$, $\pi_p = \frac{1}{2}$
2. For m = 1 to M:
   a. Compute working response $z_p = \frac{y_p - \pi_p}{\pi_p\,(\,1 - \pi_p)}$
   b. Compute weights $w_p = \pi_p$ (1 - π_p)
   c. Update

$$\phi_m = \underset{\varphi}{\operatorname{argmin}} \sum_{p=1}^{P} w_p(z_p - \phi(x_p))^2$$

$$f(x) \leftarrow f(x) + \frac{1}{2}\phi_m(x)$$

   d. Compute

$$\pi_p = \frac{1}{1 + e^{-2f(x_p)}}$$

3. Output:

$$F(x) = sign(\sum_{m=1}^{M} \phi_m(x))$$

Can we generalize further?

- Rather than rebuilding the algorithm per loss function – can we create a generic boosting algorithm across all loss functions?
- Imagine we want

$$\hat{f} = \underset{f}{\operatorname{argmin}}\, L(f)$$

Where f are the parameters of a model

- At step m let g_m be the gradient of L(f) at step f_{m-1}

$$g_{pm} = \left[\frac{\partial L(y_p, f(x_p))}{\partial f(x_p)}\right]$$

Functional Gradient Descent

$$g_{pm} = \left[\frac{\partial L(y_p, f(x_p))}{\partial f(x_p)}\right]$$

$$f_m = f_{m-1} - \rho_m g_m$$

Where ρ_m is a step length set by

$$\rho_m = \underset{\rho}{\operatorname{argmin}} L(f_{m-1} - \rho_m g_m)$$

This will not generalize, but optimize f for only a fixed size P. So we have to fit weak learners to approximate the negative gradient signal as

$$\gamma_m = \underset{\gamma}{\operatorname{argmin}} \sum_{p=1}^{P} \left(-g_{im} - \phi(x_p; \gamma)\right)^2$$

Gradient Descent Boosting

1. Initialize $f_0(x) = \underset{\gamma}{\operatorname{argmin}} \sum_{p=1}^{P} L\big(y_p, \varphi(x_p;\gamma)\big)$
2. For m = 1 to M:
    a. Compute the residual gradient using

    $$r_{pm} = -\left[\frac{\partial L(y_p, f\big(x_p\big))}{\partial f\,(x_p)}\right]$$

    b. Use a weak learner to compute γ_m which minimizes

    $$\sum_{p=1}^{P} (r_{pm} - \phi\big(x_p;\gamma_m\big))^2$$

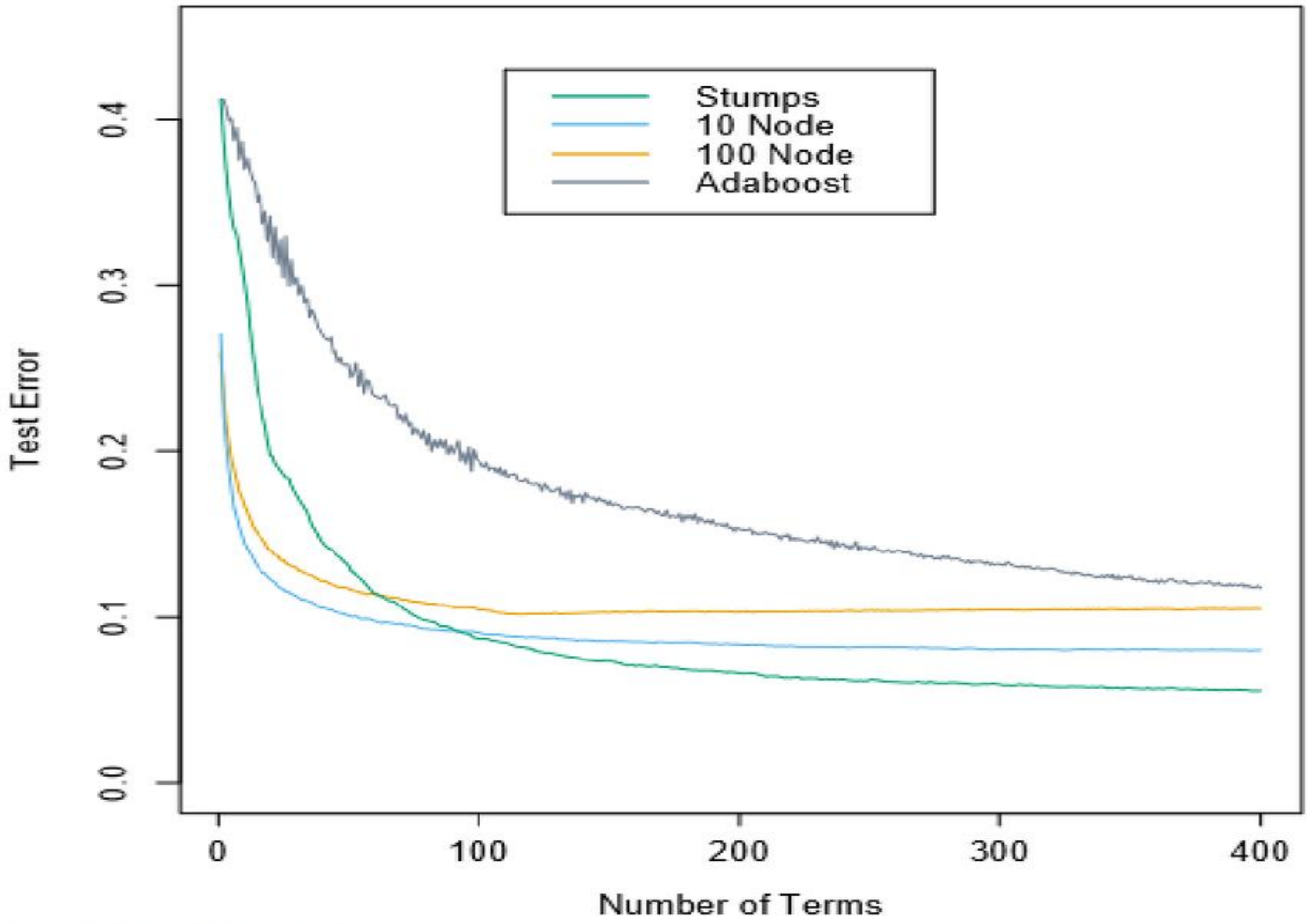
    c. Update

    $$f_m(x) = f_{m-1}(x) + \upsilon\phi(x;\gamma_m)$$

3. Output:

$$F(x) = f_m(x)$$

Boosting Comparisons



Takeaways

- Reviewed a variety of boosting algorithms for classification
- Discussed why functional gradient boosting generalizes across all kinds of loss functions
- Boosting of very weak learners creates a stronger learner over number of terms/iterations